On Singular Yamabe Obstructions

Andreas Juhl1 · Bent Ørsted2

Received: 11 March 2021 / Accepted: 31 December 2021 / Published online: 16 February 2022
© Mathematica Josephina, Inc. 2022

Abstract
We discuss the obstruction to the existence of a smooth solution of a singular version of the Yamabe problem for a hypersurface in a four-dimensional general background. This obstruction is a conformally invariant density. We derive various explicit formulas for the singular Yamabe obstruction directly from the original definition. We discuss in detail the relation to results in the literature.

Keywords Conformal geometry · Hypersurface invariant · Poincaré–Einstein metric · Singular Yamabe problem · Yamabe obstruction · Willmore functional

Mathematics Subject Classification Primary 53B20 · 53B25 · 53C18 · Secondary 53C25

1 Introduction

On a smooth manifold equipped with a Riemannian metric, the basic objects for geometry are the canonical Levi-Civita connection and the corresponding Riemann curvature tensor. Conformal geometry studies polynomials in the curvature and its derivatives transforming in simple ways under conformal changes of the metric, i.e., multiplying it by a positive smooth function. The structure of scalar conformal invariants was much illuminated by the concept of the Fefferman–Graham ambient metric [6].

Given a submanifold of a Riemannian manifold, one may in addition consider conformal invariants of the embedding, i.e., invariants which are given not only by the intrinsic metric on the submanifold induced by the metric of the ambient space,
but also from the normal geometry of the submanifold. Of special significance is the case of hypersurfaces. That theory is less developed than the conformal geometry of a given manifold.

In the classical Gauss theory of surfaces $M$ in a three-dimensional Euclidean space, the trace-free part $\tilde{L}$ of the second fundamental form $L$ is a conformal invariant. The product of the principal curvatures, i.e., the eigenvalues of the shape operator corresponding to $L$, is the intrinsic Gauss curvature $K$ which integrates for a closed $M$ to a multiple of the Euler characteristic. A celebrated global conformal invariant is the integral of the square of the mean curvature $H$ (defined as the arithmetic mean of the principal curvatures) over the closed surface $M$, the so-called Willmore functional (or Willmore energy)

$$\int_M H^2 \, dvol.$$ 

By $H^2 - K = |\tilde{L}|^2$, it differs from the obviously conformally invariant integral

$$\mathcal{W}_2 \overset{\text{def}}{=} \int_M |\tilde{L}|^2 \, dvol,$$

by a multiple of the Euler characteristic of $M$. Note that the Willmore functional also appears in string theory as the rigid string action [21].

In general, curvature invariants of a hypersurface consist of intrinsic invariants, defined by the induced metric, and extrinsic invariants, coming from the second fundamental form and the ambient metric. Whereas for a given manifold, it is known how to describe the conformally invariant scalar curvature quantities using the Fefferman–Graham ambient metric [6], an analogous description of scalar conformal invariants of a hypersurface is not known. Such a classification would also be of interest in physics [24].

Recent years have seen attempts to embed the theory of the Fefferman–Graham ambient metric and of the related Poincaré–Einstein metric into a wider framework. For instance, Albin [2] extended parts of the theory to Poincaré–Lovelock metrics including applications to $Q$-curvature. In another direction, Gover et al. [8–11] developed a tractor calculus approach to the problem of constructing higher-order generalizations of the Willmore functional $\mathcal{W}_2$. Here a central role is played by the singular Yamabe problem which replaces the Einstein condition. In [3], it was discovered that the obstruction to the smooth solvability of the singular Yamabe problem of a hypersurface of dimension $n$ is a scalar conformal invariant $B_n$. The observation of Gover et al. that $B_2 = 0$ is the Euler–Lagrange equation of $\mathcal{W}_2$ was the starting point of their theory. More generally, [13] identified the equation $B_n = 0$ as the Euler–Lagrange equations of a conformally invariant functional which he termed the Yamabe energy. This energy is an analog of the integrated (critical) renormalized volume coefficient of a Poincaré–Einstein metric which in turn is related to the integrated (critical) Branson $Q$-curvature. Notably this connection to $Q$-curvature also extends to the present setting [12,20].
Formulas for the conformally invariant obstruction in terms of classical curvature data are not known for \( n \geq 4 \). But for \( n = 3 \), such a formula for \( B_3 \) was derived in [8] from a general tractor calculus formula in [11].

In the present paper, we shall take a more classical perspective and derive formulas for \( B_3 \) directly from its very definition. We only apply standard linear algebra and tensor calculations. It confirms and partly corrects results in the literature. As technical tools, we also employ some differential identities involving \( L \). Partly these are classical such as those found by Simons, and partly these are less well known. Finally, we apply classical style arguments to relate \( B_3 \) to the variation of the conformally invariant functional

\[
\mathcal{W}_3 = \int_M (\tr(\hat{L}^3) + (\hat{L}, \hat{W})) \, dvol,
\]

which can be viewed as a natural generalizations of the classical Willmore functional \( W_2 \). This fits with Graham’s theorem [13, Theorem 3.1]. Our arguments replace a technique introduced and exploited in [8].

The formulation of the main result requires some notation. Let \( L \) be the second fundamental form, \( \hat{L} \) its trace-free part and \( H \) the mean curvature. Let \( \hat{W} \) be the Weyl tensor of the background metric. We also define two contractions \( \hat{W}_0 \) and \( \hat{W} \) of \( \hat{W} \) on \( M \) by inserting a unit normal vector \( \partial_0 \) at the last and at the first and the last slot, respectively. We let the operator \( \mathcal{D} \) act on trace-free symmetric bilinear forms \( b \) on \( M \) by

\[
\mathcal{D}(b) = \delta \delta(b) + (P, b). \tag{1.1}
\]

The operator \( \mathcal{D} \) maps trace-free symmetric bilinear forms to \( C^\infty(M) \). If the dimension \( n \) of \( M \) equals 3, then \( \mathcal{D} \) is conformally invariant in the sense that \( e^{4\phi} \mathcal{D}(b) = \mathcal{D}(b) \) for \( \phi \in C^\infty(M) \). The Levi-Civita connections on \( X \) and \( M \) are denoted by \( \bar{\nabla} \) and \( \nabla \). For more details see Sect. 2. For the definition of the obstructions \( B_n \), we refer to Sect. 4.

**Theorem 1** Let \( \iota : M^3 \hookrightarrow (X^4, g) \) be a smooth embedding. Then it holds

\[
12B_3 = 6\mathcal{D}((\hat{L}^2)_0) + 2|\hat{L}|^4 + 2\mathcal{D}(\hat{W}) - 2\hat{L}^{ij}\hat{\nabla}^0(\hat{W})_{0ij0} - 4L^{ij} \nabla^k \hat{W}_{kij0} - 4H(\hat{L}, \hat{W}) + 16(\hat{L}^2, \hat{W}) + 4|\hat{W}|^2 + 2|\hat{W}_0|^2. \tag{1.2}
\]

For a conformally flat background, Theorem 1 reduces to the identity

\[
6B_3 = 3\mathcal{D}((\hat{L}^2)_0) + |\hat{L}|^4 = \Delta(|\hat{L}|^2) - |\nabla \hat{L}|^2 + 3/2|\delta(\hat{L})|^2 - 2J|\hat{L}|^2 + |\hat{L}|^4. \tag{1.3}
\]

1 This method relies on certain distributional identities. It seems an interesting question to formulate and verify these calculations in more standard ways.
The second equality follows from Lemma 3.13. We recall the well-known fact
that for an odd-dimensional \( M \), there are Poincaré–Einstein metrics \( g_{+} \) such that the
conformal compactification \( g = r^{2} g_{+} \) is smooth \([6]\). For such a metric, it holds \( \hat{L} = 0 \),
\( \hat{\mathcal{W}} = 0 \) and even \( \hat{\mathcal{W}}_{0} = 0 \) \([9, Proposition 4.3]\). In particular, for \( n = 3 \), the above
formula confirms that \( B_{3} = 0 \). If \( \hat{L} = 0 \), then
\[
6B_{3} = D(\hat{\mathcal{W}}) + 2|\hat{\mathcal{W}}|^{2}
\]
since \( \hat{\mathcal{W}}_{0} = 0 \) (by the trace-free part of the Codazzi–Mainardi equation). Formula
(1.2) confirms the conformal invariance of \( B_{3} \) (of weight \(-4\)). In fact, the confor-
mal invariance of \( D \) implies that \( D((\hat{L}^{2})_{c}) \) and \( D(\hat{\mathcal{W}}) \) are individually conformally
invariant. Furthermore, the sum of the first three terms in the second line of (1.2) is
conformally invariant. In fact, it holds
\[
\hat{L}^{ij}(\nabla^{0}(\hat{\mathcal{W}})_{0ij0} + 2\nabla^{k}\hat{\mathcal{W}}_{kij0} + 2H\hat{\mathcal{W}}_{ij}) = (\hat{L}, B) + (\hat{L}^{2}, \hat{\mathcal{W}}) + \hat{L}^{ij}\hat{L}^{kl}\hat{\mathcal{W}}_{kijl}
\]
(see Lemma 6.27) with a conformally invariant tensor \( B \) of weight \(-1\), i.e., \( e^{\phi}\hat{B} = B \),
introduced in \([8, Lemma 2.1]\) and termed the hypersurface Bach tensor. All remaining
terms in (1.2) are individually conformally invariant.

