VARIATIONAL CALCULUS FOR HYPERSURFACE FUNCTIONALS:
SINGULAR YAMABE PROBLEM WILLMORE ENERGIES

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Abstract. We develop the calculus for hypersurface variations based on variation of
the hypersurface defining function. This is used to show that the functional gradient
of a new Willmore-like, conformal hypersurface energy agrees exactly with the ob-
struction to smoothly solving the singular Yamabe problem for conformally compact
four-manifolds. We give explicit hypersurface formulæ for both the energy functional
and the obstruction.

Keywords: Calculus of variations, conformally compact, conformal geometry, hypersurfaces, Willmore energy,
Yamabe problem
1. INTRODUCTION

Hypersurface geometry is critically important for the analysis of boundary problems in mathematics and physics. Conformal hypersurfaces form a subtle but important class of cases, particularly because of their role in treating the boundary at infinity of conformally compact structures. Naturally the fundamental problem is the construction and study of local and global invariants. The work [GW15] develops an effective approach to hypersurface geometries by treating them as conformal infinities (see also the announcement [GW13]). This approach includes a calculus for hypersurface invariants based on defining functions.

In this article we develop the corresponding variational theory; namely a hypersurface variational calculus based around defining functions. A main result is Theorem 3.11 which provides the general formula for computing variations of embeddings of hypersurface functionals by varying the underlying hypersurface defining function. A key motivation for our development of that theory was to develop an effective approach to computing the Euler–Lagrange equations corresponding to the new conformal energies of [GW15]. These functionals generalise to higher dimensions the Willmore energy [Wil65], also known as the rigid string action [Pol86]. For the crucial case of four manifolds, we show that the gradient of this functional agrees with the obstruction to smoothly solving the Yamabe problem for conformally compact structures.

The Willmore energy and its associated gradient provide important invariants for surfaces. Indeed the Willmore conjecture concerning absolute minimizers of this energy has stimulated much geometric analysis [Riv08]; the general proof of the conjecture was provided by Marques-Neves [MN14, MN13]. In physics, the Willmore energy functional has...
applications in string theory where it appears as the entanglement entropy for a three dimensional conformal field theory \cite{AGS14}. It also arises as a certain log coefficient in a holographic notion of physical observables, and is closely related to the so-called conformal anomaly \cite{GW99}. Furthermore it appears as the renormalized area of a minimal surface embedded in a hyperbolic three-manifold \cite{AM10}. An important aspect of these invariants is their conformal invariance. While the Willmore energy integrand is not surprising its gradient, with respect to variations of embeddings, is an important local conformal invariant because it has linear leading term. We call this gradient the Willmore invariant.

These applications and observations suggest a potentially significant role in geometry and physics for corresponding conformal invariants in higher dimensions. For four-dimensional hypersurfaces in Euclidean spaces, conformal energy functionals have been provided in \cite{Guv05} and \cite{Vya13}. Recently it was shown that for hypersurfaces of every dimension, there exists a conformally invariant canonical analog of both the Willmore energy and the Willmore invariant. These are generated and constructed uniformly via a singular Yamabe problem that places the hypersurface as the boundary at infinity of a conformally compact, constant scalar curvature, manifold \cite{GW13, GW15}. In each higher dimension, the analog of the Willmore invariant is called the obstruction density. This work was partly inspired by the results \cite{ACF92} of Andersson–Chruściel–Friedrich who studied boundary asymptotics for this Loewner–Nirenberg-type problem \cite{LN74}. They found that the three-manifold obstruction to smoothness was a conformal invariant and also gave some information about the corresponding obstructions in higher dimensions.

For three-manifold boundaries the obstruction density is easily shown to agree with the Willmore invariant.

In \cite{GW13, GW15} the singular Yamabe problem was recast as the tool for treating hypersurface conformal geometry that is analogous to the Fefferman-Graham Poincaré-metric as an approach to intrinsic conformal geometry. From this perspective, and using tractor calculus to re-express the Yamabe equation, the problem of computing the obstruction is reduced to a simple algorithm that also reveals the qualitative aspects of the obstruction densities and higher Willmore energies. In particular there is a dimension parity dichotomy: For each even hypersurface dimension, the obstruction density is a linear-leading-order conformal invariant that is a close analog of the Willmore invariant (and should be considered as a fundamental scalar curvature invariant); via elementary representation theory, odd dimensional hypersurfaces cannot admit linear leading order invariants.

It is an interesting problem to understand the higher Willmore energies and obstruction densities for odd dimensional hypersurfaces. A particularly important case for both mathematics and physics is when these are four-manifold boundaries. In this article we employ the general holographic formula for the obstruction density \cite{GW15} to compute the four-manifold obstruction density:

**Proposition 1.1.** The obstruction density for $d = 3$ is given by

$$B_3 = \frac{1}{6} \left[ L^{ab}(3\hat{\Pi}_{(ab)}^2 - \hat{\Pi} B_{ab} + K^2 - 7W_{ab}^{\hat{\Pi}} + 2\hat{\Pi} W_{ab} + \hat{\Pi} \hat{\Pi} \hat{\Pi} W_{abcd} + \hat{\Pi} \hat{\Pi} \hat{\Pi} W_{abc} \right].$$

Theorem \ref{thm5.10} recalls that $B_d$ is a conformally invariant density of weight $-d$, and our tensor notations are explained in Section 1.1 below, while the hypersurface invariants appearing in the above formula are introduced in Section 2. In particular $\Pi$ denotes the trace-free second fundamental form, while $L^{ab}$ is a second order, conformally invariant
differential operator (that appears in Bernstein–Gel’fand–Gel’fand (BGG) sequences) such that $L^{ab} \Pi_{ab} = \nabla^a \nabla^b \Pi_{ab} + \text{lower order terms.}$

As mentioned above, another main result in [GW15] is the construction of conformally invariant functionals that generalise the Willmore energy to higher dimensions. For a hypersurface $\Sigma$ of dimension $\bar{d}$ these take the form

$$\mathcal{I}_\bar{d} = \alpha_{\bar{d}} \int_{\Sigma} dA_{\bar{d}} N_{\bar{d}} P_{\bar{d}} N^{\bar{d}},$$

where $\alpha_{\bar{d}}$ is a non-vanishing constant and $P_{\bar{d}}$ is a uniformly constructed family of conformally invariant operators, and $N^{\bar{d}}$ is the normal tractor of [BEG94] introduced in Section 5.2. For $\bar{d}$ even, the operators $P_{\bar{d}}$ take the form $(\Delta^{\top})^{\bar{d}} + \text{lower order terms}$, so are hypersurface analogs of the GJMS operators of Graham, Jenness, Mason and Sparling [GJMS92]. For $\bar{d}$ both even and odd a holographic formula for $P_{\bar{d}}$ is known. This gives that $P_3$ takes the form $\Pi^{ab} \nabla^a_{\bar{d}} \nabla^b_{\bar{d}} + \text{lower order terms}$ (the detailed formula appears in Equation (6.2)). So for generic hypersurfaces $P_3$ is Laplacian-like. Using these results for $P_3$ yields

$$\mathcal{I}_3 = \frac{1}{6} \int_{\Sigma} dA_{\bar{d}} \Pi^{ab} \mathcal{F}_{ab},$$

where the conformally invariant Fialkow tensor takes the form $\mathcal{F}_{ab} = \Pi^{ab}_{\bar{d}} + \text{lower order terms}$; see Equation (2.7) and $\alpha_3 = \frac{1}{\bar{d}}$ has been chosen for later convenience.

Our final main result is that the functional gradient of the energy $\mathcal{I}_3$ agrees precisely with the obstruction $\mathcal{B}_3$ to the singular Yamabe problem mentioned above:

**Proposition 1.2.** With respect to hypersurface variations, the gradient of $\mathcal{I}_3$ is $\mathcal{B}_3$.

Our article is structured as follows: In Section 2 we review basic hypersurface theory and use conformal invariance as the organising principle when producing expressions for hypersurface invariants (including a novel hypersurface Bach tensor $B_{ab}$ which already appears in Proposition 1.1 above). In Section 3 we develop our hypersurface variational calculus and treat Willmore and minimal surfaces as basic examples. In Section 4 we compute the variational gradient for our four-manifold analog of the Willmore energy. Section 5 is devoted to a review of the essential tractor calculus methods needed to effectively treat the singular Yamabe problem. In Section 6 we compute the obstruction density for four-manifold hypersurfaces. We also compute the obstruction for example metrics, including a hypersurface surrounding the horizon of a Schwarzschild black hole. The appendix gives explicit formulæ for the obstruction density for manifolds of dimensions five or less (so including $B_4$) that can easily be implemented for explicit metrics using computer software packages.

1.1. Riemannian and conformal geometry conventions. We work with manifolds $M$ of dimension $d$ and embedded hypersurfaces of dimension $\bar{d} := d - 1$. When the dimension $d$ equals three or four, we often refer to the latter as surfaces and spaces, respectively. (Note that the exterior derivative will be denoted by $d$, to avoid confusion with the dimension $d$.) When $M$ is equipped with a Riemannian metric $g$, its Levi-Civita connection will be denoted by $\nabla$ or $\nabla_a$ in an abstract index notation (cf. [PR84]). The corresponding Riemann curvature tensor $R$ is

$$R(u, v)w = [\nabla_u, \nabla_v]w - \nabla_{[u, v]}w,$$

for arbitrary vector fields $u$, $v$ and $w$. In the abstract index notation, $R$ is denoted by $R_{ab} \gamma^c_d$ and $R(u, v)w$ is $u^a v^b R_{ab} \gamma^c_d w^d$. Cotangent and tangent spaces will be canonically
identified using the metric tensor, $g_{ab}$ and this will be used to raise and lower indices in the standard fashion.

The Riemann curvature can be decomposed into the trace-free \textit{Weyl curvature} $W_{abcd}$ and the symmetric \textit{Schouten tensor} $P_{ab}$ according to

$$R_{abcd} = W_{abcd} + 2g_{a[c} P_{d]b} - 2g_{b[c} P_{d]a}.$$ 

Here antisymmetrization over a pair of indices is denoted by square brackets so that $X_{[ab]} := \frac{1}{2}(X_{ab} - X_{ba})$. The Schouten and Ricci tensors are related by

$$\text{Ric}_{bd} := R_{ab}^a d = (d - 2)P_{bd} + g_{ab} J, \quad J := P_{ab}.$$ 

The scalar curvature $S_c = g^{ab} \text{Ric}_{ab}$, thus $J = S_c/(2(d - 1))$. In two dimensions the Schouten tensor is ill-defined, but we take $J = \frac{1}{2} S_c$ in that case. In dimension $d \geq 3$, the curl of the Schouten tensor gives the \textit{Cotton tensor}

$$C_{abc} := 2\nabla_d W_{ab}^d c.$$ 

In dimensions $d \geq 4$,

$$(d - 3)C_{abc} = \nabla_d W_{ab}^d c.$$ 

A conformal geometry is a manifold equipped with a conformal structure $\mathbf{c}$, namely an equivalence class of metrics with equivalence relation $g' \sim g$ when $g' = \Omega^2 g$ for $C^\infty M \ni \Omega > 0$. The corresponding Weyl tensors obey $W'^a_{ab} c = W^a_{ab} c$ and thus the Weyl tensor is a conformal invariant. Conformal invariants may also be density-valued $A$-weighted $w$ density is a section of the oriented line bundle $[\wedge^d TM]^2 \mathcal{L} =: \mathcal{E}M[w]$. Vector bundles $\mathcal{V} M$ tensored with this are denoted $\mathcal{V} M \otimes \mathcal{E}M[w] =: \mathcal{V}M[w]$. Each metric $g \in \mathbf{c}$ determines a section of $(\wedge^d T^* M)^2$ and so there is a tautological global section $g$ of $\mathcal{C}^\infty T^* M[2]$ called the \textit{conformal metric}. Hence, each $g \in \mathbf{c}$ is in $1 : 1$ correspondence with a strictly positive section $\tau \in \mathcal{E}M[1]$ via $g = \tau^{-2} g$. Such sections $\tau$ will be referred to as a \textit{true scale}, and we will often present conformally invariant formulæ in terms of a Riemannian metric $g$ by making an (arbitrary) choice of scale $\tau$. It will be clear from context where this has been done.

In situations where we are dealing with tensors built from higher rank tensors by contractions with vectors or covectors into the first slot such as $X(u, \cdot, u)$ or equivalently $u^a X_{ab}$, we will often use the notation $\tilde{X}_a$. In higher rank cases where more indices are missing, an alternating leftmost-rightmost contraction procedure has been followed, so if $X$ is rank 3, then $\tilde{X}_b$ denotes $X(u, \cdot, u)$ or equivalently $u^a X_{abc} u^c$. Contractions across multiple indices of tensors with one another will be denoted by an obvious bracket notation, for example, if $Y$ is rank two and $X$ is rank three, $X(Y, \cdot)$ denotes the covector $X_{abc} Y^{ab}$. Also, for rank two symmetric tensors $S, T$, we will have occasion to employ matrix notations such as $S_{ab}^c := S_{ac} S_{cb}^c$ and $\text{tr} ST := S_{ab} T_{ab}$. Unit weight symmetrization over groups of indices is denoted by round brackets, which we adorn with the symbol $\circ$ when projecting onto the trace-free part of this, for example $X_{(ab)} := \frac{1}{2}(X_{ab} + X_{ba}) - \frac{1}{4} g_{ab} X_{cc}$; for mixed symmetry tensors, projection onto the trace-free part of a group of indices will be indicated by the notation $\{ \}$ and their corresponding section spaces will be decorated with a subscript $\circ$. Finally, we will also use a dot product notation for inner products of vectors $g(u, v) = u_a v^a = u \cdot v$ as well as divergences $\nabla . X_b := \nabla^a X_{ab}$, and $|u| := \sqrt{u_a u^a} := \sqrt{u^2}$ denotes the length of a vector $u$. 

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2. Embedded hypersurfaces

A hypersurface $\Sigma$ is a smoothly embedded codimension 1 submanifold of a smooth manifold $M$. A function $s \in C^\infty M$ is called a defining function for $\Sigma$ if the hypersurface is given by its zero locus, i.e. $\Sigma = Z(s)$ and the exterior derivative $ds = n$ is nowhere vanishing along $\Sigma$. The covector field $n|_\Sigma$ is then a conormal to the hypersurface and $\hat{n}^a := (n^a/|n|)|_\Sigma$ is the unit conormal while $n^a|_\Sigma$ is a normal vector.

The conormal allows the tangent bundle $T\Sigma$ and the subbundle of $T M|_\Sigma$ orthogonal to $n^a$, denoted $T M^\top$, to be canonically identified. Thus we may use the same abstract indices for $T \Sigma$ as for $T M$. The projection of tensors, to hypersurface tensors will be denoted by a superscript $^\top$. Given an extension $\hat{n}^a$ of the unit normal to $M$, we will also write $v^\top := v - \hat{n} \hat{n}.v$ for vectors (and similarly for tensors) $v \in T M$. Upon restriction, these give hypersurface vectors (and tensors).