In the course of the proof of Theorem 1 we shall derive a number of equivalent
formulas for \( B_{3} \) which are of interest in special cases. In particular, we find that
\[
12B_{3} = \Delta(|\hat{L}|^{2}) + 6(\hat{L}, \text{Hess}(H)) + 6H \text{tr}(\hat{L}^{3}) + |\hat{L}|^{4} + 12|dH|^{2} \quad (1.4)
\]
for a flat background (Corollary 6.11). In \([20, Sect. 13.7]\), we derived this formula in a
different way as a consequence of a general expression for singular Yamabe obstruc-
tions \([20, Theorem 6]\). One may also derive the general case of the above formula
along this line. In \([20]\), we derived (1.3) by combining the conformal invariance of \( B_{3} \)
with (1.4) and Simons identity.

The paper is organized as follows. In Sect. 3, we derive identities for \( \delta\delta(\hat{L}^{2}) \) and
\( \Delta(|\hat{L}|^{2}) \) which are crucial for later calculations and may also be of independent interest.
They are closely related to some identities of Simons \([23]\). In Sect. 4, we define the
singular Yamabe problem and the resulting obstructions in general dimensions. In
Sect. 5, we derive a formula for \( B_{2} \) and connect it with the Willmore equation. Section 6
is devoted to the derivation of formulas for \( B_{3} \) in terms of standard curvature quantities.
The starting point will be a formula in terms of the volume expansion of \( g \) in geodesic
normal coordinates. Along the way we derive several equivalent formulas for \( B_{3} \) which
might be of interest under specific additional assumptions on the background metric
and the embedding. The proof of the main theorem, Theorem 1, is contained in the
last subsection. Here we also prove that Theorem 1 is equivalent to the arXiv version
of \([8, Proposition 1.1]\)^{2} It is here where we need the material of Sect. 3. In the final
section, we derive the right-hand side of (1.2) by variation of the functional \( \mathcal{W}_{3} \) under
normal variations of the embedding reproving a result in \([8,13]\).

\(^{2}\) The arXiv version of \([8, Proposition 1.1]\) differs from its printed version—we clarify that issue in
Remark 6.28.
In view of the possible applications to physics, such as string and membrane theory, and the principles of holography, we have tried to be very explicit throughout.

2 Notation

All manifolds $X$ are smooth. For a manifold $X$, $C^\infty(X)$ and $\Omega^p(X)$ denote the respective spaces of smooth functions and smooth $p$-forms. Let $\mathcal{X}(X)$ be the space of smooth vector fields on $X$. Metrics on $X$ usually are denoted by $g$. $\text{dvol}_g$ is the Riemannian volume element defined by $g$. The Levi-Civita connection of $g$ is denoted by $\nabla^g_X$ or simply $\nabla_X$ for $X \in \mathcal{X}(X)$ if $g$ is understood. In these terms, the curvature tensor $R$ of the Riemannian manifold $(X, g)$ is defined by $R(X, Y)Z = \nabla_X \nabla_Y (Z) - \nabla_Y \nabla_X (Z) - \nabla_{[X, Y]}(Z)$ for vector fields $X, Y, Z \in \mathcal{X}(X)$. The components of $R$ are defined by $R(\partial_i, \partial_j)(\partial_k) = R_{ijk}^l \partial_l$. We also set $\nabla_X(u) = \langle du, X \rangle$ for $X \in \mathcal{X}(X)$ and $u \in C^\infty(X)$. Ric and scal are the Ricci tensor and the scalar curvature of $g$. On a manifold $(X, g)$ of dimension $n$, we set $2(n-1) = \text{scal}$ and define the Schouten tensor $P$ of $g$ by $(n-2)P = \text{Ric} - Jg$ (if $n \geq 3$). Let $W$ be the Weyl tensor. Then the curvature tensor admits the Kulkarni–Nomizu decomposition $R = -\otimes g + W$. These conventions are as in [17].

For a metric $g$ on $X$ and $u \in C^\infty(X)$, let $\text{grad}_g(u)$ be the gradient of $u$ with respect to $g$, i.e., it holds $g(\text{grad}_g(u), V) = \langle du, V \rangle$ for all vector fields $V \in \mathcal{X}(X)$. $g$ defines pointwise scalar products $(\cdot, \cdot)$ and norms $|\cdot|$ on $\mathcal{X}(X)$, on forms $\Omega^k(X)$ and on general tensors. Then $|\text{grad}(u)|^2 = \langle du, du \rangle$. In these definitions, we use the metric as a subscript if needed for clarity. $\delta^g$ is the divergence operator on differential forms or symmetric bilinear forms. On forms, it coincides with the negative adjoint $-d^*$ of the exterior differential $d$ with respect to the Hodge scalar product defined by $g$. Let $\Delta_g = \delta^g d$ be the non-positive Laplacian on $C^\infty(X)$. On the Euclidean space $\mathbb{R}^n$, it equals $\sum_i \partial_i^2$. In addition, $\Delta$ will also denote the Bochner–Laplacian (when acting on $L$).

A metric $g$ on a manifold $X$ with boundary $M$ induces a metric $h$ on $M$. In such a setting, the curvature quantities of $g$ and $h$ will be distinguished by adding a bar to those of $g$. In particular, the covariant derivative, the curvature tensor, and the Weyl tensor of $(X, g)$ are $\tilde{\nabla}$, $\tilde{R}$ and $\tilde{W}$. Similarly, $\tilde{\text{Ric}}$ and $\tilde{\text{scal}}$ are the Ricci tensor and the scalar curvature of $g$.

A hypersurface usually is given by an embedding $\iota : M \hookrightarrow X$. Accordingly, tensors on $X$ are pulled back by $\iota^*$ to $M$. In formulas, we often omit this pull back. For a hypersurface $\iota : M \hookrightarrow X$ with the induced metric $h = \iota^*(g)$ on $M$, the second fundamental form $L$ is defined by $L(X, Y) = -h(\nabla^g_X(Y), N)$ for vector fields $X, Y \in \mathcal{X}(M)$ and a unit normal vector field $\partial_0 = N$. We set $nH = \text{tr}_h(L)$ if $M$ has dimension $n$. $H$ is the mean curvature of $M$. Let $\tilde{L} = L - hH$ be the trace-free part of $L$. Sometimes we identify $L$ with the shape operator $S$ defined by $h(X, S(Y)) = L(X, Y)$.

We use metrics as usual to raise and lower indices. In particular, we set $(L^2)_{ij} = L^k_i L_{kj} = h^{lk} L_{il} L_{kj}$ and similarly for higher powers of $L$. We always sum over repeated indices.

The 1-form $\text{Ric}_0 \in \Omega^1(M)$ is defined by $\text{Ric}_0(X) = \text{Ric}(X, \partial_0)$ for $X \in \mathcal{X}(M)$. Similarly, we write $b_0$ for the analogous 1-form defined by a bilinear form $b$ and we
let $\overline{W}_0$ be the 3-tensor on $M$ with components $\overline{W}_{ijk0}$, i.e., we always insert $\partial_0$ into the last slot. Moreover, we set $\overline{W}_{ij} = \overline{W}_{0ij0}$.

The curvatures of the background $X$ and the hypersurface $M$ are connected through the respective Gauss identities

\[
\overline{\text{Ric}}_{ij} = \text{Ric}_{ij} + L^2_{ij} - nHL_{ij} + \overline{R}_{0ij0},
\]
\[
\text{scal} = \text{scal} + |L|^2 - n^2H^2 + 2\overline{\text{Ric}}_{00},
\]
(or equivalently $\overline{J} = J + \frac{1}{2(n-1)}|\dot{L}|^2 - \frac{n}{2}H^2 + \overline{P}_{00}$)

and the Codazzi–Mainardi equation

\[
\nabla_Y (L)(X, Z) - \nabla_X (L)(Y, Z) = \overline{R}(X, Y, Z, \partial_0), \quad X, Y, Z \in \mathcal{X}(M). \tag{2.2}
\]

Taking traces in $X$ and $Z$ gives

\[
\delta(L) - ndH = (n - 1)\overline{P}_0, \tag{2.3}
\]

or equivalently

\[
\delta(\dot{L}) - (n - 1)dH = (n - 1)\overline{P}_0. \tag{2.4}
\]

3 Some Second-Order Identities Involving the Second Fundamental Form

In the present section, we derive formulas for $\delta\delta(\dot{L}^2)$ and $\Delta(|\dot{L}|^2)$ in terms of the geometry of the background and the intrinsic geometry of $M$. The second of these formulas is closely related to a well-known formula of Simons. The main results are Lemmas 3.13 and 3.14. The latter result will play an important role in Sect. 6.

We start with the discussion of some results in dimension $n = 3$.