The metric $g$ on $M$ induces a metric $\bar{g}$ on $\Sigma$ given by

$$\bar{g}_{ab} = g_{ab}|_\Sigma - \hat{n}_a \hat{n}_b.$$  

(2.1)

Given a hypersurface vector field $v^a \in \Gamma(T \Sigma)$, the Gauß formula relates the restriction to $T \Sigma$ of the Levi-Civita connection $\nabla$ on $M$ to the hypersurface Levi-Civita connection of $\bar{g}$ according to

$$\bar{\nabla}_a v^b = \nabla_\top^a v^b + \hat{n}^b \Pi_{ac} v^c.$$  

(2.2)

In the above formula, the right hand side is defined independently of how $v^a \in T \Sigma$ is extended to $v^a \in T M$. In general, we will use the term tangential for operators $O$ along $\Sigma$ if they have the property that for $v$ a smooth extension of some tensor $\bar{v}$ defined along $\Sigma$, the quantity $O \bar{v}|_\Sigma$ is independent of the choice of this extension. In the above display, the second fundamental form $\Pi_{ab} \in \Gamma(\otimes^2 T^* \Sigma)$ is given by

$$\Pi_{ab} = \nabla_\top^a \hat{n}_b.$$  

Its “averaged” trace is the mean curvature

$$H = \frac{1}{d} \Pi^a_a.$$  

We will often use bars to distinguish intrinsic hypersurface $\Sigma$ quantities from their host space counterparts. In particular, the equations of Gauß relate ambient curvatures to intrinsic ones according to

$$R^\top_{abcd} = \bar{R}_{abcd} - 2\Pi_{ac} \Pi_{db},$$  

$$\bar{\text{Ric}}_{ab} = \bar{\text{Ric}}_{ab} + \Pi^2_{ab} - dH \Pi_{ab},$$  

$$\text{Sc} - 2 \bar{\text{Ric}}(\hat{n}, \hat{n}) = \text{Sc} - \text{tr} \Pi^2 + d^2 H^2.$$  

(2.3)

The last of these recovers Gauß’ Theorema Egregium for a Euclidean ambient space. The Codazzi–Mainardi equation gives the covariant curl of the second fundamental form in terms of ambient curvature

$$\nabla_\mu \Pi_{\mu\nu} = \frac{1}{2} \hat{n}^a R^\top_{cba}.$$  

(2.4)

Finally the divergence of the Codazzi-Mainardi equation determines the Laplacian of mean curvature:

$$\bar{\Delta} H = \frac{1}{d} (\bar{\nabla} \bar{\nabla} \Pi - \hat{n} \hat{n} \bar{\text{Ric}}_{a}^a).$$  

(2.5)
2.1. Conformal hypersurfaces. The ambient conformal structure \( c \) induces a conformal structure \( \hat{c} \) on \( \Sigma \). Locally we may always assume there is a section \( \hat{n}_a \in \Gamma(T^*M[1]) \) obeying \( g_{ab} \hat{n}^a \hat{n}^b = 1 \). This conformal unit conormal plays the role of a Riemannian unit conormal. The trace-free part of the second fundamental form \( \hat{\Pi}_{ab} = \Pi_{ab} - H \hat{g}_{ab} \), defined (in a choice of scale) in terms of \( \hat{n}_a \) via Equation (2.2), is a conformally invariant section of \( \odot^2 T^* M[1] \). Thus the quantity

\[
(2.6) 
K := \text{tr} \hat{\Pi}^2 \in \Gamma(\mathcal{E}\Sigma[-2]),
\]

is a conformal density of weight \(-2\), that we call the rigidity density.

Conformal invariance of the trace-free second fundamental form \( \Pi \) and the Weyl tensor can be used to decompose the equations of Gauß and Codazzi–Mainardi equations into conformally invariant parts. First, the Ricci equation in (2.3) gives what we shall call the Fialkow–Gauß equation (cf. [Vya13])

\[
(2.7) 
\hat{\Pi}^2_{ab} - \frac{1}{2} \hat{g}_{ab} \hat{\Pi}_{cd} \hat{\Pi}^{cd} - W_{ab} = (\hat{d} - 2) \left( P^\top_{ab} - \hat{P}_{ab} + H \hat{\Pi}_{ab} + \frac{1}{2} \hat{g}_{ab} H^2 \right) =: (\hat{d} - 2) \mathcal{F}_{ab}.
\]

The left hand side of this equation is conformally invariant, which proves that the Fialkow tensor \( \mathcal{F}_{ab} \), defined by the above in dimension \( d \geq 4 \) is a conformally invariant section of \( \odot^2 T^* M[0] \). This combined with the trace-free second fundamental form gives a new distinguished density

\[
(2.8) 
L := \text{tr}(\hat{\Pi}\mathcal{F}) \in \Gamma(\mathcal{E}\Sigma[-3]),
\]

which we call the membrane rigidity density.

In dimensions \( d \geq 4 \), the trace-free part of the first Gauß equation allows the tangential part of the ambient Weyl tensor to be traded for its hypersurface counterpart:

\[
W^\top_{abcd} = W_{abcd} - 2 \Pi_{[a[c} \hat{\Pi}_{d]b]} - \frac{2}{d - 2} \left( \hat{g}_{[a[c} \hat{\Pi}_{d]b]} - \hat{g}_{b[c} \hat{\Pi}_{d]a} \right) + \frac{2}{(d - 1)(d - 2)} \hat{g}_{[a[c} \hat{g}_{d]b]} K.
\]

In dimensions \( d \geq 4 \), the third Gauß equation expresses the rigidity density in terms of the difference between ambient and hypersurface scalar curvatures:

\[
K = 2(\hat{d} - 1) \left( J - P(\hat{n}, \hat{n}) - \hat{J} + \frac{\hat{d}}{2} H^2 \right).
\]

This shows that \( J - P(\hat{n}, \hat{n}) - \hat{J} + \frac{\hat{d}}{2} H^2 \) is a conformally invariant weight \(-2\) density.

The trace-free part of the Codazzi–Mainardi equation shows that the trace-free curl of the trace-free second fundamental form is a weight 1 conformal invariant:

\[
(2.9) 
W^\top_{abc} = 2 \nabla_{\{c} \hat{\Pi}_{b]a\}}.
\]

Finally, we will need a certain novel four-manifold hypersurface invariant:

**Lemma 2.1.** Let \( \hat{d} = 3 \) and

\[
B^\hat{c}_{ab} := \hat{C}_{(ab)} + H \hat{W}_{ab} - \nabla^c \hat{W}^\top_{(ab)c}.
\]

Then \( B^\hat{c}_{ab} \) defines a symmetric, weight \(-1\) conformal hypersurface density

\[
B_{ab} \in \Gamma(\odot^2 T^* [\Sigma[-1]])
\]

given in a choice of scale \( g \in c \) by \( B^g_{ab} \).
Proof. This result can be established by examining the conformal transformation properties of the Cotton tensor, mean curvature and the divergence of the Weyl tensor:

\[
C^{\gamma \delta \rho}_{\alpha \beta \gamma} = \Omega^{-1}(C_{\alpha \beta \gamma \delta} - W_{\alpha \beta \gamma \delta} Y_d), \quad \nabla^a \nabla_b X^{ab} = \Omega^{-1}(\nabla_a \nabla_b X^{ab} + P_{ab} X^{ab}),
\]

(2.10)

\[
[\nabla^c W^{\alpha \beta \gamma \delta}_{\alpha \beta \gamma \delta}] = \Omega^{-1}(\nabla^c \nabla^{\alpha \beta \gamma \delta}_{\alpha \beta \gamma \delta} + (\delta - 4) Y_c \nabla^{\alpha \beta \gamma \delta}_{(ab)c} + (\delta - 2) \nabla^c \nabla^{\alpha \beta \gamma \delta}_{(ab)c}),
\]

where \( Y_a := \Omega^{-1} \nabla_a \Omega \). For the Cotton tensor transformation we must decompose \( Y_d = Y_d + \hat{n}^d \nabla \hat{n} \), the second term of which cancels the term in \( B^{\alpha \beta \gamma \delta}_{ab} \) produced by the mean curvature. Setting \( \delta = 3 \) and keeping only the symmetric part of the Weyl divergence terms gives the final cancellation.

\[ \square \]

Remark 2.2. Invariance of the density \( B_{ab} \) for almost Einstein structures follows from [Gov10] Proposition 4.3], where it was related to the Bach tensor. It also appeared in the construction of a tractor analog of the exterior derivative in [GLW15]. Hence we shall call \( B_{ab} \) the hypersurface Bach tensor.

2.1.1. Invariant operators. Conformally invariant operators are maps between sections conformally weighted tensor bundles. These play a fundamental role in conformal and hypersurface geometries. Quite generally we will be interested in examples of these whose target and domain have differing weights and possibly tensor types. There are two main examples that are crucial to following developments.

Proposition 2.3. Let \( d \geq 3 \) and \( X^{ab} \) be a rank 2, symmetric, weight \( -d = -d - 1 \), trace-free hypersurface tensor. The mapping, given in a choice of scale by

\[
X^{ab} \mapsto L_{ab} X^{ab} := \begin{cases} 
\nabla_a \nabla_b X^{ab} + P_{ab} X^{ab}, & d \geq 3, \\
\nabla_a \nabla_b X^{ab} + P_{ab}^{\top} X^{ab} + H \Pi_{ab} X^{ab}, & d = 2,
\end{cases}
\]

determines a conformally invariant operator mapping

\[
\Gamma(c_o^2 T \Sigma[-d]) \xrightarrow{L_{ab}} \Gamma(c_o^2 T \Sigma[-d]).
\]

Proof. In dimensions \( d \geq 3 \), the result is standard and germane to any conformal geometry from the theory of invariant differential operators based on EGG sequences, see for example [ES97]. When \( d = 2 \) one can choose a scale, and transform the metric explicitly under \( g_{ab} \rightarrow \Omega^2 g_{ab} \) and then directly verify conformal invariance using the mean curvature transformation given in Equation (2.10) as well as those for the Schouten tensor and a weight \( w \) vector \( \nu^a \) (which extends to higher rank tensors by linearity):

\[
P^{\alpha \beta \gamma \delta}_{ab} = P_{ab}^{\alpha \beta \gamma \delta} - \nabla_a Y_b + Y_a Y_b - \frac{1}{2} Y^2 g_{ab},
\]

\[
\nabla_{ab}^{\alpha \beta \gamma \delta} \nu^a = \Omega^w (\nabla_{ab}^{\alpha \beta \gamma \delta} \nu^a + (w + 1) Y_a Y_b - \nabla^{\alpha \beta \gamma \delta} \nu_b + \delta^a_{\delta} Y_v \nu^a).
\]

\[ \square \]

Observe that \( L_{ab} \) is well-defined when acting on the conformal density \( \Pi^2_{(ab)\alpha} \); we record an identity for this required in future developments:

Proposition 2.4. Along hypersurfaces in a four-manifold one has

\[
L_{ab} \Pi^2_{(ab)\alpha} = \frac{1}{3} (\nabla^a \Pi^b_{(c)})(\nabla_c \Pi_a) + \frac{1}{4} (\nabla_a \Pi_c)(\nabla_a \Pi^c) + \frac{3}{2} \Pi^{ab} \Pi_{ab} - \frac{2}{3} K - \frac{3}{2} \Pi^{ab} \Pi^{\alpha \beta} \nabla_a \nabla_{(bc)} \Pi_{\alpha \beta} + \frac{1}{2} \Pi_{ab} W_{abc} + \frac{1}{2} W_{abc} \nabla_{ab} \Pi^c.
\]
Proof. The proof is a combination of basic tensor algebra and repeated usage of the trace-free Codazzi–Mainardi Equation \((2.9)\) applied to the double divergence of \(\Pi^2_{(ab)}\). We record the main steps below:

\[
\nabla^a \nabla^b \Pi^2_{(ab)} = 2 \nabla^a (\hat{\Pi}^a_{(b)} \nabla^b \Pi^c) - \frac{1}{3} \Delta K
\]

\[
= (\nabla^a \Pi_a)(\nabla^a \Pi^a) + 2 \Pi^{ab} \nabla^c \nabla_a \Pi_{bc} + (\nabla_a \Pi_{bc})(\nabla^b \Pi^{ac}) + \hat{\Pi}^{ac}[\nabla_a, \nabla_b] \Pi^c - \frac{1}{3} \Delta K
\]

\[
= \frac{1}{3} (\nabla^a \Pi^{bc})(\nabla_a \Pi_{bc}) + \frac{1}{2} (\nabla_a \Pi_a)(\nabla^a \Pi^a) - \frac{2}{3} \Pi^{ab} \Delta \Pi_{ab} + (\nabla^a \Pi^{bc}) \hat{W}^\top_{abc}
\]

\[
+ 2 \Pi^{ab} \nabla^c \nabla_a \Pi_{bc} + \hat{\Pi}^{ac}[\nabla_a, \nabla_b] \Pi^c
\]

\[
= \frac{1}{3} (\nabla^a \Pi^{bc})(\nabla_a \Pi_{bc}) + \frac{1}{2} (\nabla_a \Pi_a)(\nabla^a \Pi^a) + \frac{2}{3} \Pi^{ab} \Delta \Pi_{ab} + \frac{1}{2} \hat{W}^\top_{abc} \hat{W}^\top_{abc}
\]

\[
- \frac{4}{3} \Pi^{ab} \nabla^c \nabla_a \Pi_{bc} + \frac{1}{3} \hat{\Pi}^{ac}[\nabla_a, \nabla_b] \Pi^c.
\]

The third line was achieved using identity

\[(2.12) \quad \Pi^{ab} \nabla_a \nabla_b = \frac{2}{3} \Pi^{ab} \Delta \Pi_{ab} - \frac{2}{3} \Delta K - 2 \text{tr}(\Pi^2 \tilde{P}) - \frac{2}{3} \Pi^{ab} \nabla^c \tilde{W}^\top_{bac}, \]

which can be proved by using Equation \((2.9)\) to rewrite \(\nabla^c \nabla_a \Pi_{bc} = \Delta \Pi_{ab} - \nabla_b \nabla_a \Pi + \text{lower order terms}\). In three dimensions, the Weyl tensor vanishes so the last term in the computation of \(\nabla^a \nabla^b \Pi^2_{(ab)}\) displayed above Equation \((2.12)\) can only contribute intrinsic Schouten and scalar curvature terms; these are precisely \(-\Pi^{ab} \Pi^2_{(ab)} + \frac{2}{3} \Delta K\) and this completes the proof. \(\square\)

The second conformally invariant hypersurface operator needed implements the Robin combination of Neumann and Dirichlet boundary conditions and was shown to be conformally invariant by Cherrier:

**Definition 2.5.** Given a weight \(w\) conformal density \(f \in \Gamma(\mathcal{E} M[w])\), we define the (conformal) Robin operator

\[(2.13) \quad \delta_n f := \nabla^n f|_\Sigma - w H f|_\Sigma.\]

**Remark 2.6.** The operation \((\nabla - \frac{w}{\Delta + 1} \nabla) f\) is the Lie derivative of the density \(f\) along the unit normal vector \(\hat{n}\), so by construction \(\delta_n f\) is a weight \(w - 1\) conformal hypersurface density. \(*\)

The Robin operator can be extended to also act on conformal tensor densities, in what follows we will need the case of a rank two, symmetric conformal tensor density:

**Lemma 2.7.** Suppose \(X_{ab} \in \Gamma(\otimes^2 T^* M[w])\) obeys \(\hat{n} . X_b|_\Sigma = 0\) then one has a conformally invariant operator given here in a scale \(g \in \mathfrak{c}\)

\[(2.14) \quad \delta_n X_{ab} := (\nabla^n X_{ab} - (w - 2) H X_{ab})|_\Sigma.\]

This defines a section of \(\Gamma(\otimes^2 T^* \Sigma[w - 1])\) in the corresponding induced scale \(\tilde{g} \in \mathfrak{c}\).

**Proof.** This is a member of a general class of results that can be obtained from the Laplace-Robin operator discussed in Section \([5,5]\) A simple proof of the statement uses
the conformal transformation property of the mean curvature given in Equation (2.10) and that for the normal derivative of a rank two tensor density:
\[
\nabla^{\Sigma} X_{ab} = \Omega^{w-1} \left( \nabla_{\Sigma} X_{ab} + (w-2) \nabla_{(a} n_{b)} - 2 \nabla_{(a} \hat{n}_{b)} + 2 \hat{n}_{(a} Y_{b)} \right).
\]

Since \(\hat{n}.X_{b}|_{\Sigma} = 0\), and the formula for \(\delta_{a}\) projects onto the tangential part of \(\nabla_{\Sigma} X_{ab}\), only the first two terms on the right hand side above survive, and the result thus follows. \(\square\)

3. Defining function variational calculus

To handle hypersurface variational problems we treat hypersurfaces in terms of defining functions. Locally any hypersurface is the zero locus of some defining function, so no generality is lost studying hypersurfaces \(\Sigma = Z(s)\) for some defining function \(s\). For simplicity we take \(M\) oriented with volume form \(\omega\); this and the conormal \(ds\) determine the orientation of \(\Sigma\). We also shall assume, again mostly for simplicity, that \(\Sigma\) is compact.