Lemma 3.1 For $n = 3$, it holds

\[
\delta\delta(\dot{L}^2) = 2\dot{L}_{jk} \nabla^j \delta(\dot{L})^k + |\nabla \dot{L}|^2 + \frac{1}{2} |\delta(\dot{L})|^2 - \frac{1}{2} |\overline{W}_0|^2 + \kappa_1 \tag{3.1}
\]

with

\[
\kappa_1 \overset{\text{def}}{=} (\nabla^i \nabla^j \dot{L}_i^k - \nabla^i \nabla^j \dot{L}_i^k) \dot{L}_{kj}. \tag{3.2}
\]

Proof. First, we calculate

\[
\delta\delta(\dot{L}^2) = \nabla^i \nabla^j \dot{L}^2_{ij} = (\nabla^i \nabla^j \dot{L}_i^k) \dot{L}_{kj} + (\nabla^i \dot{L}_i^k)(\nabla^j \dot{L}_k) + (\nabla^j \dot{L}_i^k)(\nabla^i \dot{L}_k) + \dot{L}^k_i (\nabla^i \nabla^j \dot{L}_{kj})
\]
\[
= (\nabla^i \nabla^j \dot{L}_i^k) \dot{L}_{kj} + (\nabla^j \dot{L}_i^k)(\nabla^i \dot{L}_k) + \delta(\dot{L})^k_\ell \delta(\dot{L})_{\ell k} + \dot{L}^k_i \nabla^i \delta(\dot{L})_k.
\]
In the first term, we interchange covariant derivatives. This generates the curvature term

\[ \kappa_1 \overset{\text{def}}{=} (\nabla^i \nabla^j \hat{L}^k_i) \hat{L}_{kj} - (\nabla^j \nabla^i \hat{L}^k_i) \hat{L}_{kj}. \]

In the second term, we apply the Codazzi–Mainardi equation (see (2.2))

\[ \nabla_j L_{ik} - \nabla_i L_{jk} = \bar{R}_{ijk0}. \]

Its trace-free part gives

\[ \nabla_j \hat{L}^k_i - \nabla_i \hat{L}^j_k = -\frac{1}{2} \delta(\hat{L}) \hat{L}^i_k + \frac{1}{2} \delta(\hat{L}) \hat{L}^j_k + \hat{W}_i^{jk}. \] (3.3)

In particular, we get

\[ (\nabla_j \hat{L}^k_i - \nabla_i \hat{L}^j_k) \nabla^i \hat{L}_{jk} = -\frac{1}{2} (\delta(\hat{L}), \delta(\hat{L})) + \hat{W}_i^{jk0} \nabla^i \hat{L}_{jk}. \]

But

\[ \hat{W}_{ijk0} \nabla^i \hat{L}^{jk} = \frac{1}{2} (W_{ijk0} - \nabla^i \hat{L}^{jk}) \nabla^i \hat{L}_{jk} = \frac{1}{2} \hat{W}_{ijk0} \left( \nabla^i \hat{L}^{jk} - \nabla^j \hat{L}^k_i \right) = -\frac{1}{2} \hat{W}_0^{2}. \]

where \(|\hat{W}_0|^2 \overset{\text{def}}{=} \hat{W}_{ijk0} \hat{W}^{ijk0}\). Thus

\[
(\nabla^i \hat{L}^k_i)(\nabla^i \hat{L}_{kj}) = (\nabla^i \hat{L}^k_i - \nabla_i \hat{L}^{jk}) \nabla^i \hat{L}_{kj} + (\nabla_i \hat{L}^{jk})(\nabla^i \hat{L}_{kj}) \]

\[ = (\nabla_i \hat{L}^{jk})(\nabla^i \hat{L}_{kj}) - \frac{1}{2} (\delta(\hat{L}), \delta(\hat{L})) - \frac{1}{2} |\hat{W}_0|^2 \]

\[ = (\nabla \hat{L}, \nabla \hat{L}) - \frac{1}{2} (\delta(\hat{L}), \delta(\hat{L})) - \frac{1}{2} |\hat{W}_0|^2. \]

These observations show that

\[ \delta(\hat{L}^2) = 2 \hat{L}_{jk} \nabla^i \delta(\hat{L})^k + |\nabla \hat{L}|^2 + \frac{1}{2} |\delta(\hat{L})|^2 - \frac{1}{2} |\hat{W}_0|^2 + \kappa_1, \] (3.4)

with \(\kappa_1\) as being defined in (3.2). \(\Box\)

**Lemma 3.2** Let \(n = 3\). Then

\[ \kappa_1 = 3(\hat{L}^2, P) + J|\hat{L}|^2. \]

**Proof** By definition, we have

\[ \kappa_1 = (\nabla^i \nabla^j \hat{L}^k_i - \nabla^j \nabla^i \hat{L}^k_i) \hat{L}_{kj} = \mathcal{R}^{ij} (\hat{L})^k_i \hat{L}_{kj}, \]

where \(\mathcal{R}^{ij}\) is the Ricci tensor.
where $\mathcal{R}$ denotes the curvature operator of $M$. We also observe that
\[ \mathcal{R}^{ij}(\dot{L})_i^k \dot{L}_{kj} = \mathcal{R}^{ij}(L)_i^k L_{kj}. \]

Hence by
\[ \mathcal{R}_{ij}(L)_{kl} = -L_{ij}^m R_{ijkm} - L_{k}^m R_{ijlm}, \]
and the decomposition
\[ \mathcal{R}_{ijkl} = -P_{ik} h_{jl} + P_{jk} h_{il} - P_{jl} h_{ik} + P_{il} h_{jk}, \tag{3.5} \]
(the Weyl tensor vanishes in dimension 3) we get (see also Remark 3.11)
\[ \kappa_1 = -\left( L_{i}^m R^{ij}_{km} + L^{km} R_{ij}^{im} \right) L_{kj} \]
\[ = L_{i}^m \left( P_{i}^j h_{jm} + P_{j}^i h_{im} - P_{j}^m h_{i}^j \right) L_{kj} + L^{km} \text{Ric}_m L_{kj} \]
\[ = 2(L^2, P) - 6H(L, P) + (L^2, \text{Ric}) \]
\[ = 3(L^2, P) - 6H(L, P) + J|L|^2 \]
\[ = 3(\dot{L}^2, P) + J|\dot{L}|^2. \tag{3.6} \]

Alternatively, combining the Simons’ identity (3.13) with the Gauss formula for the curvature endomorphism yields the first identity in (3.6). This completes the proof. \(\Box\)

**Example 3.3** For the flat background $\mathbb{R}^4$, it holds
\[ \kappa_1 = 3H \text{tr}(L^3) - |L|^4 = 3H \text{tr}(\dot{L}^3) + 3H^2 |\dot{L}|^2 - |\dot{L}|^4. \]

**Proof** The Gauss identity (2.1) gives
\[ J = -\frac{1}{4} |\dot{L}|^2 + \frac{3}{2} H^2, \]
and the identity
\[ \mathcal{F} \overset{\text{def}}{=} \iota^* \bar{\mathcal{P}} - \mathcal{P} + H \dot{L} + \frac{1}{2} H^2 h = \dot{L}^2 - \frac{1}{4} |\dot{L}|^2 h + \bar{\mathcal{W}}, \tag{3.7} \]
for the conformally invariant Fialkow tensor $\mathcal{F}$ of weight 0 [17, Lemma 6.23.3] implies
\[ \mathcal{P} = -\dot{L}^2 + \frac{1}{4} |\dot{L}|^2 h + H \dot{L} + \frac{1}{2} H^2 h. \]

---

3 Vyatkin [26] called the tensor $\mathcal{F}$ the Fialkow tensor. He was inspired by the discussion of Fialkow’s work [7] in [17]. The tensor $\mathcal{F}$ was proved to be conformally invariant in [25, Proposition 3.9].
Hence
\[ 3(\hat{L}^2, P) + J|\hat{L}|^2 = -3 \text{tr}(\hat{L}^4) + \frac{1}{2}|\hat{L}|^4 + 3H \text{tr}(\hat{L}^3) + 3H^2|\hat{L}|^2, \]
and it suffices to apply the identity \(2 \text{tr}(\hat{L}^4) = |\hat{L}|^4\) (Corollary 6.8). □

Now let
\[ \kappa_2 \overset{\text{def}}{=} (\hat{L}, \Delta(\hat{L})) - \frac{3}{2}\hat{L}^{ij} \nabla_j \delta(\hat{L})_i. \] (3.8)

**Lemma 3.4** For \(n = 3\), it holds
\[ \kappa_1 - \kappa_2 = \hat{L}^{ij} \nabla^k \overline{W}_{kij0}. \]

**Proof** The trace-free part of the Codazzi–Mainardi equation reads
\[ \nabla_i \hat{L}_{kj} - \nabla_k \hat{L}_{ij} - \frac{1}{2} \delta(\hat{L})_k h_{ij} + \frac{1}{2} \delta(\hat{L})_i h_{kj} = \overline{W}_{kij0}. \] (3.9)

Hence
\[ \nabla^k \nabla_i \hat{L}_{kj} - \nabla^k \nabla_k \hat{L}_{ij} - \frac{1}{2} \nabla^k \delta(\hat{L})_k h_{ij} + \frac{1}{2} \nabla^k \delta(\hat{L})_i h_{kj} = \nabla^k \overline{W}_{kij0}. \]

We commute the covariant derivatives in the first term and obtain
\[ \hat{L}^{ij} \nabla_i \delta(\hat{L})_j + \kappa_1 - (\hat{L}, \Delta(\hat{L})) + \frac{1}{2} \hat{L}^{ij} \nabla_j \delta(\hat{L})_i = \hat{L}^{ij} \nabla^k \overline{W}_{kij0}. \]

Therefore, we get
\[ \frac{3}{2} \hat{L}^{ij} \nabla_i \delta(\hat{L})_j - (\hat{L}, \Delta(\hat{L})) + \kappa_1 = \hat{L}^{ij} \nabla^k \overline{W}_{kij0}. \]

In other words, we have
\[ \kappa_1 - \kappa_2 = \hat{L}^{ij} \nabla^k \overline{W}_{kij0}. \]

The proof is complete. □

One should compare this result with [8, (2.12)].