Hypersurface invariants are defined as follows (see [GW15] Definition 2.6):

**Definition 3.1.** A scalar Riemannian pre-invariant is a mapping \(P\) which assigns a smooth function \(P(s; g)\) to each Riemannian \(d\)-manifold \((M, g)\) and hypersurface defining function \(s\), satisfying:

(i) \(P(s; g)\) is natural; for any diffeomorphism \(\phi : M \to M\) we have

\[
P(\phi^*s, \phi^*g) = \phi^*P(s; g).
\]

(ii) If \(s' = vs\) for some smooth, positive function \(v\) then

\[
P(s; g)|_{\Sigma\Sigma} = P(vs; g)|_{\Sigma\Sigma}, \text{ where } \Sigma = Z(s).
\]

(iii) \(P\) is given by a universal polynomial expression such that, given a local coordinate system \((x^a)\) on \((M, g)\), \(P(s, u; g)\) is given by a polynomial in the variables

\[
g_{ab}, \partial_1 g_{bc}, \cdots, \partial_k \partial_1 \cdots \partial_k g_{bc}, (\det g)^{-1}, \omega_{a_1 \cdots a_d},
\]

\[
s, \partial_1 s, \cdots, \partial_k \partial_1 \cdots \partial_k s, |ds|^2 \left(\frac{1}{g}\right),
\]

for some positive integers \(k, \ell\). Here \(\partial_a\) means \(\partial/\partial x^a\), \(g_{ab} = g(\partial_a, \partial_b)\), \(\det g = \det(g_{ab})\) and \(\omega_{a_1 \cdots a_d} = \omega(\partial_{a_1}, \cdots, \partial_{a_d})\).

A scalar Riemannian invariant of a hypersurface \(\Sigma\) is the restriction \(P(\Sigma; g) := P(s; g)|_{\Sigma}\) of a pre-invariant \(P(s; g)\) to \(\Sigma\).

**Remark 3.2.** A hypersurface invariant \(P\) depends only on the data \((M, g, \Sigma)\). For point (i) note that if \(\Sigma = Z(s)\), then \(\phi^{-1}(\Sigma)\) is a hypersurface with defining function \(\phi^*s\). In (ii), the requirement \(s' = vs\) means that \(s'\) and \(s\) are are two compatibly oriented defining functions with \(Z(s) = Z(s') =: \Sigma\). In (iii), since we are ultimately interested in hypersurface invariants, there is no loss of generality studying defining functions such that \(|ds|^2 \neq 0\) everywhere in \(M\), since we may, if necessary replace \(M\) by a local neighborhood of \(\Sigma\).

The definition extends to tensor-valued hypersurface pre-invariants and invariants by considering tensor-valued functions \(P\) and requiring the coordinate components of the image satisfy conditions (ii), (iii), and the obvious adjustment of (i). The term hypersurface invariant will be taken to mean either tensor or scalar valued hypersurface invariants.

*
Local Riemannian invariants, constructed in the usual way, provide trivial examples of hypersurface preinvariants. Examples of preinvariants that depend non-trivially on both $s$ and $g$ are given below:

**Example 3.3.** Given a hypersurface defining function $s$, examples of preinvariants are

\[ \mathcal{P}_a(s; g) = \frac{\nabla_a s}{|\nabla s|} \quad \text{and} \quad \mathcal{P}_{ab}(s; g) = \nabla_a \left( \frac{\nabla_b s}{|\nabla s|} \right) - \frac{\nabla_a s}{|\nabla s|} \frac{\nabla^c s}{|\nabla s|} \nabla_c \left( \frac{\nabla_b s}{|\nabla s|} \right). \]

Upon restriction to $\Sigma = \mathcal{Z}(s)$, these give the unit conormal and second fundamental form hypersurface invariants. It is important to note that for distinguished choices of defining function $s$, these expressions simplify considerably. For example, if $s$ obeys $|\nabla s| = 1$, then the second fundamental form is $\Pi_{ab} = (\nabla_a \nabla_b s)|_{\Sigma}$, but the quantity $\nabla_a \nabla_b s$ is, of course, not a preinvariant.

We now consider integrals $\int_{\Sigma} dA_g \cdot$ over a hypersurface, where $dA_g$ is the volume element of the induced metric $\bar{g}_{ab}$. Let $s$ be a defining function for $\Sigma$. Then, since (see Equation (2.1))

\[ \bar{g} = \left( g - \frac{ds \otimes ds}{|ds|^2} \right)|_{\Sigma}, \]

choosing coordinates $(x^a) = (s, y^i)$ where $g(ds, dy^i)|_{\Sigma} = 0$, it follows that

\[ \sqrt{\det g} \bigg|_{\Sigma} = \sqrt{\det \bar{g}} \bigg|_{\Sigma}. \]

Thus we have the following:

**Proposition 3.4.** Let $\Sigma$ be a smoothly embedded, compact hypersurface in $M$, with defining function $s$, and let $\mathcal{P}$ be a hypersurface invariant for $\Sigma$ with preinvariant $\mathcal{P}(s; g)$. Then

\[ (3.1) \quad \int_{\Sigma} dA_g \mathcal{P} = \int_M dV_g |\nabla s| \delta(s) \mathcal{P}(s; g), \]

where $\bar{g}$ is the pullback of the metric $g$ to $\Sigma$.

In the above $\delta(s)$ is the Dirac delta distribution. The above formula is standard, see for example [OF03] for its use in the theory of implicit surfaces. This has the advantage of allowing us to perform surface integrals over hypersurface invariants $\mathcal{P}$ in terms of (often far simpler) extensions to $M$.

**Remark 3.5.** The distributional identities $x \delta(x) = 0$ and $\delta(f(x)) = \sum_{x_0 \in \mathcal{Z}(f)} \frac{\delta(x-x_0)}{|f(x_0)|}$ for functions $f$ with simple roots, imply $|\nabla(v s)| \delta(v s) = |\nabla s| \delta(s)$. Thus, the integrand $|\nabla s| \delta(s) \mathcal{P}(s; g)$ on the right hand side of (3.1) can be loosely viewed as distributional hypersurface preinvariant.

Moving now to variational considerations, let $\mathcal{P}$ be a hypersurface invariant. The variation of the functional $I(\Sigma) = \int_{\Sigma} dA_g \mathcal{P}$, with respect to the embedding of the hypersurface $\Sigma$, is defined by

\[ (3.2) \quad \delta I := \frac{dI(\Sigma_t)}{dt} \bigg|_{t=0} = \frac{d}{dt} \int_{\Sigma_t} dA_g \mathcal{P}(\Sigma_t; g) \bigg|_{t=0}. \]

Here $\Sigma_t$ denotes a smooth, one parameter family of hypersurfaces such that $\Sigma_0 = \Sigma$ and $\Sigma_t = \Sigma$ outside a compactly supported subset of $M$. Also, $\bar{g}_t$ is the pullback of the metric $g$ to $\Sigma_t$. 

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Variational Calculus and the Singular Yamabe Problem

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Our strategy is, without loss of generality, to consider a family of hypersurfaces \( \Sigma_t = Z(s_t) \) where \( s_t \) is the family of defining functions
\[
s_t := s + tu
\]
for some smooth, compactly supported \( \delta s := u \in C^\infty M \). Thus \( I(\Sigma_t) = I(Z(s_t)) \). In general we will use \( \delta \) to denote the operation \( f(s) \mapsto \left( \frac{df(s+tu)}{dt} \right)_{t=0} =: \delta f \).

Using Equation (3.1) the variational formula (3.2) becomes
\[
\delta I = \frac{d}{dt} \int_M dV_g \left| \nabla s_t \right| \delta(s_t) \mathcal{P}(s_t; g) \bigg|_{t=0}.
\]
This reformulation leads to the following Lemma which is needed for our key variational Theorem 3.11 and is also a useful computational tool:

**Lemma 3.6.** Let \( \mathcal{P} \) be a hypersurface preinvariant with corresponding hypersurface invariant \( \tilde{\mathcal{P}} \). Consider a compactly supported variation \( \delta s \) of a defining function \( s \) for a hypersurface \( \Sigma \). Then
\[
(3.4) \quad \delta \left( \int_\Sigma dA_g \tilde{\mathcal{P}} \right) = \int_M dV_g \left| \nabla s \right| \delta(s) \left[ \delta \mathcal{P} - \frac{\delta s}{\left| \nabla s \right|} (\nabla \hat{n} + \nabla \hat{n}) \mathcal{P} \right],
\]
where \( \hat{n} := (\nabla s)/|\nabla s| \).

**Proof.** Let \( \chi \) be a (fixed) compactly supported cutoff function taking the value 1 on an open neighborhood of the support of \( \delta s \). Then
\[
\delta \left( \int_\Sigma dA_g \tilde{\mathcal{P}} \right) = \delta \left( \int_M dV_g \chi |\nabla s| \delta(s) \mathcal{P} \right)
\]
\[
= \int_M dV_g \chi \left[ (\nabla \hat{n}) \delta s \delta(s) \mathcal{P} + |\nabla s| \delta'(s) \delta s \mathcal{P} + |\nabla s| \delta(s) \delta \mathcal{P} \right]
\]
\[
\quad - \int_M dV_g \chi \left[ - (\nabla \hat{n}) \delta s \delta(s) \mathcal{P} - \delta(s) \delta \delta s \tilde{\mathcal{P}} + |\nabla s| \delta(s) \delta \mathcal{P} \right].
\]
Here we used that the derivative of \( \chi \) vanishes where \( \delta s \) has support and \( \nabla \hat{n} \delta(s) = |\nabla s| \delta'(s) \). Also, here and in the above, \( \delta'(s) \) can be interpreted in the usual distributional sense. In the second line above we performed an integration by parts using that the integrand has compact support. The result follows using Equation (3.1). \( \square \)

**Remark 3.7.** When \( \mathcal{P} \) (and thus also \( \tilde{\mathcal{P}} \)) is a density of weight \( -\tilde{d} \), the integral \( \int_\Sigma dA_g \tilde{\mathcal{P}} \) is conformally invariant. In this case the operator appearing in the second term of Equation (3.4) is the Lie derivative of \( \mathcal{P} \) along \( \hat{n} \). Along \( \Sigma \) this becomes
\[
\left( (\nabla \hat{n} + \nabla \hat{n}) \mathcal{P} \right) \bigg|_\Sigma = \delta \mathcal{P},
\]
where \( \delta \mathcal{P} \) is Cherrier’s conformally invariant Robin operator; see Definition 2.5. This motivates the notation of the definition that follows.

**Definition 3.8.** Let \( \Sigma \) be a hypersurface and let \( f \in C^\infty M \) (or a density of any weight). Then we define
\[
\delta_k f = \nabla \hat{n} f |_{\Sigma} - k H \tilde{f},
\]
where \( \tilde{f} = f |_{\Sigma} \) and \( k \in \mathbb{C} \).
To compute the variational gradient of $\int_{\Sigma} dA_{\hat{g}} \mathcal{P}$, it remains to express the first term on the right-hand side of Equation (3.4) in the form $\int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) \hat{\delta} s \mathcal{P}'$ with some local formula for $\mathcal{P}'$ where

$$\hat{\delta} s := \frac{\delta s}{|\nabla s|}.$$ We have introduced the quantity $\hat{\delta} s$ for homogeneity reasons: Observe that the integral $\int_{\Sigma} dA_{\hat{g}} \mathcal{P}$ being differentiated on the left-hand side of (3.4) is independent of the defining function $s$, so in particular is unchanged upon replacing $s$ with $vs$, for any positive, smooth function $v$. Thus $\delta \left( \int_{\Sigma} dA_{\hat{g}} \mathcal{P} \right) =: \delta I(s, \delta s) = \delta I(vs, v\delta s)$. It is easy to verify the identity

$$\frac{v \delta s}{|\nabla (vs)|} = \frac{\delta s}{|\nabla (s)|},$$

so that along $\Sigma$, $\hat{\delta} s$ enjoys the same homogeneity property as $\delta I$. To rewrite $\delta I$ with $\hat{\delta} s$ undifferentiated, we will need the following “integration by parts” lemma:

**Lemma 3.9.** Let $s$ be a defining function and suppose $C^a \in \Gamma(TM)$. Moreover let $B$ be a test function (i.e., smooth with compact support). Then

$$\int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) C^{a} \nabla_{a}^\top B = - \int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) B \nabla_{a}^\top C^{\top a},$$

where $\nabla^\top = \nabla - \hat{n} \nabla \hat{n}$, $\hat{n}_a = (\nabla_a s) / |\nabla s|$ and $C^{\top} := C - \hat{n} \cdot C$.

**Proof.** First, not forgetting the dependence of $\nabla^\top$ on $\hat{n}$, we use that $B$ is a test function and integrate by parts to compute

$$\int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) C^{a} \nabla_{a}^\top B = - \int_{\mathcal{M}} dV_{g} B \left[ \nabla_{a}^\top (|\nabla s| \delta(s) C^{\top a}) - |\nabla s| \delta(s) C^{\top b} \nabla_{a}^\top (\hat{n}_a^b \hat{n}_b) \right].$$

Next, a straightforward computation shows that

$$\nabla_{a} \hat{n}_a = \frac{\nabla_{a} |\nabla s|}{|\nabla s|}.$$ Using the distributional identity $\nabla^\top \delta(s) = 0$, the result follows. \qed

**Remark 3.10.** When $C^a$ and $B$, respectively, take values in sections of some tensor bundle over $\mathcal{M}$ and its dual and these are appropriately contracted to form a scalar, the natural extension of the above Lemma follows immediately.

The variation $\delta \mathcal{P}$ of a preinvariant is linear in the variation $u = \delta s$ and its derivatives up to some finite order $k$. If all derivatives on the variation $u$ are tangential derivatives $\nabla^\top u$, $(\nabla^\top)^2 u, \ldots, (\nabla^\top)^k u$, we can use the above lemma to integrate these by parts. In fact, as we shall prove in Theorem 3.11, this is always the case. That is, we show there is a well-defined notion for the functional derivative $\frac{\delta \mathcal{P}}{\delta s}$ of a preinvariant determined by

$$\int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) \delta \mathcal{P} := \int_{\mathcal{M}} dV_{g} |\nabla s| \delta(s) \hat{\delta} s \mathcal{P}' \delta s,$$

for compactly supported variations $\delta s$. We now give our main variational theorem:
Theorem 3.11. Let $\Sigma$ be a hypersurface with defining function $s$ and let $\mathcal{P}$ be a hypersurface invariant with corresponding preinvariant $\mathcal{P}$. Then for compactly supported variations,

$$
\delta \int_{\Sigma} dA_g \mathcal{P} = \int_M dV_g |\nabla s| \delta(s) \frac{\delta \mathcal{P}}{\delta s} (\delta_{\hat{n}} - (\nabla_{\hat{n}} + \nabla \cdot \hat{n}) \mathcal{P}),
$$

where $\hat{n} = (\nabla s)/|\nabla s|$.

Proof. Thanks to Lemma 3.6, we need only verify the well definedness of $\frac{\delta \mathcal{P}}{\delta s}$ in Equation (3.6). Our first step is to construct coordinates $(s, x^i)$ where $i = 1, \ldots, d$ such that the vector field $\frac{\partial}{\partial s}$ is orthogonal to constant $s = \varepsilon$ hypersurfaces $\Sigma^\varepsilon := Z(s - \varepsilon)$. This is achieved by integrating the vector fields $g^{-1}(ds, \cdot)$ and using the flow along their integral curves to push forward coordinates $x^i$ on $\Sigma = \Sigma_0$ to $\Sigma^\varepsilon$.