**Corollary 3.5** Let \(n = 3\). Then
\[ \kappa_2 = 3(\hat{L}^2, P) + J|\hat{L}|^2 - \hat{L}^{ij} \nabla^k \overline{W}_{kij0}. \] (3.10)
Corollary 3.6 Let \( n = 3 \). Then

\[
(\tilde{L}, \Delta(\tilde{L})) = 3(\tilde{L}, \text{Hess}(H)) + 3(\tilde{L}^2, P) + J|\tilde{L}|^2 + 3\tilde{L}^{ij} \nabla_i(\tilde{P}_0)_j - \tilde{L}^{ij} \nabla^k \tilde{W}_{ki0}.
\]

**Proof** We calculate

\[
(\tilde{L}, \Delta(\tilde{L})) = \frac{3}{2} \tilde{L}^{ij} \nabla_j \delta(\tilde{L})_i + \kappa_2 \quad \text{(by (3.8))}
\]

\[
= 3(\tilde{L}, \text{Hess}(H)) + 3\tilde{L}^{ij} \nabla_j \tilde{P}_{0i} + \kappa_2 \quad \text{(by Codazzi–Mainardi)}.
\]

Now we apply Corollary 3.5. \( \square \)

Alternatively, we outline how Corollary 3.6 can be derived by using a Simons type formula. We continue the discussion in general dimensions. First, we prove

Lemma 3.7 In general dimensions, it holds

\[
\nabla_k \nabla_l (L)_{ij} = \nabla_i \nabla_j (L)_{kl} - \nabla_l \nabla_k (L)_{ij} = \nabla_k \tilde{R}_{lij0} - R_{ki}^m L_{mj} - R_{ki}^m j L_{lm}.
\]

**Proof** We start with the Codazzi–Mainardi equation

\[
\nabla_i (L)_{lj} - \nabla_l (L)_{ij} = \tilde{R}_{lij0}
\]

(see (2.2)). Differentiation gives

\[
\nabla_k \nabla_i (L)_{lj} - \nabla_k \nabla_l (L)_{ij} = \nabla_k \tilde{R}_{lij0}.
\]

Now we commute the derivatives in the first term using

\[
\nabla_k \nabla_i (L)_{lj} = \nabla_k \nabla_i (L)_{lj} = R_{ki}^m L_{mj} + R_{ki}^m j L_{lm}.
\]

Hence

\[
\nabla_i \nabla_k (L)_{lj} - \nabla_k \nabla_i (L)_{lj} = \nabla_k \tilde{R}_{lij0} - R_{ki}^m L_{mj} - R_{ki}^m j L_{lm}. \quad (3.11)
\]

Similarly, we differentiate the Codazzi–Mainardi equation

\[
\nabla_j (L)_{kl} - \nabla_k (L)_{jl} = \tilde{R}_{kjl0},
\]

and obtain

\[
\nabla_i \nabla_j (L)_{kl} - \nabla_i \nabla_k (L)_{jl} = \nabla_i \tilde{R}_{kjl0}. \quad (3.12)
\]

Adding (3.11) and (3.12) proves the assertion. \( \square \)
Lemma 3.7 implies
\[ (\nabla^i \nabla^j (L)_{ik} - \nabla^i \nabla^j (L)_{jk}) L^i_j = (\nabla^i \nabla^j (L)_{ik} - \nabla^k \nabla^i (L)_{ij}) L^i_j \] (by the symmetry of \( L \))
\[ = R_{ikm} L^{mj} L^{kj} + R_{ikm} L^{jm} L^i_j. \]

One can easily check that this identity also holds if \( L \) is replaced by \( \hat{L} \). This reproves (3.6).

Now taking a trace in Lemma 3.7 gives

**Lemma 3.8** In general dimensions, it holds
\[ \Delta (L)_{ij} = n \text{Hess}_{ij} (H) - \nabla^k \hat{R}_{kij0} + \nabla_i (\text{Ric}_0) j + R_{ikm} L^m_j - R_{kijm} L^{km}. \]

In particular, this gives a

**Second Proof of Corollary 3.6.** Let \( n = 3 \). Lemma 3.8 and \((L, \Delta(L)) = (\hat{L}, \Delta(\hat{L})) + 3H \Delta(H)\) imply
\[ (\hat{L}, \Delta(\hat{L})) = 3(\hat{L}, \text{Hess}(H)) + L^{ij} \nabla_i (\text{Ric}_0) j - L^{ij} \nabla^k \hat{R}_{kij0} \]
\[ + L^{ij} R_{ikm} L^m_j - L^{ij} R_{kijm} L^{km} \]
\[ = 3(\hat{L}, \text{Hess}(H)) + (L^2)^{im} R_{ikm} - L^{ij} L^{kl} R_{kijl} \]
\[ + L^{ij} \nabla_i (\text{Ric}_0) j - L^{ij} \nabla^k \hat{R}_{kij0}. \]

Now
\[ (L^2)^{im} R_{ikm} = (L^2)^{ij} \text{Ric}_{ij} = (L^2, P) + J|L|^2, \]
and (3.5) implies
\[ L^{ij} L^{kl} R_{kijl} = -2(L^2, P) + 6H (L, P). \]

Hence
\[ (\hat{L}, \Delta(\hat{L})) = 3(\hat{L}, \text{Hess}(H)) + 3(L^2, P) + J|L|^2 \]
\[ - 6H (L, P) + 2L^{ij} \nabla_i (\hat{P}_0) j - L^{ij} \nabla^k \hat{R}_{kij0}. \]

In order to simplify this formula, we note that
\[ 3(L^2, P) + J|L|^2 - 6H (L, P) = 3(\hat{L}^2, P) + J|\hat{L}|^2, \]
and
\[ \nabla^k \hat{R}_{kij0} = \nabla^k (\hat{P}_0) k h_{ij} - \nabla_j (\hat{P}_0) i + \nabla^k \overline{W}_{kij0}. \]
Hence
\[
(\hat{L}, \Delta(\hat{L})) = 3(\hat{L}, \text{Hess}(H)) + 3(\hat{L}^2, P) + J|\hat{L}|^2 + 3L^{ij}\nabla_i(\bar{P}_0)_j
- 3H\nabla^k(\bar{P}_0)_k - L^{ij}\nabla^k \bar{W}_{kj0}.
\]

The last term is unchanged if we replace \(L\) by \(\hat{L}\). This completes the proof. \(\square\)

Combining Lemma 3.7 with some arguments using the Gauss formula relating the curvature tensors of \(X\) and \(M\) leads to the following well-known identities which are due to Simons [16,22,23,26].

**Proposition 3.9** For any hypersurface \(M^n \hookrightarrow X^{n+1}\) with the second fundamental form \(L\), it holds
\[
\nabla_i \nabla_j (L)_{kl} = \nabla_k \nabla_l (L)_{ij} + L_{ij} L^2_{kl} - L_{kl} L^2_{ij} - L_{il} L^2_{jk} - L_{jk} L^2_{il}
- L_i^m \tilde{R}_{jklm} - L_j^m \tilde{R}_{iklm} + L^m_k \tilde{R}_{lijm} + L^m_l \tilde{R}_{kijm}
+ L_{ij} \tilde{R}_{0kl0} - L_{kl} \tilde{R}_{0ij0} + \tilde{\nabla}_l (\tilde{R})_{kjl0} + \tilde{\nabla}_k (\tilde{R})_{lij0}.
\]

(3.13)

Taking a trace gives
\[
\Delta(L)_{ij} = n \text{Hess}_{ij}(H) + nH L^2_{ij} - L_{ij}|L|^2
+ L_i^r \tilde{R}_{ikrs} + L_j^r \tilde{R}_{jkrs} - 2L^{rs} \tilde{R}_{rijs}
+ nH \tilde{R}_{0ij0} - L_{ij} \text{Ric}_{00} + \tilde{\nabla}_k (\tilde{R})_{ikj0} + \tilde{\nabla}_i (\tilde{R})_{jk0}.
\]

(3.14)

For flat backgrounds, Proposition 3.9 specializes to

**Proposition 3.10** For any hypersurface \(M^n \hookrightarrow \mathbb{R}^{n+1}\) with the second fundamental form \(L\), it holds
\[
\nabla_i \nabla_j (L)_{kl} = \nabla_k \nabla_l (L)_{ij} + L_{ij} L^2_{kl} - L_{kl} L^2_{ij} - L_{il} L^2_{jk} - L_{jk} L^2_{il}.
\]

(3.15)

Hence
\[
\Delta(L) = n \text{Hess}(H) + nH L^2 - |L|^2
\]

(3.16)

and
\[
\frac{1}{2} \Delta(|L|^2) = n(L, \text{Hess}(H)) + |\nabla L|^2 + nH \text{tr}(L^3) - |L|^4.
\]

(3.17)

In the remaining part of this section, we assume that \(n = 3\).

**Remark 3.11** The first part of Proposition 3.9 again confirms Lemma 3.2. In fact, by the symmetry of \(L\), we obtain
\[
(\nabla^i \nabla^j (L)_{ki} - \nabla^j \nabla^i (L)_{ki}) L^k_j = (\nabla^i \nabla^j (L)_{ki} - \nabla^k \nabla^i (L)_{ji}) L^k_j.
\]

\(\Box\) Springer
In this identity, one can replace $L$ by $\hat{\mathcal{L}}$. Hence (3.13) implies
\[
\kappa_1 = (L^2)^{kl} \tilde{R}_{kiil} - L^{il} L^{jk} \tilde{R}_{kilj}.
\]

By the Gauss identity, we obtain
\[
\kappa_1 = 3H \text{tr}(L^3) - |L|^4 + (L^2)^{kl} R_{kiil} - L^{il} L^{jk} R_{kilj}
\]
\[+ (L^2)^{kl}(L_{ki} L_{il} - L_{kl} L_{ii}) - L^{il} L^{jk}(L_{ki} L_{ij} - L_{kj} L_{il})
\]
\[= (L^2)^{kl} R_{kiil} - L^{il} L^{jk} R_{kilj}.
\]

The remaining arguments are as in the proof of Lemma 3.2.

**Remark 3.12** For flat backgrounds, it holds $\kappa_2 = \kappa_1 = 3H \text{tr}(L^3) - |L|^4$ (Example 3.3). Hence (3.17) implies
\[
\frac{1}{2} \Delta(|\dot{\mathcal{L}}|^2) = 3(\dot{\mathcal{L}}, \text{Hess}(H)) + |\nabla \dot{\mathcal{L}}|^2 + 3H \text{tr}(L^3) - |L|^4.
\]

Moreover, Lemma 3.1 (together with $\delta(\dot{\mathcal{L}}) = 2dH$) gives
\[
\delta \delta(\dot{\mathcal{L}}^2) = 4(\dot{\mathcal{L}}, \text{Hess}(H)) + |\nabla \dot{\mathcal{L}}|^2 + 2|dH|^2 + 3H \text{tr}(L^3) - |L|^4.
\]

As a consequence, we find the difference formula
\[
\frac{1}{2} \Delta(|\dot{\mathcal{L}}|^2) - \delta \delta(\dot{\mathcal{L}}^2) = -(\dot{\mathcal{L}}, \text{Hess}(H)) - 2|dH|^2. \tag{3.18}
\]

Now combining Lemma 3.1 with (3.8), we obtain
\[
\delta \delta(\dot{\mathcal{L}}^2) = \frac{4}{3}(\dot{\mathcal{L}}, \Delta(\dot{\mathcal{L}})) + |\nabla \dot{\mathcal{L}}|^2 + \frac{1}{2}|\delta(\dot{\mathcal{L}})|^2 - \frac{1}{2}|W_0|^2 - \frac{4}{3}\kappa_2 + \kappa_1.
\]

Hence
\[
\delta \delta((\dot{\mathcal{L}}^2)_o) = \delta \delta(\dot{\mathcal{L}}^2) - \frac{1}{3} \Delta(|\dot{\mathcal{L}}|^2)
\]
\[= \delta \delta(\dot{\mathcal{L}}^2) - \frac{2}{3}|\nabla \dot{\mathcal{L}}|^2 - \frac{2}{3}(\dot{\mathcal{L}}, \Delta(\dot{\mathcal{L}}))
\]
\[= \frac{2}{3}(\dot{\mathcal{L}}, \Delta(\dot{\mathcal{L}})) + \frac{1}{3}|\nabla \dot{\mathcal{L}}|^2 + \frac{1}{2}|\delta(\dot{\mathcal{L}})|^2 - \frac{1}{2}|W_0|^2 - \frac{1}{3}\kappa_1 + \frac{4}{3}(\kappa_1 - \kappa_2). \tag{3.19}
\]

Thus, using
\[
(P, (\dot{\mathcal{L}}^2)_o) = (P, \dot{\mathcal{L}}^2) - \frac{1}{3} |\dot{\mathcal{L}}|^2,
\]

Lemmas 3.2 and 3.4, we obtain
Lemma 3.13

\[
\delta \delta ((\hat{L}^2)_o) + (P, (\hat{L}^2)_o) = \frac{2}{3} (\hat{L}, \Delta \hat{L}) + \frac{1}{3} |\nabla \hat{L}|^2 + \frac{1}{2} |\delta (\hat{L})|^2 - \frac{2}{3} |J\hat{L}|^2
- \frac{4}{3} \hat{L}^{ij} \nabla^k (\hat{W}_0)_{kij} - \frac{1}{2} |\overline{W}_{ikj0}|^2.
\]

Lemma 3.13 confirms [8, Proposition 2.4] up to the sign of the term $|\overline{W}_0|^2$.

The following result extends the difference formula (3.18) to general backgrounds. It will play an important role in Sect. 6.

Lemma 3.14

It holds

\[
\Delta (|\hat{L}|^2) - 2 \delta \delta (\hat{L}^2) = -2 (\hat{L}, \text{Hess}(H)) - 2 (\hat{L}, \nabla (\overline{P}_0))
- |\delta (\hat{L})|^2 - 2 \hat{L}^{ij} \nabla^k \overline{W}_{kij0} + |\overline{W}_0|^2. \tag{3.20}
\]

Proof We recall that

\[
\Delta (|\hat{L}|^2) = 2 (\hat{L}, \Delta (\hat{L})) + 2 |\nabla (\hat{L})|^2
= 6 (\hat{L}, \text{Hess}(H)) + 2 \kappa_1 + 6 (\hat{L}, \nabla (\overline{P}_0)) - 2 \hat{L}^{ij} \nabla^k \overline{W}_{kij0} + 2 |\nabla (\hat{L})|^2
\]

(by Lemmas 3.2, 3.6) and

\[
2 \delta \delta (\hat{L}^2) = 8 (\hat{L}, \text{Hess}(H)) + 8 (\hat{L}, \nabla (\overline{P}_0)) + 2 |\nabla (\hat{L})|^2 + |\delta (\hat{L})|^2 - |\overline{W}_0|^2 + 2 \kappa_1
\]

(by (3.4) and $\delta (\hat{L}) = 2dH + 2\overline{P}_0$ (Codazzi–Mainardi)). The difference of both sums equals

\[
- 2 (\hat{L}, \text{Hess}(H)) - 2 (\hat{L}, \nabla (\overline{P}_0)) - |\delta (\hat{L})|^2 - 2 \hat{L}^{ij} \nabla^k \overline{W}_{kij0} + |\overline{W}_0|^2. \tag{3.21}
\]

The proof is complete. \qed

Note that the left-hand side of (3.20) is a total divergence, i.e., integrates to 0 on a closed $M$. On the other hand, the sum of the first three terms on the right-hand side of (3.20) also is a total divergence. In fact, the identity

\[
(\hat{L}, \nabla \omega) + (\delta (\hat{L}), \omega) = \delta (\omega; \hat{L}), \quad \omega \in \Omega^1 (M),
\]

shows that

\[
- 2 (\hat{L}, \text{Hess}(H)) - 2 (\hat{L}, \nabla (\overline{P}_0)) = 2 (\delta (\hat{L}), dH) + 2 (\delta (\hat{L}), \overline{P}_0),
\]

up to a divergence term. By the Codazzi–Mainardi equation $2dH + 2\overline{P}_0 = \delta (\hat{L})$, this sum equals $|\delta (\hat{L})|^2$. This proves the claim. The fact that the additional terms on the
right-hand side of (3.20) also form a total divergence can be seen as follows. Partial integration gives

\[-2 \int_M \hat{L}^{ij} \nabla^k \hat{W}_{kij0} dvol_h = 2 \int_M \nabla^k (\hat{L})^{ij} \hat{W}_{kij0} dvol_h.\]

By the trace-free part of the Codazzi–Mainardi equation

\[\nabla_k (\hat{L})_{ij} - \nabla_i (\hat{L})_{kj} - \frac{1}{2} \delta (\hat{L})_{ij} h_{kj} + \frac{1}{2} \delta (\hat{L})_{kj} h_{ij} = \hat{W}_{i k j0} = -\hat{W}_{kij0},\]

and partial integration, this integral equals

\[2 \int_M \nabla^i (\hat{L})^{kj} \hat{W}_{kij0} dvol_h - 2 \int_M \hat{W}^{kj0}_{kij0} \hat{W}_{kij0} dvol_h = -2 \int_M \hat{L}^{kj} \nabla^i \hat{W}_{kij0} dvol_h - 2 \int_M |\hat{W}_{kij0}|^2 dvol_h.\]

Hence

\[\int_M \left(-4 \hat{L}^{kj} \nabla^i \hat{W}_{kij0} + 2|\hat{W}_{kij0}|^2\right) dvol_h = 0.\]

This proves the claim.