Since $\delta s$ has compact support, we may write the variation $\delta s = u \in C^\infty M$ in the coordinates $(s, x^i)$ as

$$u(s, x^i) = u(0, x^i) + s U(s, x^i),$$

for some smooth, bounded, function $U$. Now we decompose the one parameter family of defining functions in Equation (3.3) according to

$$s_i = s' + tu_0,$$

where the function $u_0$ is defined in these coordinates by $u_0 = u(0, x^i)$. Now note that $1 + t U(s, x^i)$ is a positive function for $t$ small, because $U$ is bounded. (So $s' = s(1 + t U(s, x^i))$ is also a defining function.) Thus for all such $t$ we have that $I(\Sigma) := \int_{\Sigma} dA_g \mathcal{P}$ satisfies

$$I(\Sigma) = I(Z(s)) = I(Z(s')).$$

Now from the construction of $I$ it follows that $I(t_1, t_2) := I(Z(s + t_1 s U + t_2 u_0))$ is differentiable as a function on $\mathbb{R}^2$. From this and the previous observation it follows that

$$\delta I = \frac{dI(s + tu_0)}{dt} \bigg|_{t=0}.$$

Next, from the definition of a preinvariant it follows that the variation $\delta I$ is a sum of terms of the form

$$\int_M dV_g |\nabla s| \delta(s) C^{\alpha_1 \ldots \alpha_k} \nabla_{a_1} \cdots \nabla_{a_k} u,$$

for some smooth tensors $C^{\alpha_1 \ldots \alpha_k}(s; g)$. However, the above coordinate argument shows that we may replace this by

$$\int_M dV_g |\nabla s| \delta(s) C^{\alpha_1 \ldots \alpha_k} \nabla_{a_1} \cdots \nabla_{a_k} u_0.$$

However, since $\nabla_{\hat{n}} u_0 = 0$, we have $\nabla u_0 = (\nabla - \hat{n} \nabla_{\hat{n}}) u_0 =: \nabla^\top u_0$. An easy induction shows that we can reexpress the integral as a sum of terms

$$\int_M dV_g |\nabla s| \delta(s) \tilde{C}^{\alpha_1 \ldots \alpha_k} \nabla^\top_{a_1} \cdots \nabla^\top_{a_k} u,$$

where we written $u$ not $u_0$ because $\nabla^\top s = 0$ and $s \delta(s) = 0$ (and $\tilde{C}^{\alpha_1 \ldots \alpha_k}$ are some smooth tensors). Integrating all $\nabla^\top s$ by parts according to Lemma 3.9 then establishes Equation (3.6). \qed
Corollary 3.12. Let $\Sigma$ be a hypersurface with defining function $s$ and let $\mathcal{P}$ be a hypersurface invariant with corresponding preinvariant $\check{\mathcal{P}}$. Then
\[
\frac{\delta \mathcal{P}}{\delta s} \bigg|_{\Sigma} - \delta_{\bar{a}} \mathcal{P} \quad \text{and} \quad \frac{\delta \mathcal{P}}{\delta s} - (\nabla_{\hat{n}} + \nabla\hat{n})\mathcal{P}
\]
are a hypersurface invariant and its corresponding preinvariant.

Example 3.13. Let $\hat{n}_a = \nabla_a s / |\nabla s|$ where $s$ is a defining function for $\Sigma$. Then
\[
\mathcal{P}(s; g) = \nabla_a \hat{n}_a
\]
is a preinvariant for $d$ times the mean curvature. Noting that
\[
\delta \hat{n}_a = \nabla_a \delta s / |\nabla s|,
\]
it follows that
\[
\delta \mathcal{P} = \nabla_a \left( \nabla_a \delta s / |\nabla s| \right) = \left[ \Delta^\top - |\nabla_a \log |\nabla s||^2 + (\Delta^\top \log |\nabla s|) \right] \delta s,
\]
where $\nabla_a^\top := \nabla_a - \hat{n}_a \nabla_{\hat{n}}$ and $\Delta^\top := g^{ab} \nabla_a \nabla_b^\top$. Notice $\delta \mathcal{P}$ does not contain normal derivatives $\nabla_{\hat{n}}$ acting on $\delta s$. Thus
\[
\frac{\delta P}{\delta s} = \Delta^\top \log |\nabla s| - |\nabla_a \log |\nabla s||^2.
\]
This is not a preinvariant, but it is not difficult to verify that $\frac{\delta P}{\delta s} - (\nabla_{\hat{n}} + \nabla\hat{n})\mathcal{P}$ is and along $\Sigma$ this equals the hypersurface invariant
\[
- \text{tr } \Pi^2 + d^2 H^2 + \text{Ric}(\hat{n}, \hat{n}) = Sc - \text{Ric}(\hat{n}, \hat{n}) - \hat{Sc}.
\]
Here the last equality relied on Equation (2.3).

3.1. Variational methods and identities. We now explain our strategy for computing variations and collect some key identities. Using Theorem 3.11, hypersurface variations are given in terms of preinvariants. To express preinvariants in terms of standard hypersurface invariants, we take advantage of property (ii) of Definition 3.1 which allows us to choose any defining function when evaluating preinvariants along $\Sigma$. In a computational context we are often concerned with expressions built from a sum of terms which separately are not preinvariants even though their sum is. Therefore in calculations it is important to use the same choice of defining function for every term.

Given any hypersurface in a Riemannian manifold there is locally a defining function $s$ satisfying
\[
|\nabla s| = 1.
\]
Defining functions with this property are dubbed unit defining functions. Since unit defining functions are determined by the hypersurface embedding, they provide a good choice for computations. In fact, there is a recursive solution to the formal problem of finding a smooth unit defining function $s_1$ given a defining function $s$ for a hypersurface such that
\[
|\nabla s_1| = 1 + s^\ell f,
\]
for $\ell \in \mathbb{Z}_{\geq 1}$ arbitrarily large and $f \in C^\infty M$ (see GW15 Section 2.2). This explicitly relates the jets of $s$ to hypersurface invariants. We employ the notation $\hat{=} \equiv$ for equalities relying on this choice while $\Sigma \equiv$ is used when evaluating quantities along $\Sigma$.

In general we abuse notation by using the same symbols for preinvariants as for their corresponding hypersurface invariant when the former has been explicitly chosen. Let
us tabulate some commonly used choices for preinvariants as well as their expressions in terms of a unit defining function:

| $\frac{1}{n}$ | Preinvariant | Invariant |
|--------------|-------------|----------|
| $n_a := \nabla_a s$ | $\frac{\nabla_a s}{|\nabla s|}$ | $\hat{n}_a$ |
| $g_{ab} - n_a n_b$ | $\gamma_{ab} := g_{ab} - \hat{n}_a \hat{n}_b$ | $\hat{g}_{ab}$ |
| $\nabla_a n_b$ | $\nabla_a \hat{n}_b$ | $\Pi_{ab}$ |
| $\frac{1}{d-1} \nabla_a n^a$ | $\frac{1}{d-1} \nabla_a \hat{n}^a$ | $H$ |
| $\nabla_a n_b - \frac{(g_{ab} - n_a n_b) \nabla_c n_c}{d-1}$ | $\nabla_a \hat{n}_b - \gamma_{ab} H$ | $\hat{\Pi}_{ab}$ |

So for example, off the hypersurface the notation $\hat{n}_a$ means $(\nabla_a s)/|\nabla s|$ and an expression like $\nabla n H$ denotes $\frac{1}{d-1} \nabla \nabla^\top \hat{n}^a$. The label $\top$ is employed to denote projection of tensors on M to their part perpendicular to the unit vector $\hat{n}$, and $\nabla^\top := \nabla - \hat{n} \nabla \hat{n}$.

Our first key variational identity was given in Example 3.13, but we repeat it for completeness:

\[
\delta \hat{n}^a = \frac{\nabla^a \delta s}{|n|} - \frac{n^a}{|n|^2 \nabla \hat{n} \delta s} = 1. \nabla^a \delta \Sigma \Rightarrow \nabla^a \delta s,
\]

where $\delta s := \delta s|\Sigma = 1 = \delta s|\Sigma = 1$. Thus

\[
(\delta \Pi_{ab})^\top = \left[ \nabla^\top a \left( \frac{\nabla^\top b \delta s}{|n|} - \frac{\nabla^\top a \delta s}{|n|} \nabla \hat{n} \hat{n} \right) \nabla \hat{n}_{b} \right] = \left[ \nabla^\top a \nabla^\top b \delta s \right]^\top \Sigma = \nabla^\top a \nabla^\top b \delta s.
\]

Importantly, in the above computations, we first varied preinvariant expressions for invariants and only thereafter specialized these to a unit defining function.

In a functional setting, we can use Equation (3.8) to give a useful lemma for computing variations of functionals involving the second fundamental form:

**Lemma 3.14.** Let $K^{ab} \in \Gamma((\bigotimes^2 T\Sigma)$ and $s$ be a unit defining function with $\delta s| = \delta s| \Sigma = 1$. Then

\[
\int_{\Sigma} dA \bar{g} K^{ab} (\delta \Pi_{ab})|\Sigma = \frac{1}{d-1} \int_{\Sigma} dA \bar{g} \delta s| \nabla \nabla_{b} K^{ab}.
\]

Finally, one more technical lemma is required:

**Lemma 3.15.** Let $X_{ab}$ be a rank two, symmetric tensor on $M$ satisfying $\hat{n}^a X_{ab} = 0$. Then

\[
[\nabla \hat{n} X_{ab} - \gamma_{ab} \gamma^{cd} \nabla \hat{n} X_{cd} - \nabla \hat{n} (X_{(ab)c})] = 0\,
\]

We leave the proof to the reader.

### 3.2. Examples

As a first example, we consider the problem of extremizing the area of an embedded hypersurface. The relevant functional is

\[
I = \int_{\Sigma} dA \bar{g}.
\]

Using Theorem 3.11 we have

\[
\delta I = -\int_{\Sigma} dA \bar{g} \delta s| (\delta_{-1} 1) = -d \cdot \int_{\Sigma} dA \bar{g} \delta s| H,
\]

which recovers the standard vanishing mean curvature $H$ condition for minimal surfaces.
A second example is the variation of the Willmore energy for surfaces (in Lorentzian signature, this is the rigid string action of Pol86):

\[ I_2 = -\frac{1}{6} \int \sigma dA \hat{g} K, \]

where \( K \) is the rigidity density of Equation (2.6). Using Theorem 3.6 we find

\[ \delta I_2 = -\frac{1}{6} \int \sigma dA \hat{g} (\delta K) + \frac{1}{6} \int dA \hat{g} \delta s | \delta \hat{n} K. \]

Using Equation (3.9), and observing that only the variations of \( II_{ab} \) contribute when the preinvariant \( K \) is written in terms of \( II_{ab} \) and \( \gamma_{ab} \), the first of the terms above becomes

\[ -\frac{1}{3} \int \sigma dA \hat{g} \delta s | \nabla_a \nabla_b \hat{II}_{ab}. \]

The second term requires that we compute a normal derivative of \( K \):

\[ \delta_n K - 2HK = \nabla_n K = 2\hat{II}_{ab} \nabla_n \hat{II}_{ab} = 2\hat{II}_{ab} | [\nabla_n, \nabla_a] n_b \]

\[ = 2\hat{II}_{ab} [-P_{ab} - \hat{II}_{ab} - 2H\hat{II}_{ab}] = -2 \text{tr}(\hat{II} P) - 4HK, \]

where we have used Equation (2.13) as well as that the Weyl tensor vanishes for \( d < 4 \) and for surfaces \( \text{tr} \hat{II}^3 = 0. \) Assembling the above we find

\[ \delta I_2 = -\frac{1}{3} \int \sigma dA \hat{g} \delta s | (\nabla_a \nabla_b + P_{ab} + H\hat{II}_{ab}) \hat{II}_{ab}. \]

Thus, using Equation (2.11), we obtain the following:

**Proposition 3.16.** With respect to hypersurface variations the gradient of the Willmore energy \( I_2 \) is

\[ -\frac{1}{3} L_{ab} \hat{II}_{ab}. \]

Thus the Willmore equation is \( L_{ab} \hat{II}_{ab} = 0. \) Note that the Willmore invariant displayed in the above Proposition is manifestly conformally invariant because \( L_{ab} \) is the invariant operator of Proposition 2.3. For Euclidean host spaces, using Equation (2.5), the Willmore equation takes the more familiar form

\[ \hat{\Delta} H + 2H(H^2 - K) = 0, \]

where \( K = \frac{1}{2} Sc \) is the Gauß curvature.

4. **The Conformal Four-Manifold Hypersurface Energy Functional**

Our main variational result, as stated in Proposition 1.2 is that the obstruction density \( B_3 \) for spaces agrees with the variational gradient of the rigid membrane functional

\[ I_3 = \frac{1}{6} \int \sigma dA \hat{g} L, \]

where the membrane rigidity density \( L \) is given in Equation (2.8). In this section we prove Proposition 1.2.

We begin by using Theorem 3.6 to write the variation as

\[ \delta I_3 = \frac{1}{6} \int \sigma dA \hat{g} (\delta L) | \sigma - \frac{1}{6} \int dA \hat{g} \delta s | \delta \hat{n} L. \]
To compute the first of these terms, we use the Fialkow Equation (2.7) to write
\[ L = \text{tr} \hat{\Pi}^3 - \hat{W}(\hat{n}, \hat{\Pi}, \hat{n}) , \]
so that
\[ \int dA_g(\delta L)_{|\Sigma} = \int dA_g [3\Pi_{ab}^2 \delta \Pi^{ab} - (\delta \Pi^{ab}) \hat{W}_{ab} - 2\Pi^{ab} \hat{W}_{bac} \delta n^c]_{|\Sigma} . \]
Using Equations (3.7) and (3.9), this becomes
\[ \int dA_g \delta L = \frac{1}{6} \int dA_g \delta s \left[ 3\nabla^a \nabla^b \hat{\Pi}_{(ab)\circ}^2 - \nabla^a \nabla^b \hat{W}_{ab} + 2\nabla^c (\hat{\Pi}^{ab} \hat{W}_{bac}^\top) \right]_{|\Sigma} , \]
where the final two terms in the last line were obtained using Equation (2.7) to rewrite the final term of the first line.

To compute the second term in \( \delta \mathcal{L}_3 \), we employ Lemma 3.15 to first calculate the normal derivative of the second fundamental form:
\[ (\nabla_n \hat{\Pi}_{ab})^\top = (\nabla_n \Pi_{ab})^\top - (n^a \nabla_c \hat{W}_{bc})^\top - \hat{W}_{ab} - \hat{P}_{(ab)\circ} \hat{\Pi}_{(ab)\circ}^2 \]
\[ = 2\hat{W}_{ab} - \hat{P}_{(ab)\circ} - 2\hat{\Pi}_{(ab)\circ}^2 - H\hat{\Pi}_{ab} , \]
where in the final step we have used the Fialkow Equation (2.7). Additionally, we must compute a normal derivative of the Weyl tensor:
\[ \nabla_n \hat{W}_{ab} = n^a \nabla_c \hat{W}_{bad} = (g^{dc} - \hat{g}^{dc}) \nabla_c \hat{W}_{bad} \]
\[ = \hat{\Pi}^d \hat{W}_{dabc} + n^c \nabla^d \hat{W}_{dabc} - \nabla^c \hat{W}_{bc}^\top \]
\[ = \hat{\Pi}^d \hat{W}_{dabc} - 3\hat{H} \hat{W}_{ab} + n^c C_{bca} - \nabla^c \hat{W}_{bac}^\top + \hat{\Pi}_{a} \hat{W}_{cb}^\top . \]
Orchestrating the above results we find
\[ \delta_n L := \delta_n L + 3H \delta L = \frac{1}{6} \int dA_g \delta s \left[ 3\nabla^a \nabla^b \hat{\Pi}_{(ab)\circ}^2 + 3\hat{P}^{ab} \hat{\Pi}_{(ab)\circ}^2 - \nabla^a \nabla^b \hat{W}_{ab} - \hat{W}(n, \hat{\Pi}, \hat{n}) \right]_{|\Sigma} , \]
\[ = 3\hat{P}^{ab} \hat{\Pi}_{(ab)\circ}^2 - \hat{W}(n, \hat{\Pi}, \hat{n}) - 3\hat{H} \hat{W}_{ab} - \hat{P}_{(ab)\circ} \hat{\Pi}_{(ab)\circ}^2 \]
\[ - 7 \hat{W}(n, \hat{\Pi}, \hat{n}) + K^2 + \hat{P}^{ab} \hat{W}_{dabc} + 2\hat{W}_{ab} \hat{W}_{ab}^\top . \]
Using these, the variation \( \delta \mathcal{L}_3 \) becomes
\[ \delta \mathcal{L}_3 = \frac{1}{6} \int dA_g \delta s \left[ 3\nabla^a \nabla^b \hat{\Pi}_{(ab)\circ}^2 + 3\hat{P}^{ab} \hat{\Pi}_{(ab)\circ}^2 - \nabla^a \nabla^b \hat{W}_{ab} - \hat{W}(n, \hat{\Pi}, \hat{n}) \right]_{|\Sigma} , \]
\[ + \hat{\Pi}^a \nabla^c \hat{W}_{bac}^\top - C(n, \hat{\Pi}) - 3\hat{H} \hat{W}(n, \hat{\Pi}, \hat{n}) + \hat{W}_{bac}^\top \hat{W}_{bac}^\top \]
\[ - 7 \hat{W}(n, \hat{\Pi}, \hat{n}) + K^2 + \hat{P}^{ab} \hat{W}_{dabc} + 2\hat{W}_{ab} \hat{W}_{ab}^\top \right]_{|\Sigma} . \]
This result can be written in a manifestly conformally invariant way using the operator \( L^{ab} \) of Proposition (2.11) and the hypersurface Bach tensor of Lemma 2.1:
\[ \delta \mathcal{L}_3 = \frac{1}{6} \int dA_g \delta s \left[ L^{ab} [3\Pi_{(ab)\circ}^2 - \hat{W}_{ab} - \hat{P}^{ab} B_{ab} + K^2 + \hat{W}_{bac}^\top \hat{W}_{bac}^\top \]
\[ - 7 \hat{W}(n, \hat{\Pi}, \hat{n}) + \hat{P}^{ab} \hat{W}_{dabc} + 2\hat{W}_{ab} \hat{W}_{ab}^\top \right] . \]
This shows that the tensor
\[ B_3 = \frac{1}{6} \left[ L^{ab}(3\Pi_{(ab)c}^{(kl)} - W_{abc}) - \Pi^{ab}B_{ab} + K^2 - 7W_{abc} + 2W_{abc} + \Pi^{cd}W_{abcd} + W_{abc} \right] \]
is the variational gradient and completes the proof of Proposition 5.2.