4 The Singular Yamabe Problem and the Obstruction

The material in this section rests on [3] and [11].

Let \((X^{n+1}, g)\) be a compact manifold with boundary \(M\) of dimension \(n\). The singular Yamabe problem asks to find a defining function \(\sigma\) of \(M\) so that

\[\text{scal}(\sigma^{-2} g) = -n(n + 1).\]  

(4.1)

The conformal transformation law of scalar curvature shows that

\[\text{scal}(\sigma^{-2} g) = -n(n + 1)|d\sigma|^2_g + 2n\sigma \Delta_g (\sigma) + \sigma^2 \text{scal}(g).\]

Following [11], we write this equation in the form

\[\text{scal}(\sigma^{-2} g) = -n(n + 1) S(g, \sigma),\]

where

\[S(g, \sigma) \overset{\text{def}}{=} |d\sigma|^2_g + 2\rho \sigma, \quad (n + 1)\rho \overset{\text{def}}{=} -\Delta_g (\sigma) - \sigma J \quad \text{and} \quad 2nJ = \text{scal}(g).\]
In these terms, \( \sigma \) is a solution of (4.1) iff \( S(g, \sigma) = 1 \). Although such \( \sigma \) exists and is unique, in general, \( \sigma \) is not smooth up to the boundary. The smoothness is obstructed by a locally determined conformally invariant scalar function on \( M \) which is called the singular Yamabe obstruction.

In order to describe the structure of a solution \( \sigma \) of the singular Yamabe problem more precisely, we use geodesic normal coordinates. Let \( r \) be the distance function of \( M \) for the background metric \( g \). Then there are uniquely determined coefficients \( \sigma(k) \in C^\infty(M) \) for \( 2 \leq k \leq n + 1 \) so that the smooth defining function

\[
\sigma_F \overset{\text{def}}{=} r + \sigma(2)r^2 + \cdots + \sigma(n+1)r^{n+1}
\]

satisfies

\[
S(g, \sigma_F) = 1 + Rr^{n+1}
\]

with a smooth remainder term \( R \). The coefficients are recursively determined. In geodesic normal coordinates, the metric \( g \) takes the form \( dr^2 + h_r \) with a one-parameter family \( h_r \) of metrics on \( M \). The condition (4.3) is equivalent to

\[
|d\sigma_F|^2_g - \frac{2}{n+1} \sigma_F \Delta_g(\sigma_F) - \frac{1}{n(n+1)} \sigma_F^2 \text{scal}(g) = 1 + Rr^{n+1}.
\]

We write the left-hand side of this equation in the form

\[
\partial_r(\sigma_F)^2 + h_r^{ij} \partial_i(\sigma_F) \partial_j(\sigma_F)
- \frac{2}{n+1} \sigma_F \left( \partial_r^2(\sigma_F) + \frac{1}{2} \text{tr}(h_r^{-1}h_r') \partial_r(\sigma_F) + \Delta_h(\sigma_F) \right)
- \frac{1}{n(n+1)} \sigma_F^2 \text{scal}(g),
\]

and expand this sum into a Taylor series in the variable \( r \). Then the vanishing of the coefficient of \( r^k \) for \( k \leq n \) is equivalent to an identity of the form

\[
(k - 1 - n)\sigma(k+1) = LOT,
\]

where LOT involves only lower-order Taylor coefficients of \( \sigma \). The latter relation also indicates that there is a possible obstruction to the existence of an improved solution \( \sigma'_F \) which contains a term \( \sigma(n+2)r^{n+2} \) and satisfies \( S(g, \sigma'_F) = 1 + Rr^{n+2} \). Following [3], we define the singular Yamabe obstruction by

\[
\mathcal{B}_n \overset{\text{def}}{=} \left( r^{-n-1}(S(g, \sigma_F) - 1) \right) |_{r=0}.
\]

Since \( \sigma_F \) is determined by \( g \), \( \mathcal{B}_n \) is a functional of \( g \). It is a key result that \( \mathcal{B}_n \) is a conformal invariant of \( g \) of weight \(- (n + 1) \). More precisely, we write \( \hat{\mathcal{B}}_n \) for the obstruction defined by \( \hat{g} = e^{2\varphi} g \) with \( \varphi \in C^\infty(X) \). Then

\( \heartsuit \) Springer
Lemma 4.1 ([13]) \( e^{(n+1)r^2(\varphi)} \hat{\mathcal{B}}_n = \mathcal{B}_n \).

Let us be a bit more precise about the above algorithm. We set \( S_k = \sum_{j=1}^{k} \sigma(j) \) so that \( S_{n+1} = \sigma_F \). Then the coefficients of \( \sigma_F \) are recursively determined by the conditions

\[
S(S_k) = 1 + O(r^k).
\]

More precisely, we recursively find

\[
S(S_k) = 1 + r^{k-1}(c(n-k+2)\sigma(k) + \cdots) + \cdots
\]

with \( c = 2k/(n+1) \). Then the condition \( S(S_k) - 1 = O(r^k) \) with an unknown coefficient \( \sigma(k) \) is satisfied iff the coefficient of \( r^{k-1} \) in this expansion vanishes. This can be solved for \( \sigma(k) \) if \( k = 2, 3, \ldots, n+1 \). In the case \( k = n+1 \), we obtain

\[
S(S_{n+1}) = 1 + O(r^{n+1}),
\]

and the restriction of the latter remainder is the obstruction \( \mathcal{B}_{n+1} \).

In the following, we shall need explicit formulas for the coefficients \( \sigma(k) \) for \( k \leq 4 \).

First, we consider flat backgrounds. We approximately solve the equation \( S(g, \sigma_F) = 1 \) for the flat metric \( g \) by differentiation of the relation

\[
\partial_r(\sigma_F)^2 + h^{ij}_{\sigma_F} \partial_i(\sigma_F) \partial_j(\sigma_F) - \frac{2}{n+1} \sigma_F \left( \partial^2_r(\sigma_F) + \frac{1}{2} \text{tr}(h^{-1}_r h') \partial_r(\sigma_F) + \Delta h_r(\sigma_F) \right) = 0 \quad (4.6)
\]

in the variable \( r \). Then, for general \( n \geq 3 \), we find the solution

\[
\sigma_F = r + \frac{r^2}{2} H - \frac{r^3}{3(n-1)} |\hat{\mathcal{L}}|^2 + r^4 \sigma_{(4)} + \cdots \quad (4.7)
\]

with the coefficient

\[
\sigma_{(4)} = \frac{1}{24(n-2)} \left( 6 \text{tr}(\hat{\mathcal{L}}^3) + \frac{7n-11}{n-1} H |\hat{\mathcal{L}}|^2 + 3\Delta(H) \right). \quad (4.8)
\]

Note that \( \sigma_{(3)} \) is singular for \( n = 1 \) and \( \sigma_{(4)} \) is singular for \( n = 2 \). In particular, we have

\[
\sigma_F = r + \frac{r^2}{2} H - \frac{r^3}{6} |\hat{\mathcal{L}}|^2 + \frac{r^4}{24} \left( 6 \text{tr}(\hat{\mathcal{L}}^3) + 5H |\hat{\mathcal{L}}|^2 + 3\Delta(H) \right) + \cdots
\]

if \( n = 3 \) ([14, (2.16–2.18)]). These results are determined by the conditions

\[
S(S_2) = 1 + O(r^2), \quad S(S_3) = 1 + O(r^3), \quad S(S_4) = 1 + O(r^4).
\]
In particular, the obstructions $B_2$ and $B_3$ are the restrictions of the remainder terms in the second and the third expansions. More precisely, for $B_2 (n = 2)$, we find

$$B_2 = \left(r^{-3}(S(S_3) - 1)\right) |_0 = -\frac{1}{3}(H|\hat{L}|^2 + \Delta(H)) - \frac{2}{3} \operatorname{tr}(\hat{L}^3). \quad (4.9)$$