5. Conformal hypersurfaces and the singular Yamabe problem

We define here a singular Yamabe problem as the boundary version of the classical
Yamabe problem of finding a conformally related metric with constant scalar curva-
ture \[ \text{Maz91, ACF92}. \]

Problem 5.1. Given a \( d \geq 3 \)-dimensional Riemannian manifold \( (M, g) \) with boundary
\( \Sigma := \partial M \), find a smooth defining function \( u \) on \( M \) satisfying the conditions:
(1) \( u \) is a defining function for \( \Sigma \) (i.e., \( \Sigma \) is the zero set of \( u \), and \( du \neq 0 \) \( \forall x \in \Sigma \));
(2) \( g^\sigma := u^{-2}g \) has scalar curvature \( Sc^{g^\sigma} = -d(d - 1) \).

Where \( 0 < u := \rho^{-2/(d-2)} \), part (2) of this problem is governed by the Yamabe equation
\[ \left[ -4 \frac{d - 1}{d - 2} \Delta^g + Sc^g \right] \rho + d(d - 1) \rho \frac{d + d - 2}{d - 2} = 0. \]

But since \( u \) is a defining function, to deal with boundary aspects the equation can be
usefully recast: Since each \( g \in c \) is in 1:1 correspondence with a true scale \( \tau \in \Gamma(\mathcal{E}M[1]) \),
setting the smooth defining function \( u = \sigma/\tau \), the Yamabe equation becomes
\[ S(\sigma) := \left( \nabla^2 \right)^2 2 \frac{d}{d} \sigma \left( \Delta + \frac{Sc}{2(d - 1)} \right) \sigma = 1. \]

In the above \( \Delta := g^{ab}\nabla_a \nabla_b \) and all index contractions are performed with the conformal
metric \( g \) and its inverse. It follows easily that the quantity \( S(\sigma) \) on the left hand side of
Equation (5.1) is conformally invariant. Note that \( S(\sigma) = -\frac{Sc^{g^\sigma}}{d(d-1)} \). Also, because \( u \)
is a defining function, \( \sigma \) is a defining density: this is a section of \( \Gamma(\mathcal{E}M[1]) \) with zero locus
\( \mathcal{E}(\sigma) = \Sigma \) and such that for any Levi-Civita connection in the conformal class \( \nabla \sigma \neq 0 \)
along \( \Sigma \); see Section 5.3 below.

Development of the asymptotic analysis of the singular Yamabe problem as well as
uncovering its fundamental role in the theory of conformal hypersurface invariants uses
the tractor calculus treatment of conformal geometries. We next review key aspects of
that theory.

5.1. Conformal geometry and tractor calculus. Although there is no distinguished
connection on the tangent bundle \( TM \) for a \( d \)-dimensional conformal manifold \( (M, c) \),
there is a canonical metric \( h \) and linear connection \( \nabla^\ell \) (preserving \( h \)) on a related higher
rank vector bundle known as the tractor bundle \( T^A M \). This is a rank \( d + 2 \) vector bundle
equipped with a canonical tractor connection \( \nabla^A \) [Tho26, BEG94]. The bundle \( T^A M \) is
not irreducible but has a composition series given by the semi-direct sum
\[ T^A M = \mathcal{E}M[1] \oplus \mathcal{E}aM[1] \oplus \mathcal{E}M[-1]. \]

There is a canonical bundle inclusion \( \mathcal{E}M[-1] \to T^A M \), with \( T^*M[1] \) a subbundle of the
quotient by this, as well as a surjective bundle map \( T^A M \to \mathcal{E}M[1] \). We denote by \( X^A \)
the canonical section of \( T^A M[1] := T^A M \otimes \mathcal{E}M[1] \) giving the first of these:
\[ X^A : \mathcal{E}M[-1] \to T^A M, \]
and term \( X \) the canonical tractor.
A choice of metric \( g \in c \) determines an isomorphism (or splitting)

\[
\mathcal{T}M \overset{\mathcal{E}M[1]}{\rightarrow} E_M[1] \oplus E^*M[1] \oplus E_M[-1].
\]

We may write, for example, \( U \overset{g}{\rightarrow} (\sigma, \mu_a, \rho) \), or alternatively \([U^A]_g = (\sigma, \mu_a, \rho)\), to mean that \( U \) is an invariant section of \( \mathcal{T}M \) and \((\sigma, \mu_a, \rho)\) is its image under the isomorphism \((5.3)\); often the dependence on \( g \in c \) is suppressed when this is clear by context. Changing to a conformally related metric \( \hat{g} = \Omega^2 g \) gives a different isomorphism, which is related to the previous one by the transformation formula

\[
(\sigma, \mu_a, \rho)^{(\hat{g})} = (\Omega \sigma, \Omega(\mu_a + \sigma \gamma_a), \Omega^{-1}(\rho - g^{bc} \gamma_b \mu_c - \frac{1}{2} \sigma g^{bc} \gamma_b \gamma_c))^g,
\]

where \( \gamma_b \) is the one-form \( \Omega^{-1} d\Omega \).

In terms of the above splitting, the tractor connection is given by

\[
\nabla^T_a \left( \begin{array}{c} \sigma \\ \mu_b \\ \rho \end{array} \right) := \left( \begin{array}{c} \nabla_a \sigma - \mu_a \\ \nabla_a \mu_b + g_{ab} \rho + P_{ab} \sigma \\ \nabla_a \rho - P_{ac} \mu^c \end{array} \right).
\]

We will often recycle the Levi-Civita notation to also denote the tractor connection; it is the only connection we shall use on \( \mathcal{T}M \), its dual, and tensor powers. Its curvature is the tractor-endomorphism valued two form \( \mathcal{R}^2 \), in the above splitting this acts as

\[
\mathcal{R}^2_{ab} \left( \begin{array}{c} \sigma \\ \mu_c \\ \rho \end{array} \right) = [\nabla_a, \nabla_b] \left( \begin{array}{c} \sigma \\ \mu_c \\ \rho \end{array} \right) = \left( \begin{array}{c} 0 \\ W_{abc} \mu^c + C_{abc} \sigma \\ -C_{abc} \mu^c \end{array} \right).
\]

For \([U^A] = (\sigma, \mu^a, \rho)\) and \([V^A] = (\tau, \nu^a, \kappa)\), the conformally invariant, signature \((d + 1, 1)\), tractor metric \( h \) on \( \mathcal{T}M \) given by

\[
h(U, V) = h_{AB} U^A V^B = \sigma \kappa + g_{ab} \mu^a \nu^b + \rho \tau =: U V,
\]

is preserved by the tractor connection, i.e., \( \nabla^T h = 0 \). It follows from this formula that \( X_A = h_{AB} X^B \) provides the surjection by contraction \( \iota(X) : \mathcal{T}M \rightarrow E[1] \). The tractor metric \( h_{AB} \) and its inverse \( h^{AB} \) are used to identify \( \mathcal{T}M \) with its dual and to raise and lower tractor indices. The notation \( V^2 \) is shorthand for \( V_A V^A = h(V, V) \).

Tensor powers of the standard tractor bundle \( \mathcal{T}M \), and tensor products thereof, are vector bundles that are also termed tractor bundles. We shall denote a tractor bundle of arbitrary tensor type by \( \mathcal{T}^\Phi M \) and write \( \mathcal{T}^\Phi M[w] \) to mean \( \mathcal{T}^\Phi M \otimes E_M[w] \); \( w \) is then said to be the weight of \( \mathcal{T}^\Phi M[w] \).

Closely linked to \( \nabla^T \) is an important second order conformally invariant differential operator

\[
D^A : \Gamma(\mathcal{T}^\Phi M[w]) \rightarrow \Gamma(\mathcal{T}^\Phi M[w - 1]),
\]

known as the Thomas (or tractor) D-operator. Here \( \mathcal{T}^\Phi M[w - 1] := \mathcal{T}^A \otimes \mathcal{T}^\Phi M[w - 1] \). In a scale \( g \),

\[
[D^A]_g = \left( \begin{array}{c} (d + 2w - 2) w \\ (d + 2w - 2) \nabla_a \\ -(\Delta^g + J w) \end{array} \right),
\]

where here \( \Delta = g^{ab} \nabla_a \nabla_b \), and \( \nabla \) is the coupled Levi-Civita-tractor connection \( [\text{BEG94}, \text{Tho26}] \). The following variant of the Thomas D-operator is also useful.
Definition 5.2. Suppose that \( w \neq 1 - \frac{d}{2} \). The operator

\[
\hat{D}^A : \Gamma(T^\Phi M[w]) \rightarrow \Gamma(T^{\Phi'} M[w - 1])
\]

is defined by

\[
\hat{D}^A T := \frac{1}{d + 2w - 2} D^A T.
\]

Remark 5.3. We term the critical value \( w = 1 - \frac{d}{2} \) the Yamabe weight, since one then has

\[
D^A = -X^A \Box_Y,
\]

where the operator \(-\Box_Y : \Gamma(T^\Phi M[1 - \frac{d}{2}]) \rightarrow \Gamma(T^\Phi M[-1 - \frac{d}{2}])\) is the conformally invariant, tractor-coupled, Yamabe operator given by \( \Delta - \frac{d-2}{2} J \) in a choice of scale. *

The Thomas D-operator is null, in the sense that

\[
D^A \circ D_A = 0;
\]

this operator identity can easily be derived from Equation (5.7). The Thomas D-operator is not, however, a derivation. Its failure to obey a Leibniz rule is captured by the following Proposition, a result which was first observed in [JTW13] and proved in [GW15]:

Proposition 5.4. Let \( T_i \in \Gamma(T^\Phi M[w_i]) \) for \( i = 1, 2 \), and \( h_i := d + 2w_i, h_{12} := d + 2w_1 + 2w_2 - 2 \) with \( h_i \neq 0 \neq h_{12} \). Then

\[
\hat{D}^A(T_1 T_2) - (\hat{D}^A T_1) T_2 - T_1 (\hat{D}^A T_2) = -\frac{2}{d + 2w_1 + 2w_2 - 2} X^A (\hat{D} B T_1) (\hat{D} B T_2).
\]

We shall also need the following Lemma which is easily verified by direct application of Equation (5.7) or the modified Leibniz rule (5.8) in tandem with the identity

\[
\hat{D}^A X^B = h^{AB}.
\]

Lemma 5.5. Let \( T \in \Gamma(T^\Phi M[w]) \). Then

\[
D_A (X^A T) = (d + w)(d + 2w + 2) T.
\]

5.2. Conformal hypersurfaces and tractors. The basis for a conformal hypersurface calculus [Gov10, Gra03, Sta05, Vya13, GW15] is a unit tractor object \( N^A \in \Gamma(T\Sigma)\) (from [BEG94]) corresponding to the conformal unit conormal \( \hat{n} \), termed the normal tractor. This is defined along \( \Sigma \), in a choice of scale, by

\[
[N^A] = \begin{pmatrix} \hat{n}^a \\ -H \end{pmatrix} \Rightarrow N_A N^A = 1.
\]

The subbundle \( T\Sigma^\top \) orthogonal to the normal tractor (with respect to the tractor metric \( h \)) along \( \Sigma \) is canonically isomorphic to the intrinsic hypersurface tractor bundle \( T\Sigma \), see [BG01] and [Gov10, Section 4.1]. This is the conformal tractor analog of the Riemannian isomorphism between the intrinsic tangent bundle \( T\Sigma \) and the subbundle \( T\Sigma^\top \) of \( T\Sigma \) orthogonal to \( \hat{n}^a \) along \( \Sigma \). This isomorphism identifies these bundles and thus we use the same abstract index for \( T\Sigma \) and \( T\Sigma \). In explicit computations in a given choice of scale, we will need to relate sections given in corresponding splittings of the
ambient and hypersurface tractor bundles. In terms of sections expressed in a scale \( g \in c \) (which determines \( \tilde{g} \in \tilde{e} \)), the isomorphism is given by

\[
(5.12) \quad [V^A]_g := \begin{pmatrix} v^+ \\ v_a \\ v^- \end{pmatrix} \mapsto \begin{pmatrix} v^+ \\ v_a - \tilde{n}_a H v^+ \\ v^- + \frac{1}{2} H^2 v^+ \end{pmatrix} = [U^A B]_{\tilde{g}} [V^B]_{\tilde{g}} =: [\tilde{V}^A]_{\tilde{g}},
\]

where \( V^A \in \Gamma(\mathcal{T} M^\top) \), \( \tilde{V}^A \in \Gamma(\mathcal{T} \Sigma) \) and the \( SO(d+1,1) \)-valued matrix

\[
[U^A B]_{\tilde{g}} := \begin{pmatrix} 1 & 0 & 0 \\ -\tilde{n}_a H & \delta_a^b & 0 \\ -\frac{1}{2} H^2 & \tilde{n}_b H & 1 \end{pmatrix}.
\]

In the above the canonical isomorphism between \( T^* M^\top|_{\Sigma} \) and \( T^* \Sigma \) defined by the unit normal vector \( \tilde{n} \) is used to identify sections of these bundles.

The ambient tractor connection \( \nabla \) obeys an analog of the classical Gauß formula relating it to the intrinsic tractor connection \( \bar{\nabla} \) of \((\Sigma, c)\) which is known as the Fialkow–Gauß formula ([Gra03, Sta05, Vya13] or in our current notation [GW15, Proposition 7.14]) because the Fialkow tensor of Equation (2.7) encodes the difference between these two connections along \( \Sigma \). As in the Gauß case, the tractor-coupled operator \( \nabla^\top := \nabla - \tilde{n} \nabla \tilde{n} \) is well-defined along \( \Sigma \) irrespective of how tensors are extended to the ambient. For future use, we record some identities for this operator acting on the normal tractor:

**Lemma 5.6.** Along \( \Sigma \), tangential, tractor-coupled gradients of the normal tractor are given in a choice of scale by

\[
(5.13) \quad \nabla^\top_a N^C = \begin{pmatrix} 0 \\ \tilde{\Pi}_{ac} \\ \frac{\nabla \tilde{n}_a}{d-1} \end{pmatrix}, \quad \nabla^\top_a \nabla^\top_b N^C = \begin{pmatrix} -\tilde{\Pi}_{ab} \\ \nabla^\top_a \tilde{\Pi}_{bc} - \frac{1}{d-1} \tilde{g}_{ac} \nabla^\top b \tilde{\Pi}_b \\ -\frac{1}{d-1} \nabla^\top_a \nabla^\top b \tilde{\Pi}_b - \tilde{\Pi}_{ac}^T P_{ac}^T \end{pmatrix},
\]

while the tangential, tractor-coupled operator \( \Delta^\top := g^{ab} \nabla^\top_a \nabla^\top_b \) gives

\[
(5.14) \quad \Delta^\top N^C = \begin{pmatrix} 0 \\ \frac{d-2}{d-1} \nabla_c \tilde{\Pi}_c - n_c K \\ \nabla \nabla \tilde{\Pi} + (d-1) P_{ab} \tilde{\Pi}_{ab} \end{pmatrix}.
\]

**Proof.** Since \( \nabla^\top \) is tangential, the first identity follows directly from [GW15, Corollary 6.7]. The third identity follows directly from the second, both of which only require a direct application of Equation (5.13). \( \square \)

**Remark 5.7.** Note that expressions such as \( \nabla^\top_a \tilde{\Pi}_{bc} \) in the above Lemma are well-defined along \( \Sigma \) since \( \nabla^\top \) is tangential. It is obviously possible to further develop the second and third identities using the Gauß formula (2.2) and (for \( d \geq 3 \)) the Fialkow–Gauß Equation (2.7).