Since for $n = 2$ the term $\operatorname{tr}(\hat{L}^3)$ vanishes, we get

$$B_2 = -\frac{1}{3}(H|\hat{L}|^2 + \Delta(H)).$$

Similarly, for $n = 3$, we get

$$B_3 = (r^{-4}(S(S_4) - 1)) |_0$$

$$= \frac{1}{12} \left(|\hat{L}|^4 - 6H\Delta(H) + \Delta(|\hat{L}|^2) + 6H \operatorname{tr}(\hat{L}^3) + 3|dH|^2 - 3\Delta'(H)\right),$$

where $\Delta_{hr} = \Delta_h + r\Delta'_h + \cdots$. By the variation formula $\Delta'(u) = -2(L, \operatorname{Hess}(u)) - 3(dH, du)$ (see the proof of Lemma 6.2), this leads to

$$12B_3 = \Delta(|\hat{L}|^2) + 6(\hat{L}, \operatorname{Hess}(H)) + |\hat{L}|^4 + 6H \operatorname{tr}(\hat{L}^3) + 12|dH|^2. \quad (4.10)$$

For general background, we shall express the coefficients $\sigma(k)$ in terms of the volume coefficients $v_k$ of $h_r$, which are defined by the expansion

$$v(r) = \sum_{k \geq 0} r^k v_k$$

of

$$v(r) \overset{\text{def}}{=} \frac{d\operatorname{vol}(h_r)}{d\operatorname{vol}(h)} = \frac{(\det(h_r))/\det(h)}{\frac{1}{2}.}$$

This is convenient since the identity

$$\frac{v'(r)}{v(r)} = \frac{1}{2} \operatorname{tr}(h_r^{-1}h'_r) \quad (4.11)$$

provides natural formulas for the expansion of the coefficient $\operatorname{tr}(h_r^{-1}h'_r)$ in (4.4).

Note that for the background $\mathbb{R}^{n+1}$ it holds

$$v(r) = \det(\operatorname{Id} + rL) \quad (4.12)$$

(see [15, Sect. 3.4]). Hence $v_{n+1} = 0$ in this case. For a general backgrounds, the volume coefficient $v_{n+1}$ does not vanish, however.

The calculation of the remainder term in the expansion of $\mathcal{S}(S_k)$ requires $k$ normal derivatives of the Eq. (4.6). Since the expansion of $S_k$ has a vanishing zeroth-order
term, this amounts to take $k - 1$ derivatives of the trace term. In turn, this involves volume coefficients of the metric $h_r$ up to order $k$. In general, we find

$$B_n \overset{\text{def}}{=} (r^{-(n+1)}(S(\sigma F) - 1))|_0 = (\cdots) - 2v_{n+1}. $$

In particular, $B_2$ involves the coefficient $v_3$ and $B_3$ involves $v_4$.

Now, the above algorithm shows that, for general backgrounds and in general dimensions, the coefficients $\sigma(2)$ are given by the formulas

$$\sigma(2) = \frac{1}{2n} v_1,$$

$$\sigma(3) = \frac{2}{3(n-1)} v_2 - \frac{1}{3n} v_1^2 + \frac{1}{3(n-1)} \bar{J},$$

$$\sigma(4) = \frac{3}{4(n-2)} v_3 - \frac{9n^2 - 20n + 7}{12n(n-1)(n-2)} v_1 v_2 + \frac{6n^2 - 11n + 1}{24n^2(n-2)} v_3^3$$

$$+ \frac{2n-1}{6n(n-1)(n-2)} v_1 \bar{J} + \frac{1}{4(n-2)} \bar{J}' + \frac{1}{4(n-2)} \Delta(\sigma(2)).$$

These formulas also can be derived from the description of the solution $\sigma$ of the singular Yamabe problem in [8, Appendix]. We omit the details.

The observation that $\sigma(4)$ has a (formal) pole at $n = 2$ reflects the fact that there is no approximate solution $\sigma_F$ up to order $r^4$ in that dimension. Similarly, $\sigma(5)$ has a pole at $n = 3$—we shall not display an explicit formula for $\sigma(5)$, however. The obstruction to the existence of a smooth solution in $n = 3$ is defined in terms of $S(S_4)$.

In the flat case, the identity (4.12) implies that the volume coefficients $v_k$ are given by the elementary symmetric polynomials $\sigma_k(L)$ in the eigenvalues of the shape operator defined by $L$. Hence Newton’s formulas show that

$$v_1 = nH,$$

$$v_2 = \frac{1}{2} (nH)^2 - \frac{1}{2} |L|^2,$$

$$v_3 = \frac{1}{6} (nH)^3 - \frac{1}{2} nH |L|^2 + \frac{1}{3} \text{tr}(L^3).$$

A combination of these formulas with (4.13) reproduces the expressions in (4.7) and (4.8).

5 The Singular Yamabe Obstruction $B_2$

In this section, we derive an explicit formula for the obstruction $B_2$ from its definition in Sect. 4. This reproves a result in [3]. We also briefly recall the relation to the conformal Willmore functional $W_2$. 
Let \( n = 2 \). The formula for \( B_2 \) in terms of volume coefficients reads

\[
B_2 \overset{\text{def}}{=} (r^{-3}(S(S_3) - 1))|_0 = -2v_3 - \frac{1}{12}v_1^3 + \frac{1}{3}v_1v_2 - \frac{2}{3}\Delta(\sigma(2)) - \frac{2}{3}v_1\bar{J} - \frac{2}{3}\bar{J}'.
\] (5.1)

We recall that the term \( v_3 \) vanishes in \( n = 2 \) in the flat case but not in the curved case. In the flat case, this formula reduces to (4.9). The proof easily follows using \( v_1 = 2H, v_2 = H^2 - |\hat{L}|^2/2 \) (see (4.14)) and \( \sigma(2) = H/2 \). In the general case, the formulas for the volume coefficients in Lemma 6.4 imply

\[
B_2 = \left( \frac{1}{3}\tilde{\nabla}_0(\overline{Ric})_{00} - \frac{1}{6}\text{scal} \right) - \frac{1}{3}H\text{scal} + H\overline{Ric}_{00} - \frac{2}{3}(\bar{L}, \bar{G}) - \frac{1}{3}\Delta(H) - \frac{1}{3}H|\hat{L}|^2
\]

using \( \text{tr}(L^3) = 0 \) in dimension \( n = 2 \). Now the second Bianchi identity implies

\[
\frac{1}{3}\tilde{\nabla}_0(\overline{Ric})_{00} - \frac{1}{6}\text{scal}' = -\frac{1}{3}\delta(\bar{P}_0) + \frac{1}{3}(\bar{L}, \bar{P}) - H\overline{Ric}_{00} + \frac{1}{3}H\text{scal}
\]

(see [20, (13.6.5)]). Hence using \( (\bar{L}, \bar{G}) = (\bar{L}, \bar{P}) \) we find

\[
B_2 = -\frac{1}{3}(\Delta(H) + H|\hat{L}|^2 + \delta(\bar{P}_0) + (\bar{L}, \bar{P})).
\] (5.2)

By Codazzi–Mainardi \( dH = \delta(\bar{L}) - \overline{Ric}_0 \), this formula is equivalent to

\[
B_2 = -\frac{1}{3}(\delta \delta(\bar{L}) + H|\hat{L}|^2 + (\bar{L}, \bar{P})).
\]

The latter formula for the obstruction was first derived in [3, Theorem 1.3].

**Remark 5.1** The coefficient \( \sigma(4) \) has a simple (formal) pole in \( n = 2 \). Moreover, (4.13) implies

\[
\text{Res}_{n=2}(\sigma(4)) = \frac{3}{4}v_3 + \frac{1}{32}v_1^3 - \frac{1}{8}v_1v_2 + \frac{1}{4}v_1\bar{J} + \frac{1}{4}\bar{J}' + \frac{1}{4}\Delta(\sigma(2)).
\]

This formula shows the residue formula

\[
\text{Res}_{n=2}(\sigma(4)) = -\frac{3}{8}B_2
\]

being a special case of [20, Lemma 16.3.9]).

Let \( K \) be the Gauss curvature of a surface \( M \hookrightarrow \mathbb{R}^3 \). By \( 2(H^2 - K^2) = |\hat{L}|^2 \), the equation \( \Delta(H) + H|\hat{L}|^2 = 0 \) is equivalent to

\[
\Delta(H) + 2H(H^2 - K) = 0.
\]
This equation is well known as the Willmore equation for a surface $M$. It is the Euler–Lagrange equation of the Willmore functional

$$\mathcal{W}_2 = \int_M |\hat{\nabla}|^2 \, d\text{vol}_h$$

for variations of the embedding of $M$ [27, Sect. 7.4]. In other words, $B_2$ provides the Euler–Lagrange equation of $\mathcal{W}_2$ [27]. This fact extends to the curved case (for details see [20, Sect. 13.9]).

### 6 The Singular Yamabe Obstruction $B_3$

In this section, we determine explicit formulas for the obstruction $B_3$. We shall start by expressing the definition (4.5) in terms of volume coefficients of the background metric and two normal derivatives of the scalar curvature. We simplify that result by repeated applications of the second Bianchi identity. A sequence of further transformations finally leads to Theorem 1.