5.3. **Singular Yamabe problem asymptotics and defining densities.** Given a hypersurface \( \Sigma \), a section \( \sigma \in \Gamma(\mathcal{E}[1]) \) is said to be a **defining density** for \( \Sigma \) if \( \Sigma = \mathcal{Z}(\sigma) \) and \( \nabla \sigma \) is nowhere vanishing along \( \Sigma \), where \( \nabla \) is the Levi-Civita connection for some
The conformal analog of the exterior derivative of a defining function is then provided by the tractor field

\[ I_A^\sigma := \hat{D}^A \sigma = (\sigma, \nabla_a \sigma, -\frac{1}{d}(\Delta + J)\sigma) =: (\sigma, n_a, \rho). \]

In Riemannian signature for any defining density \( \sigma \), we have that

\[ I_2^\sigma > 0 \]

holds in a neighbourhood of \( \Sigma \). More generally, any section \( \sigma \in \Gamma(\mathcal{E}M[1]) \) such that \( I_A^\sigma \) is nowhere vanishing is called a \emph{scale}, \( I_A^\sigma \) is its \emph{scale tractor} and the data \((M, c, \Sigma)\) is an \emph{almost Riemannian structure} (or geometry). The following proposition, whose proof follows directly from Equations (5.15) and (5.6), shows that almost Riemannian geometries are a natural setting for the singular Yamabe problem:

**Proposition 5.8** (see [Gov10]). For \( \sigma \in \Gamma(\mathcal{E}[1]) \) the quantity \( S(\sigma) \) of Equation (5.1) is the squared length of the corresponding scale tractor:

\[ S(\sigma) = I_2^\sigma := h_{AB} I_A^\sigma I_B^\sigma. \]

Indeed, the Yamabe equation (5.1) now reads simply

\[ I_2^\sigma = 1. \]

Thus, the asymptotic version of the singular Yamabe Problem 5.1 is stated as follows:

**Problem 5.9.** Find a smooth defining density \( \bar{\sigma} \) such that

\[ I_2^{\bar{\sigma}} = 1 + \bar{\sigma}^d A_\ell, \]

for some smooth \( A_\ell \in \Gamma(\mathcal{E}[-\ell]) \), where \( \ell \in \mathbb{N} \cup \{\infty\} \) as high as possible.

The above problem was solved in [GW13, GW15], that result is captured by the following Theorem whose proof may be found in [GW15]:

**Theorem 5.10.** Let \( \sigma \) be a defining density for a hypersurface \( \Sigma \) and \( \sigma_0 := \sigma/\sqrt{I_2^\sigma} \), then there exist smooth densities \( A_k \in \Gamma(\mathcal{E}[\Sigma][-k]) \) such that

\[ \bar{\sigma} = \sigma_0 \left( 1 + A_1 \sigma_0 + A_2 \sigma_0^2 + \cdots + A_d \sigma_0^d \right) \]

solves

\[ I_2^{\bar{\sigma}} = 1 + \sigma_0^d B_\sigma, \]

for some smooth \( B_\sigma \in \Gamma(\mathcal{E}[d]) \). For \( 1 \leq k \leq d \) the densities \( A_k \) are determined by the recursion

\[ \bar{\sigma}_k = \bar{\sigma}_{k-1} \left[ 1 - \frac{d}{2} \frac{I_{2k-1}^\sigma - 1}{(d-k)(k+1)} \right], \]

where \( \bar{\sigma}_{k-1} := \sigma_0(1 + \sum_{j=1}^{k-1} \sigma_j A_j) \) solves \( I_{2k-1}^\sigma = 1 + \sigma^{k-1} C \) for smooth \( C \in \Gamma(\mathcal{E}[1-k]) \).

Moreover, for any true scale \( \tau \in \Gamma(\mathcal{E}[1]) \),

\[ \sigma' = \bar{\sigma} \left[ 1 + \frac{d}{2} \log(\bar{\sigma}/\tau) \frac{I_2^{\bar{\sigma}} - 1}{d+1} \right] \]

solves

\[ I_2^{\sigma'} = 1 + \sigma^{d+1} \left( C' + D \log(\sigma/\tau) + D' \log^2(\sigma/\tau) \right) \]

for smooth \( C', D, D' \in \Gamma(\mathcal{E}[d-1]) \). Finally, given two defining functions \( \sigma \) and \( \bar{\sigma} \) for \( \Sigma \), then

\[ B_\sigma\big|_\Sigma = B_{\bar{\sigma}}\big|_\Sigma =: B_d. \]
The last statement of this theorem implies that the density $\mathcal{B}_d$ is uniquely determined by $(M, c, \Sigma)$. Since it obstructs a smooth all orders solution to the singular Yamabe problem we term it the \textit{obstruction density}. The solution $\bar{s}(\sigma)$ is determined uniquely by the recursion up to the order of the obstruction. Thus, up to the given order, $\bar{s}$ is a canonical scale defining the hypersurface $\Sigma$ and whose scale tractor has unit length to accuracy $\sigma^d$, so is termed a \textit{conformal unit defining density}.

5.4. Conformal hypersurface invariants and canonical extensions. A Riemannian hypersurface invariant $\mathcal{P}(\Sigma; g) := \mathcal{P}(s; g)|_\Sigma$ with the property $\mathcal{P}(\Omega s, \Omega^2 g) = \Omega^w \mathcal{P}(s; g)$ is termed a \textit{conformal hypersurface covariant}. This determines an invariant section $\mathcal{P}(\sigma, g) \in \Gamma(\mathcal{E}M[w])$ where $\sigma$ is a defining density. Thus $\mathcal{P}(\sigma, g)|_\Sigma$ is called a \textit{conformal hypersurface invariant}. As for the Riemannian case, this definition extends to tensor and therefore also tractor-valued invariants.

Since the conformal unit scale $\bar{s}$ is a unique defining density, up to the addition of terms $\bar{s}^{d+1} S$ for $S \in \Gamma(\mathcal{E}M[-d])$, it follows that any conformal density $\mathcal{P}(\bar{s}(\sigma), g)$, where $\bar{s}(\sigma)$ is determined in terms a given defining density $\sigma$ via Equation (5.18) of Theorem 5.10 gives a conformal hypersurface invariant $\mathcal{P}(\bar{s}(\sigma), g)|_\Sigma$ so long as the formula for $\mathcal{P}$ involves jets of $\bar{s}$ of order $\leq d$. (In fact, $\mathcal{P}(\bar{s}(\sigma), g)$ is a density-valued preinvariant.) This construction provides \textit{holographic formulae} for conformal hypersurface invariants, see [GW15, Section 6.2].

Example 5.11. The scale tractor for the conformal unit defining density gives a holographic formula for the normal tractor

$$I_\sigma^A|_\Sigma = \bar{D}^A \bar{s}|_\Sigma = N^A.$$ 

This result was first proved in [Gov10].

Moreover, in the above example we may view the conformal unit defining density as providing a canonical extension $I_\sigma^A$ of the normal tractor $N^A$. A short computation (in a choice of scale) shows that

$$\nabla_a I_\sigma^B = \left( \begin{array}{c} \nabla_a n_b + P_{ab} \bar{s} + g_{ab} \rho \\ 0 \end{array} \right),$$

where $\rho := -\frac{1}{\pi} (\Delta \bar{s} + J \bar{s})$ as in Equation (5.15). Comparing this with Equation (5.13) gives a holographic formula for the trace-free second fundamental form

$$\bar{H}_{ab} = (\nabla_a n_b + P_{ab} \bar{s} + g_{ab} \rho)|_\Sigma.$$ 

Hence we have the following canonical extensions of the trace-free second fundamental form and rigidity density

$$(5.19) \quad \bar{H}_{ab} := \nabla_a n_b + P_{ab} \bar{s} + g_{ab} \rho \quad \text{and} \quad K := (\nabla_a n_b + P_{ab} \bar{s} + g_{ab} \rho)(\nabla^a n_b + P^{ab} \bar{s} + g^{ab} \rho).$$

The above formulae are now well-defined in $M$ rather than only along $\Sigma$. These extensions are canonical up to a finite order determined by Theorem 5.10.

5.5. The Laplace–Robin operator and tangential operators. By contracting the scale tractor and Thomas D-operator, we can build a new operator that plays two roles: that of the ambient Laplace operator and of a conformally invariant boundary Robin-type Dirichlet-plus-Neumann operator [Gov07]. Thus we call the operator

$$I \cdot D : \Gamma(\mathcal{T}^\Phi M[w]) \longrightarrow \Gamma(\mathcal{T}^\Phi M[w-1]),$$
the Laplace–Robin operator. Calculated in some scale \( g \in c \)

\[
I \cdot D = -\sigma \Delta + (d + 2w - 2) \left[ \nabla_n - \frac{w}{d} (\Delta \sigma) \right] - \frac{2w}{d} (d + w - 1) \sigma J,
\]

where \( n = \nabla \sigma \). Hence this is a Laplace-type operator which is degenerate along \( \Sigma = \mathcal{Z}(\sigma) \). Indeed, along \( \Sigma \) the Laplace–Robin operator becomes first order. In particular, for a conformal unit defining scale, along \( \Sigma \) and in a choice of scale we have

\[
I_\sigma \cdot D = (d + 2w - 2) (\nabla_n - wH) .
\]

Hence, for \( w \neq 1 - \frac{d}{2} \) and in the spirit of the Section 5.4 along \( \Sigma \) the Laplace-Robin operator is a operator-valued holographic formula for the Robin operator \( \delta \tilde{H} \) as given in Equation (2.13) (recall that for a conformal unit defining density, along \( \Sigma \) one has \( \nabla \sigma = \nabla \). Given a natural density, tensor or tractor field \( f \) along \( \Sigma \), it is often the case that we can fix an extension \( \tilde{f} \) off \( \Sigma \), that is canonical to some order using the conformal unit defining density, such as those given in Equation (5.19). In that case we will denote the Robin operator by

\[
\delta_R \tilde{f} = \left\{ \begin{array}{ll} 
I_\sigma \tilde{D} f|_\Sigma, & w \neq 1 - \frac{d}{2}, \\
\nabla_n f|_\Sigma + \frac{d-2}{2} H \tilde{f}, & w = 1 - \frac{d}{2} .
\end{array} \right.
\]

In light of this, we will often use the same notation for \( f \) and \( \tilde{f} \).

Combining the conformal unit defining density and the Laplace–Robin operator allows successive normal derivatives of canonically extended conformal hypersurface invariants to be defined up to the order of the obstruction. The canonical extensions of the normal tractor and intrinsic canonical tractor are the scale tractor \( I_\sigma^A \) and the ambient canonical tractor \( X^A \), respectively. The following Lemma gives one normal derivative acting on these:

**Lemma 5.12.** The Robin operator acting on the canonically extended canonical and normal tractors gives:

\[
(5.21) \quad \delta_R X^A = N^A, \quad \delta_R N^A = \frac{K X^A}{d - 1} .
\]

**Proof.** The first identity is a direct consequence of Equation (5.9). For the second we compute in a scale

\[
\delta_R N^A = \nabla_n I^A_\sigma|_\Sigma = \begin{pmatrix} 0 \\
\nabla_n n_a - H n_a \\
\n\nabla_n \rho - P(n, n) \end{pmatrix} .
\]

To complete the proof we need the normal derivatives of the canonical extensions of \( n_a \) and \( \rho \) determined by \( I^A_\sigma \). These were computed in [GW15, Lemmas 6.1 and 6.6] and, along \( \Sigma \) are:

\[
(5.22) \quad \nabla_n n_a = H n_a, \quad \nabla_n \rho = P(n, n) + \frac{K}{d - 1} .
\]

□

The Laplace–Robin operator has one further crucial role to play. In [GW14], it was shown that by viewing the scale \( \sigma \) as an operator mapping \( \Gamma(\mathbb{T}^\Phi \mathcal{M}[w]) \rightarrow \Gamma(\mathbb{T}^\Phi \mathcal{M}[w + 1]) \) and acting by multiplication, then the commutator of this with the Laplace–Robin operator acting on weight \( w \) tractors obeys

\[
[I_\sigma \cdot D, \sigma] = -I_\sigma^2 (d + 2w) .
\]
This identity underlies a solution-generating \( \mathfrak{sl}(2) \) algebra. A particular consequence of this is that the operator

\[
P_k^\sigma := \left( -\frac{1}{I_2^\sigma} I_\sigma \cdot D \right)^k
\]
is tangential when acting on weight \( w = \frac{k-d+1}{2} \) tractors. Specializing to the conformal unit defining density gives a differential operator

\[
P_k : \Gamma(\mathcal{T}^k \mathcal{M} \left[ \frac{k-d+1}{2} \right]) \big|_\Sigma \rightarrow \Gamma(\mathcal{T}^k \mathcal{M} \left[ \frac{-k-d+1}{2} \right]) \big|_\Sigma,
\]
which is completely determined by the data \((M, c, \Sigma)\) [GW15, Section 8.1]. We call this the extrinsic conformal Laplace operator. For \( k \) even the operator \( P_k \) is \((\Delta^\top)^d + \text{L.O.T.}\), up to multiplication by a non-vanishing constant, where “L.O.T.” stands for terms of lower derivative order involving both intrinsic and extrinsic curvature quantities.

6. Singular Yamabe obstruction densities

Given a unit conformal defining density, the obstruction density \( B_\bar{d} \) has a simple holographic formula whose leading structure is given in terms of the extrinsic conformal Laplace operator [GW15, Theorem 8.11]:

**Theorem 6.1.** The obstruction density is given by

\[
B_\bar{d} = 2^n \bigg[ \Sigma_B^A \left( P_{\bar{d}} N_B^A + (-1)^{d-1} [\bar{I} D^{d-1} (X^B K)] \big|_\Sigma \right) \bigg],
\]

where the rigidity density \( K \) is canonically extended off \( \Sigma \) by the formula \( K = P_{AB} P^{AB} \) with \( P^{AB} := D^A I^B \). Also, the projector \( \Sigma_B^A := \delta_B^A - N^A N_B \).

The main aim of this section is to compute \( B_3 \) using the above holographic formula. The canonical extension of the rigidity density \( K \) stated in the theorem is the same as that given in Equation (5.19). Also, in hypersurface dimensions \( \bar{d} = 2, 3 \), the extrinsic conformal Laplacians acting on weight zero tractors are given by

\[
P_2 = \Delta^\top,
\]

\[
P_3 = -8 \bar{\bar{\Pi}}^{ab} \bar{\nabla}_a \bar{\nabla}_b - 8 \bar{\nabla}. \bar{\Pi} \bar{\nabla}^\top - 4 n^a \left( R_{ab}^{\#} \circ \nabla^b + \nabla^b \circ R_{ab}^{\#} \right).
\]

**Proposition 6.2.** If \( \bar{d} = 2 \), then

\[
P_2 N_C = -X^C L_{ab} \bar{\Pi}^{ab} - N^C K, \quad \bar{d} = 2.
\]

**Proof.** Using Equations (6.2) and (5.14), we have for \( \bar{d} = 2 \),

\[
P_2 N_C = \Delta^\top N_C = \begin{pmatrix}
0 & -n^C K \\
-\nabla \nabla . \bar{\Pi} - P_{ab} \bar{\Pi}^{ab}
\end{pmatrix}.
\]

Using Equation (2.11) the quoted result follows. □

**Remark 6.3.** Our computation of \( B_3 \) relies on a \( \bar{d} = 3 \) version of the above Proposition.

The second term in Equation (6.1) involves normal derivatives of the canonically extended rigidity density \( K \). The following proposition provides the first of these.
Proposition 6.4. The canonically extended trace-free second fundamental form $\hat{\Pi}_{ab}$, rigidity density $K$ and membrane rigidity density $L$ obey

\begin{equation}
(\delta_R \hat{\Pi}_{ab})^\top = -\hat{\Pi}_{ab}^2 + \hat{W}_{ab} + \frac{1}{2} \hat{g}_{ab}K, \quad \delta_R K = -2(\bar{d} - 2)L.
\end{equation}

Proof. We begin by computing a normal derivative of the canonical extension of $\hat{\Pi}_{ab}$:

\begin{align*}
\nabla_n \hat{\Pi}_{ab} &= \nabla_n \nabla_a n_b + g_{ab} \nabla_n \rho + \sigma \nabla_n P_{ab} + P_{ab} \nabla_n \sigma \\
&= \hat{n}_{ab} - (\nabla_a n_c) \nabla^c n_b - \nabla_a \nabla_b (\rho \sigma) + g_{ab} \nabla_n \rho + P_{ab} + \sigma (\nabla_n - 2\rho) P_{ab} \\
&= \hat{n}_{ab} - \hat{\Pi}_{ab}^2 + \rho \hat{\Pi}_{ab} - 2n_{(a} \nabla_{b)} \rho + g_{ab} \nabla_n \rho + P_{ab} \\
&\quad + \sigma \left[ (\nabla_n - 3\rho) P_{ab} + 2\hat{\Pi}^c_{(a} \hat{P}^b_{c)} - \nabla_a \nabla_b \rho \right] + O(\sigma^2).
\end{align*}

(6.4)

Projecting onto the tangential piece of this quantity along $\Sigma$, and using Equation (5.22) we find

\begin{equation}
(\nabla_n \hat{\Pi}_{ab})^\top_{\Sigma} = -\hat{\Pi}_{ab}^2 + \hat{W}_{ab} + \frac{1}{2} \hat{g}_{ab}K - H \hat{\Pi}_{ab}.
\end{equation}

Using Equation (2.14), we have

\begin{equation}
(\delta_R \hat{\Pi}_{ab})^\top_{\Sigma} = [((\nabla_n + H) \hat{\Pi}_{ab})^\top_{\Sigma} = -\hat{\Pi}_{ab}^2 + \hat{W}_{ab} + \frac{1}{2} \hat{g}_{ab}K.
\end{equation}

The second equation follows by noting that $\delta_R K = 2\hat{\Pi}^{ab} \delta_R \hat{\Pi}_{ab}$ and using the above result. □

Remark 6.5. Recalling that the Willmore energy functional (3.10) for embedded surfaces is the integral of the rigidity density $K$ and its analog (1.1) for embedded spaces is the integral of the membrane rigidity density $L$, we see from Equation 6.3 that the Robin operator relates the two integrands for these functionals. It would be interesting to investigate whether this phenomenon holds in higher dimensions $\bar{d} = 2k$ to $\bar{d} = 2k + 1$ ($k \in \mathbb{Z}_{\geq 2}$).

Using Propositions 6.3 and 6.2 as well as Equations (5.21) and (5.10), we arrive at an explicit formula for the obstruction density for surfaces.

Proposition 6.6. The obstruction density for $\overline{d} = 2$ is given by

\begin{equation}
\mathcal{B}_2 = -\frac{1}{3} L^{ab} \hat{\Pi}_{ab}.
\end{equation}

Comparing the above with Proposition 3.16 verifies again that the obstruction density and the gradient of the Willmore energy $\mathcal{I}_2$ agree.

6.1. Four-manifold obstruction density. Our goal is now to find hypersurface formula for the $\overline{d} = 3$ obstruction density and thus prove Proposition 1.1. We begin by calculating $P_{3N}$.

Proposition 6.7. When $\overline{d} = 3$,

\begin{equation}
P_{3N} = 4 B' X^B + \frac{4}{3} \left[ U^{-1} \right]^B_C D^C K - 4(\delta_R K) N^B,
\end{equation}
where
\begin{equation}
B' = L^{ab}(2\tilde{\Pi}_{(ab)} - \tilde{W}_{ab}) - \tilde{\Pi}^{ab}B_{ab} + \frac{1}{2}K^2 - 3W(\tilde{n}, \tilde{\Pi}, \tilde{n}) + \tilde{W}_{ab}\tilde{W}^{ab} + \frac{1}{2}\tilde{W}_{abc}\tilde{W}^{abc}.
\end{equation}

Proof. Using Equation (6.13), the first two terms in \(\mathcal{P}_3N^C\) appearing in Equation (6.2) can be written explicitly as
\[8K\]
\[
\begin{pmatrix}
-8\tilde{\Pi}^{ab}\tilde{\nabla}_a\tilde{\Pi}_{bc} - 4\tilde{\Pi}^b\tilde{\nabla}_b\tilde{\Pi}_c + 8n_c(\text{tr} \tilde{\Pi}^3 + HK) \\
4\tilde{\Pi}^{ab}\tilde{\nabla}_a\tilde{\nabla}_b + 4\tilde{\nabla}_a\tilde{\nabla}_b + 8\text{tr}(\tilde{\Pi}^2\tilde{P}^T)
\end{pmatrix}.
\]

To compute the remaining two terms of \(\mathcal{P}_3N^C\), we make use of the tractor curvature and connection formulæ in Equations (5.5) and (5.4), respectively, as well as Equation (5.13), and find
\[
n^a\nabla^b \circ \mathcal{R}^N_{ab} N^C \text{ is related to } n^a\nabla^b \circ \nabla^T N^C \text{ as follows:}
\]
\[
\begin{pmatrix}
0 \\
-W_{abc}\tilde{\Pi}^{ab} \\
-\nabla^b\tilde{C}_b - W(n, \tilde{P}^T, n)
\end{pmatrix},
\]
\[
\begin{pmatrix}
0 \\
-W_{abc}\tilde{\Pi}^{ab} \\
-C(n, \tilde{\Pi})
\end{pmatrix}.
\]

In the first equation we have made use of the four-manifold identity \(\nabla^bW_{bad} = C_{eda}\). Orchestrating, we have
\[
\mathcal{P}_3N^C = \left(-8\tilde{\Pi}^{ab}\tilde{\nabla}_a\tilde{\Pi}_{bc} - 4\tilde{\Pi}^b\tilde{\nabla}_b\tilde{\Pi}_c - 8W(n, \tilde{\Pi}, c)^T + 8n_c(\text{tr} \tilde{\Pi}^3 - W(n, \tilde{\nabla}, n) + HK)\right) + \frac{8K}{4}\left(-8\tilde{\Pi}^{ab}\tilde{\nabla}_a\tilde{\Pi}_{bc} + 4\tilde{\nabla}_a\tilde{\nabla}_b\tilde{\Pi}_c + 8\text{tr}(\tilde{\Pi}^2\tilde{P}^T) - 4C(n, \tilde{\Pi}) - 4\tilde{\nabla}_b\tilde{C}_b - 4W(n, \tilde{P}^T, n)\right).
\]

This expression can be simplified by comparing it with the boundary Thomas D-operator acting on the rigidity density,
\begin{equation}
\frac{4}{3}[U^{-1}]^{B}_C D^{C'}K = \begin{pmatrix} 1 & 0 & 0 \\ n_bH & \delta^e_b & 0 \\ -\frac{1}{2}H^2 & -n^eH & 1 \end{pmatrix} \begin{pmatrix} 8K \\ -4\nabla_eK \\ -\frac{1}{3}(\Delta - 2)K \end{pmatrix} = \begin{pmatrix} 8K \\ -4\nabla_bK + 8n_bHK \\ -\frac{4}{3}(\Delta - 2)K - 4H^2K \end{pmatrix}.
\end{equation}

Here we have used the isomorphism (5.12) between sections of \(T\Sigma\) and \(TM^T\). To match this expression with terms appearing in \(\mathcal{P}_3N^C\) as displayed above, we make use of the trace-free Mainardi Equation (2.9) to obtain the identity
\[
\frac{1}{2}\nabla_eK = \tilde{\Pi}^{ab}\nabla_e\tilde{\Pi}_{ab} = \tilde{\Pi}^{ab}\nabla_a\tilde{\Pi}_{bc} + \frac{1}{2}\tilde{\Pi}^b\nabla_a\tilde{\Pi}_b + W_{abc}\tilde{\Pi}^{abc}.
\]

Using this identity, Equation (2.12), the Fialkow Equation (2.7) as well as Proposition 6.3 we have
\[
\mathcal{P}_3N^B = \frac{4}{3}[U^{-1}]^{B}_C D^{C'}K - 4N^B\delta_KK + 4B'X^B,
\]
with $B'$ given by

$$
B' = \frac{2}{3} \nabla^a \tilde{\Pi}^b \nabla_a \Pi_{bc} + (\nabla^a \tilde{\Pi}_a)(\nabla^b \tilde{\Pi}^b) + \frac{4}{3} \tilde{\Pi}^{ab} \Delta \tilde{\Pi}_{ab} - \frac{4}{3} \tilde{\Pi}^{ab} \nabla_c \tilde{W}_{abc} - 3 W(n, \tilde{\Pi}^2, n) + \frac{1}{2} K^2 + \tilde{W}_{ab} \tilde{W}_{ab} + 2 \tilde{\Pi}^{ab} \nabla_c \tilde{W}_{abc} - \nabla^b \tilde{C}_b - W(n, P, n) - C(n, \tilde{\Pi}) - H W(n, \tilde{\Pi}, n) .
$$

It remains only to show that this last expression reduces to that stated in the proposition. This follows directly from Proposition 2.4 and the identities

$$
\tilde{C}_b = \nabla^c \tilde{W}_{ab} + \tilde{W}_{abc} \tilde{\Pi}_{bc} = \nabla^b \tilde{W}_{ab} + \tilde{\Pi}^{ab} \nabla_c \tilde{W}_{abc} + \frac{1}{2} \tilde{W}_{abc} \tilde{W}_{abc} ;
$$

these are direct consequences of Equation (1.2) and (2.9). Noting that $n = \hat{n}$ along $\Sigma$ completes the proof. □

We now turn to the second term in the holographic formula (6.1). We first need the following technical result:

**Lemma 6.8.** Let $T \in \Gamma(T^\phi \mathcal{M}[-2])$ and $\tilde{d} = 3$. Then

$$
I \cdot D^2 (X^C T) \Sigma = -2 D^C T .
$$

**Proof.** The key to the proof is to note that for $d = 4$, the tractor $X^C T$ has ambient Yamabe weight $w = -1$, so that

$$
I \cdot D (X^B T) = -\sigma \Box_Y (X^B T) .
$$

Acting with the remaining $I \cdot D \Sigma = -2 \delta_R$ (at this weight) and calculating explicitly using the tractor connection (5.4) gives the identity stated. □

Our result for two canonical normal derivatives of the rigidity density multiplied by the canonical tractor is given by the following:

**Proposition 6.9.** Let $\tilde{d} = 3$. Then,

$$
(6.7) \quad I \cdot D^2 (X^C K) \Sigma = 4 X^B B'' - \frac{4}{3} [U^{-1}] B^C D^C K + 4 N^B \delta_R K ,
$$

where

$$
(6.8) \quad B'' = L^{ab} \tilde{\Pi}_{\langle ab \rangle}^2 + \frac{1}{2} K^2 - 4 W(\hat{n}, \tilde{\Pi}^2, \hat{n}) + \hat{\tilde{W}}_{ab} \hat{\tilde{W}}_{ab} + \tilde{\Pi}^{ab} \tilde{\Pi}^{cd} \tilde{W}_{abcd} + \frac{1}{2} \hat{\tilde{W}}_{abcd} \hat{\tilde{W}}_{abcd} .
$$

**Proof.** Using Lemma 6.8 we must compare

$$
-2 D^C K = \begin{pmatrix} -8 K \\ 4 \nabla^c K \\ 2(\Delta - 2 J) K \end{pmatrix}
$$

with Equation (6.6). This yields Equation (6.7) with

$$
(6.9) \quad B'' = \frac{1}{2} \nabla^2 n K + 2 H \delta_R K + \frac{1}{6} \Delta K - \frac{3}{2} H^2 K - \frac{1}{3} \tilde{K} - \frac{1}{4} K^2 - P(n, n) K .
$$

It remains to show that this expression reduces to Equation (6.8). For that, we need to compute two normal derivatives of the canonically extended rigidity density $K$. Returning to Equation (6.4), we see that the following normal derivatives of curvature terms...
appear in \( \frac{1}{2} \nabla_n^2 K \):

\[
\nabla_n \tilde{R}_{ab} + 2 \nabla_n P_{ab} = (\nabla_n n^d) R_{dabc} n^e + n^e n^d \nabla_c (R_{dabc} n^e) + 2 \nabla_n P_{ab}
\]

\[
\sum H \tilde{R}_{ab} + (g^{cd} - \tilde{g}^{cd}) \nabla_c (R_{dabc} n^e) + 2 \nabla_n P_{ab}
\]

\[
= H \tilde{R}_{ab} + \nabla^d (R_{dabc} n^e) + \nabla_d \tilde{R}_{ab} + 2 \nabla_n P_{ab}
\]

\[
= H \tilde{R}_{ab} + (\nabla^d n^e) R_{dabc} - n^e (\nabla_c R_{dabc} d) + \nabla_d \tilde{R}_{ab} + 2 \nabla_n P_{ab}
\]

\[
\sum H \tilde{R}_{ab} + (H \tilde{g}^{dc} + H g^{dc}) R_{dabc} + n^e \nabla_c R_{dabc} - g_{ab} \nabla_n J + \nabla_d \tilde{R}_{ab}.
\]

In the fourth line above we used the Bianchi identity for the Riemann tensor. Upon contraction with \( \tilde{H}^{ab} \) the above yields

\[
\tilde{H}^{ab} (\nabla_n \tilde{R}_{ab} + 2 \nabla_n P_{ab}) = W(n, \tilde{H}^2, n) - HW(n, \tilde{H}, n) - 3H \text{ tr}(\tilde{H} P) + \tilde{H}^{ab} \tilde{g}^{cd} W_{cabd}
\]

\[
- \text{ tr}(\tilde{H}^2 P) + \tilde{H}^{ab} \nabla_a \tilde{P}_b + K P(n, n) - \tilde{H}^{ab} \nabla^d \tilde{W}_{b \tilde{a} d}.
\]

Combining the above expression and Equation (6.4), we have

\[
\tilde{H}^{ab} (\nabla_n \tilde{R}_{ab} + 2 \nabla_n P_{ab}) = W(n, \tilde{H}^2, n) - HW(n, \tilde{H}, n) - 3H \text{ tr}(\tilde{H} P) + \tilde{H}^{ab} \tilde{g}^{cd} W_{cabd}
\]

\[
- \text{ tr}(\tilde{H}^2 P) + \tilde{H}^{ab} \nabla_a \tilde{P}_b + K P(n, n) - \tilde{H}^{ab} \nabla^d \tilde{W}_{b \tilde{a} d}.
\]

Here we have used Equations (5.22), (6.4) and (2.7) as well as the following consequence of the Mainardi Equation (2.3) is needed:

\[
\tilde{H}^{ab} \nabla_a \nabla_b H = \frac{1}{3} \tilde{H}^{ab} \Delta \tilde{H}_{ab} - \tilde{H}^{ab} \nabla_a \tilde{P}_b - \frac{1}{3} J K - \text{ tr}(\tilde{H}^2 P) - \frac{1}{3} \tilde{H}^{ab} \nabla^c \tilde{W}_{bac}.
\]

The computation of \( \nabla_n^2 K \) also requires the cross term \( (\nabla_n \tilde{H}_{ab})(\nabla_n \tilde{H}^{ab}) \). Again using Equation (6.4), we have

\[
\nabla_n \tilde{H}_{ab} = \nabla \tilde{H}_{ab} - n_b \nabla_a K - n_a \nabla_b K - H \tilde{H}_{ab} - \tilde{H}_{ab} + \frac{1}{2} g_{ab} K.
\]

Contracting this identity on itself we find

\[
(\nabla_n \tilde{H}_{ab})(\nabla_n \tilde{H}^{ab}) = \tilde{W}_{ab} \tilde{W}^{ab} - 2HW(n, \tilde{H}, n) - 2W(n, \tilde{H}^2, n) + \frac{1}{2} (\nabla_n \tilde{H}_{ab})(\nabla_n \tilde{H}^{ab})
\]

\[
+ H^2 K + 2H \text{ tr}(\tilde{H}^3) + \frac{1}{2} K^2.
\]

Orchestrating this and Equation (6.10), we have

\[
\frac{1}{2} \nabla_n^2 K = \frac{1}{2} (\nabla_n \tilde{H})(\nabla_n \tilde{H}) + \frac{1}{3} \tilde{H}^{ab} \Delta \tilde{H}_{ab} + \frac{3}{4} K^2 - 4W(n, \tilde{H}^2, n) + \tilde{W}_{ab} \tilde{W}^{ab} + \frac{1}{2} H^2 K
\]

\[
- 4HW(n, \tilde{H}, n) + 4H \text{ tr}\tilde{H}^3 - \frac{1}{3} J K + \tilde{H}^{ab} \tilde{g}^{cd} W_{cabd} + P(n, n) K - \frac{4}{3} \tilde{H}^{ab} \nabla^c \tilde{W}_{bac}.
\]
Substituting this result into Equation (6.9) and simplifying gives
\[ B'' = \frac{1}{3} \nabla^b \Pi_{bc} + \frac{1}{2} (\nabla \Pi) (\nabla \Pi)^n + \frac{2}{3} \Pi_{ab} \Delta \Pi_{ab} - \frac{2}{3} J K - \frac{4}{3} \Pi^{ab} \nabla^c \omega^b_{bac} \]
\[ - 4W(n, \Pi^2, n) + \frac{1}{2} K^2 + \Pi_{ab} W^{ab} + \Pi^{cd} W_{cabc} . \]

Using Proposition 2.4 gives the result (6.8), which completes the proof.

We now complete the proof of Proposition 1.1 giving the obstruction density for four-manifolds:

Proof of Proposition 1.1. Using Equation (6.1) and Propositions 6.7 and 6.9, the obstruction density is given by
\[ B_3 = \frac{1}{72} \hat{D}^A [4X_A(B' + B'')] . \]

Substituting the formulæ (6.5) and (6.8) for \( B' \) and \( B'' \) into the above and using Lemma 5.10 gives the result.

6.2. Examples and umbilicity. Our results can be easily applied to explicit metrics and hypersurfaces. As we shall explain below, this gives both an independent check of our computations and also generates interesting examples.

For surfaces, total umbilicity suffices to ensure vanishing of the obstruction density (this follows by inspection of the formula for \( B_2 \) given in Proposition 6.6). The following proposition shows this is not true in dimension \( \bar{d} = 3 \).

Proposition 6.10. Total umbilicity (i.e., vanishing of \( \Pi \) everywhere) is not a sufficient condition for the obstruction density to vanish.

Proof. See the explicit counterexample on the third line of the table below.

Remark 6.11. There is no in principle difficulty constructing examples of umbilic hypersurfaces with non-vanishing obstruction density in dimensions \( \bar{d} > 3 \). Also, albeit in Lorentzian signature, the Schwarzschild example below provides another \( \bar{d} = 3 \) example of this.

In the following table we give some sample four manifold metrics, hypersurfaces and their obstruction density \( B_3 \). Additionally, \( \hat{\sigma} \) denotes the conformal unit density in the scale determined by the quoted metric, \( H \) the mean curvature, \( \Pi \) the trace-free second fundamental form and \( L \) the membrane rigidity density. Non-vanishing expressions that are too long to be displayed are denoted by a \( \star \). These results were generated with the aid of a computer software package [PM01].

| \( ds^2 \) | \( \Sigma \) | \( \hat{\sigma} \) | \( H \) | \( \Pi \) | \( B_3 \) | \( L \) |
|---|---|---|---|---|---|---|
| \( dx^2 + (1 + \alpha x)(dy^2 + dz^2 + dw^2) \) | \( x = 0 \) | \( x + \frac{1}{4} y^2 - \frac{1}{8} y^3 + \frac{1}{32} y^4 x \) | \( \frac{x}{2} \) | \( 0 \) | \( 0 \) | \( 0 \) |
| \( dx^2 + (1 + \alpha x)dy^2 + (1 - \alpha x)dz^2 + dw^2 \) | \( x = 0 \) | \( x - \frac{1}{8} y^3 \) | \( 0 \) | \( \frac{1}{72} (dy^2 - dx^2) \) | \( \frac{1}{72} \) | \( 0 \) |
| \( dx^2 + (1 + x)dy^2 + (1 + w)dx^2 + (1 + y)dw^2 \) | \( x = 0 \) | \( \star \) | \( 0 \) | \( 0 \) | \( \star \) | \( 0 \) |
| \( -(1 - \frac{2M}{r})dt^2 + \frac{dr^2}{1 - \frac{2M}{r}} + d\Omega^2 \) | \( r = R + 2M \) | \( \star \) | \( \star \) | \( \star \) | \( \star \) | \( \star \) |

The first line of the table gives a metric and an umbilic but non-minimal hypersurface for which the obstruction density vanishes. In the second line, the hypersurface is minimal but non-umbilic. The third line is particularly interesting, the hypersurface is both umbilic and minimal, yet the obstruction density does not vanish. Finally in the fourth
line, we use the fact that all local formulæ presented in this paper can be extended to Lorentzian structures (provided the conormal is nowhere null), and study a spherical shell of radius \( R \) in the Schwarzschild metric. The conormal \( dr \) is spacelike for \( R > 0 \), timelike for \( R < 0 \) and lightlike at the horizon \( R = 0 \), so that strictly the formulæ presented below apply only to the spacelike case. In that case the second fundamental form is given by

\[
H = \frac{1}{3} \frac{M + 2R}{\sqrt{R(R + 2M)^3}}, \quad \tilde{II} = -\frac{1}{3} (M - R) \sqrt{\frac{R + 2M}{R}} \left( \frac{2Rdt^2}{(R + 2M)^3} + d\Omega^2 \right),
\]

so that the hypersurface \( \Sigma \) is neither minimal nor umbilic, save for the distinguished radius \( R = M \) where umbilicity holds. At that value the membrane rigidity density also vanishes; at general \( R \) it is given by

\[
L = \frac{2(M - R)(M^2 + 6MR + R^2)}{R\sqrt{R(R + 2M)^3}}.
\]

The obstruction density is

\[
\mathcal{B}_3 = \frac{2M^4 + 4M^3R + 30M^2R^2 - 8MR^3 - R^4}{27R^2(R + 2M)^6}
\]

and has one simple real root in the region \( R > -2M \) at \( R/M \approx 2.9 \).

Finally let us explain how the formulæ for the obstruction density can be generated without simply computing each term in Proposition 1.1. This is based on the two iterative recursions given in [GW15, Lemma 2.4 and Proposition 4.9]. Firstly, given a four manifold with metric \( g \) and hypersurface \( \Sigma \) labeled by a defining function \( s \), we improve the defining function to

\[
s_0 = \frac{s}{|\nabla s|}
\]

which ensures that \( |\nabla s_0|_\Sigma = 1 \). It is highly propitious to work with a unit defining function \( s_1 \) with \( |\nabla s_1| = 1 \). For applications, it suffices to require \( |\nabla s_1| = 1 + s^\ell f \) for smooth \( f \) and \( \ell \) of sufficiently high order. This is achieved using the recursion of [GW15, Lemma 2.4]. For the first three examples tabulated above, \( s_1 = x \) is already a unit defining function, but for the Schwarzschild case, we performed this algorithm explicitly using the computer software package [PM01].

Supposing now that \( s \) is a unit defining function, we next improve this to a conformal unit defining density evaluated in the scale determined by the metric \( g \). This can be achieved using the recursion of [GW15, Proposition 4.9]. In practice this simply amounts to repeatedly computing the leading failure of \( I^2_\sigma \) to equal unity and then adding a next to leading correction to \( \sigma \) to correct for this. In Appendix A we present the first four improvement terms for a unit defining function \( s \) as well as the corresponding obstruction densities for hypersurface dimensions \( d \) = 1, 2, 3 and 4. These were computed using the symbolic manipulation software [KUVV12]. We have verified their correctness by checking that the resulting \( I^2_\sigma \) equals unity to the required order for explicit metric and hypersurface examples, including those given above.

We note that the result for \( B_4 \) quoted in the appendix, when evaluated along \( \Sigma \) gives the obstruction density for five-manifold hypersurfaces expressed in terms of a unit defining function. This is a novel result that is simple to use in practical applications. There is no in principle difficulty employing the unit defining function identities of Sections 3 and 4 and their higher order analogs to evaluate \( B_5 \) in terms of hypersurface invariants.
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Appendix A. Conformal unit defining function formulæ and five-manifold obstruction density

Let $s$ be a defining function for a hypersurface $\Sigma$ in a $d$-dimensional Riemannian manifold $(M, g)$. The following formulæ improve this to $s_k$ which determines a defining density $\sigma_k$ in the scale $g$ such that

$$I^2_{\sigma_k} = 1 + \sigma^k f, \quad k < d,$$

for some smooth $f \in \Gamma(\mathcal{E}M[-k])$:

$$s_0 = s$$

$$s_1 = s_0 + \frac{1}{2(d-1)} s^2 \nabla.n$$

$$s_2 = s_1 + \frac{1}{6(d-2)(d-1)} s^3 (2(\nabla.n)^2 - (d-4) \nabla.n \nabla.n + 2(d-1) J)$$

$$s_3 = s_2 + \frac{1}{24(d-3)(d-2)(d-1)} s^4 \left( \frac{5d - 6}{d - 1} (\nabla.n)^3 - 4(2d - 9) \nabla.n \nabla.n \nabla.n + (d - 4)(d - 6) \nabla.n \nabla.n + 3(d - 2) \Delta \nabla.n + 4(2d - 3) \nabla.n J - 2(d - 6)(d - 1) \nabla.n J \right)$$

$$s_4 = s_3 + \frac{1}{120(d-4)(d-3)(d-2)(d-1)} s^5 \left( \frac{13d^6 - 62d^5 + 100d^4 - 48}{(d-2)(d-1)^2} (\nabla.n)^4 ight.$$

$$+ \frac{398d^2 - 880d^3 + 49d^4 + 576}{(d-2)(d-1)^2} (\nabla.n)^2 \nabla.n \nabla.n + \frac{13d^3 - 156d^2 + 524d - 384}{d-1} \nabla.n \nabla.n \nabla.n \nabla.n$$

$$+ \frac{25d^2 - 94d + 72}{d-1} \nabla.n \Delta \nabla.n + \frac{11d^4 - 149d^3 + 668d^2 - 1112d + 576}{(d-2)(d-1)} (\nabla.n \nabla.n)^2$$

$$- \frac{(d - 4)(d - 6)(d - 8) \nabla.n \nabla.n - (3d^2 - 22d + 16)(d - 3)}{d-1} (\nabla.n \nabla.n)^2$$

$$- 4(d - 4)(d - 3) \nabla.n \nabla.n - 3(d - 2)(d - 8) \nabla.n \nabla.n + 2(13d^2 - 58d + 72)/(d-2) (\nabla.n \nabla.n)^2 J$$

$$- \frac{4(4d^3 - 35d^2 + 88d - 72)}{d-2} (\nabla.n \nabla.n) J + \frac{4(d - 4)(d - 3)(d - 1)}{d-2} J^2$$

$$- 6(3d - 4)(d - 6) \nabla.n \nabla.n J + 8(d - 3)(d - 1) \Delta J + 2(d - 8)(d - 6)(d - 1) \nabla.n^2 J \right).$$
When \( k = d \), we have \( I^2 = 1 + \sigma^d \bar{B}_d \) where the obstruction density \( B_d = B_d|_{\Sigma} \). Thus the following determine the obstruction density in dimensions \( d = 2, 3, 4 \) and 5.

\[
B_1 = -(\nabla.n)^2 - \nabla_n n \cdot n - J
\]

\[
B_2 = -\frac{1}{12} \left( 2\Delta \nabla.n + 2\nabla_n^2 \nabla.n + 8 \nabla.n \nabla_n \nabla.n + 3 (\nabla.n)^3 + 8 \nabla.n J + 8 \nabla_n J \right)
\]

\[
B_3 = -\frac{1}{108} \left( 9 \nabla_n \Delta \nabla.n + 12 \nabla_n \Delta \nabla.n + 6 \nabla_n \nabla^2_n \nabla.n + 3 (\nabla \nabla.n)^2 + 6 (\nabla.n)^2 \nabla_n \nabla.n + 4 (\nabla.n)^4 + 9 \Delta J + 18 \nabla^2_n J + 36 \nabla.n \nabla_n J + 18 \nabla_n \nabla.J + 18 (\nabla.n)^2 J \right)
\]

\[
B_4 = \frac{1}{46080} \left( -312 \nabla.n (\nabla_n \nabla.n)^2 + 352 \nabla.n (\nabla^2_n \nabla.n) - 155 \nabla.n^2 \nabla.n^3 + 44 \nabla.n^2 (\nabla^2_n \nabla.n) - 832 \nabla.n^3 (\nabla_n \nabla.n) + 480 (\nabla_n \nabla.n)(\nabla^2_n \nabla.n) + 96 (\nabla_n^4 \nabla.n) + 32 \Delta \nabla^2_n \nabla.n + 288 \nabla.n \Delta \nabla_n \nabla.n + 256 \nabla_n \Delta \nabla_n \nabla.n + 96 (\nabla_n \nabla.n)(\nabla^a_n \nabla.n) + 552 \nabla.n (\nabla_n \nabla.n)(\nabla^a_n \nabla.n) - 608 (\nabla_n \nabla.n) \nabla_n \nabla^a \nabla.n - 1436 \nabla.n^2 \Delta \nabla.n - 1248 (\nabla_n \nabla.n) \Delta \nabla.n - 2176 \nabla.n \Delta \nabla.n \nabla.n - 864 \nabla_n \Delta \nabla.n - 288 \Delta^2 \nabla.n - 2304 \nabla.n (\nabla_n \nabla.n) J - 832 \nabla.n^3 J - 640 (\nabla^2_n \nabla.n) J - 384 (\Delta \nabla.n) J + 1024 \nabla.J + 512 \nabla_n J - 2496 \nabla.n^2 \nabla_n J - 2304 (\nabla_n \nabla.n)(\nabla_n J + 1536 \nabla.n J - 2432 \nabla.n \nabla^2_n J - 768 \nabla_n^3 J - 256 \Delta \nabla_n J - 512 (\nabla_n \nabla.n) \nabla^a J - 2176 \nabla.n \Delta J - 2048 \nabla_n \Delta J \right).
\]

The above yields \( B_1 = B_1|_{\Sigma} = 0 \) and it is not difficult to show that \( B_2|_{\Sigma} \) agrees with \( B_2 \) as in Proposition 6.6. The expressions above for \( B_3 \) and \( B_4 \) provide an efficient way to compute the obstruction densities \( B_3 \) and \( B_4 \) for explicit metrics, but expressing the above formulae in terms of standard hypersurface invariants is rather tedious. For \( (M, g) \) flat and \( d = 3 \), this computation was performed in [GW15] and agrees with our generally curved expression for \( B_3 \) given in Proposition 6.6.

References

[ACF92] L. Andersson, P. T. Chruściel and H. Friedrich, On the regularity of solutions to the Yamabe equation and the existence of smooth hyperboloidal initial data for Einstein’s field equations, Comm. Math. Phys. 149(3), 587–612 (1992).

[AGS14] A. F. Astaneh, G. Gibbons and S. N. Solodukhin, What surface maximizes entanglement entropy?, Phys. Rev. D90(8), 085021 (2014), 1407.4719.

[AM88] P. Aviles and R. C. McOwen, Complete conformal metrics with negative scalar curvature in compact Riemannian manifolds, Duke Math. J. 56(2), 395–398 (1988).

[AM10] S. Alexakis and R. Mazzeo, Renormalized area and properly embedded minimal surfaces in hyperbolic 3-manifolds, Comm. Math. Phys. 297(3), 621–651 (2010).

[BEG94] T. N. Bailey, M. G. Eastwood and A. R. Gover, Thomas’s structure bundle for conformal, projective and related structures, Rocky Mountain J. Math. 24(4), 1191–1217 (1994).

[BG01] T. Branson and A. R. Gover, Conformally invariant non-local operators, Pacific J. Math. 201(1), 19–60 (2001).

[ES97] M. Eastwood and J. Slovák, Semiholonomic Verma modules, J. Algebra 197(2), 424–448 (1997).
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