#### 6.1 $B_3$ in Terms of Volume Coefficients

For $n = 3$, the formulas in (4.13) read

$$\sigma(2) = \frac{1}{6} v_1, \quad \sigma(3) = \frac{1}{9} (3v_2 - v_1^2) + \frac{1}{6} \bar{J}$$

and

$$\sigma(4) = \frac{1}{108} (81v_3 - 42v_1v_2 + 11v_1^3) + \frac{5}{36} v_1 \bar{J} + \frac{1}{4} \bar{J}' + \frac{1}{4} \Delta(\sigma(2)).$$

These quantities define $S_4$. We also recall the expansion $\Delta_{h_r} = \Delta_h + r \Delta'_h + \cdots$. In these terms, we obtain

**Lemma 6.1** It holds

$$B_3 \overset{\text{def}}{=} (r^{-4}(S(S_4) - 1))|_0 = -2v_4 + \frac{1}{2} v_1 v_3 + \frac{1}{3} v_2^2 - \frac{7}{18} v_1^2 v_2 + \frac{2}{27} v_1^4$$

$$- \frac{1}{3} \bar{J} v_2 - \frac{5}{12} \bar{J}' v_1 - \frac{1}{4} \bar{J}''$$

$$- \frac{1}{2} \Delta(\sigma(3)) - \frac{1}{3} v_1 \Delta(\sigma(2)) - \frac{1}{2} \Delta'(\sigma(2)) + |d\sigma(2)|^2.$$

This result follows by direct evaluation of the definition of $B_3$. We omit the details. By a substantial calculation, the formula (6.1) also can be derived from the results in [8, Appendix].
In the remaining part of this section, we evaluate this formula. First of all, we calculate the last line in (6.1).

**Lemma 6.2** It holds

\[
-\frac{1}{2} \Delta (\sigma_3) - \frac{1}{3} v_1 \Delta (\sigma_2) - \frac{1}{2} \Delta' (\sigma_2) + |d \sigma_2|^2 \\
= \frac{1}{12} \Delta (|\hat{L}|^2) + \frac{1}{2} (\hat{L}, \text{Hess} (H)) + \frac{1}{6} \Delta (\bar{P}_{00}) + \frac{1}{2} (dH, \text{Ric}_0) + |dH|^2.
\]

**Proof** We recall that \( v_1 = 3H \). By

\[
\sigma_2 = \frac{1}{2} H \quad \text{and} \quad \sigma_3 = \frac{1}{6} (-|\hat{L}|^2 - 2\bar{P}_{00}),
\]

we obtain

\[
-\frac{1}{2} \Delta (\sigma_3) - \frac{1}{3} v_1 \Delta (\sigma_2) - \frac{1}{2} \Delta' (\sigma_2) + |d \sigma_2|^2 \\
= \frac{1}{12} \Delta (|\hat{L}|^2) + \frac{1}{6} \Delta (\bar{P}_{00}) - \frac{1}{2} H \Delta H - \frac{1}{4} \Delta' (H) + \frac{1}{4} |dH|^2.
\]

Now the variation formula [5, Proposition 1.184]

\[
(d/dt)|_0 (\Delta_{g+\delta h}(u)) = -(\nabla^g (du), h)_g - (\delta_g (h), du)_g + \frac{1}{2} (d (\text{tr}_g (h)), du)_g \quad (6.2)
\]

for the Laplacian implies (for \( h = 2L \) and \( g = h \))

\[
\Delta' (u) = -2 (L, \text{Hess} (u)) - 2 (\delta (L), du) + 3 (dH, du).
\]

By Codazzi–Mainardi, it holds \( \delta (L) = 3dH + 2\bar{P}_0 = 3dH + \text{Ric}_0. \) Hence

\[
\Delta' (u) = -2 (L, \text{Hess} (u)) - 3 (dH, du) - 2 (\text{Ric}_0, du).
\]

These results imply the assertion. \( \Box \)

### 6.2 The Volume Coefficients

The volume coefficients \( v_j \) can be expressed in terms of the Taylor coefficients of \( h_r \). These relations follow by Taylor expansion of the identity (4.11) in the variable \( r \) and solving the resulting relations for \( v_j \). We find

\[
2v_1 = \text{tr}(h_{(1)}), \\
8v_2 = \text{tr}(h_{(1)})^2 + 4 \text{tr}(h_{(2)}) - 2 \text{tr}(h_{(1)}^2), \\
48v_3 = \text{tr}(h_{(1)})^3 + 12 \text{tr}(h_{(1)}) \text{tr}(h_{(2)}) + 24 \text{tr}(h_{(3)}) - 6 \text{tr}(h_{(1)}) \text{tr}(h_{(2)}^2)
\]
Lemma 6.3 In general dimensions, it holds

$$ h_{(1)} = 2L, \ h_{(2)} = L^2 - \bar{G} \text{ and } 3(h_{(3)})_{ij} = -\bar{\nabla}_0(\bar{R})_{0ij0} - 2L_i^k \bar{G}_{jk} - 2L_j^k \bar{G}_{ik}, $$

where $\bar{G}_{ij} \overset{\text{def}}{=} \bar{R}_{0ij0}$.

As consequences, we find explicit formulas for the volume coefficients $v_k$ for $k \leq 3$.

Lemma 6.4 In general dimensions, it holds

$$ v_1 = nH, $$
$$ 2v_2 = -\bar{Ric}_{00} - |\bar{L}|^2 + n(n-1)H^2 = \bar{Ric}_{00} + \text{scal} - \text{scal}, $$
$$ 6v_3 = -\bar{\nabla}_0(\bar{Ric})_{00} + 2(\bar{L}, \bar{G}) - (3n-2)H\bar{Ric}_{00} $$
$$ + 2\text{tr}(\bar{L}^3) - 3(n-2)H|\bar{L}|^2 + n(n-1)(n-2)H^3. $$

These formulas coincide with the corresponding terms in the expansion of the volume form in [1, Theorem 3.4]. Note that this is obvious for $v_1$ and $v_2$ but requires to apply the Gauss identities (2.1) for $v_3$. Equivalent formulas can be found in [14, Sect. 2].

The coefficient $v_4$ is more involved. It depends on $h_{(k)}$ for $k \leq 3$ and $\text{tr}(h_{(4)})$. We shall not discuss an explicit formula for $h_{(4)}$. For our purpose, it will be enough to prove the following formula for the quantity $\text{tr}(h_{(4)})$.

Lemma 6.5 In general dimensions, it holds

$$ 12\text{tr}(h_{(4)}) = -\bar{\nabla}_0^2(\bar{Ric})_{00} - 6L^i^j \bar{\nabla}_0(\bar{R})_{0ij0} - 4(L^2, \bar{G}) + 4(\bar{G}, \bar{G}). \quad (6.3) $$

Proof A calculation of Christoffel symbols shows that

$$ \bar{R}_{0jk0} = \frac{1}{4}g^{ab}g_{aj}g_{bk} - \frac{1}{2}g''_{jk} \quad (6.4) $$
[20, Sect. 13.2.5]. The assertion then follows by evaluating the second-order derivative in \( r \) of this equation followed by contraction with \( h^{jk} \). Here are the details. Differentiating (6.4) twice in \( r \) at \( r = 0 \) yields

\[
\partial_r^2(\tilde{R}_{0jk0}) = \frac{1}{4}(g^{ab})''g'_{aj}g'_{bk} + \frac{1}{4}g^{ab}(g_{aj})'''g'_b + \frac{1}{4}g^{ab}g'_{aj}(g_{bk})'''
\]

\[
+ \frac{1}{2}(g^{ab})'(g_{aj})''g'_b + \frac{1}{2}(g^{ab})'(g_{aj})'(g_{bk})'' + \frac{1}{2}g^{ab}(g_{aj})''(g_{bk})'' - \frac{1}{2}g^{ab}_{jk}
\]

\[
= 2(3L^2 + \bar{G})^{ab}_{jk}L_{ak}L_{jk} + 3h^{ab}(h_{(3)})_{aj}L_{bk} + 3h^{ab}L_{aj}(h_{(3)})_{bk}
\]

\[
- 4L^{ab}(L^2 - \bar{G})_{aj}L_{bk} - 4L^{ab}L_{aj}(L^2 - \bar{G})_{bk}
\]

\[
+ 2h^{ab}(L^2 - \bar{G})_{aj}(L^2 - \bar{G})_{bk} - 12(h_{(4)})_{jk}
\]

using \((h_r^{-1})_{ij} = h^{ij} - 2L^{ij}r + (3(L^2)^{ij} + \bar{G}^{ij})r^2 + \cdots \). Hence

\[
h^{jk}\partial_r^2(\tilde{R}_{0jk0})
\]

equals

\[
- 2L^{ij}\bar{\nabla}_0(\bar{R})_{0ij0} - 2(L^2, \bar{G}) + 2(\bar{G}, \bar{G}) - 12 \text{tr}(h_{(4)}).
\] (6.5)

On the other hand, we calculate

\[
h^{jk}\partial_r^2(\tilde{R}_{0jk0}) = \partial_r^2((h_r^{-1})_{jk}\tilde{R}_{0jk0}) - 2(h_r^{-1})'_{jk}\partial_r(\tilde{R}_{0jk0}) - (h_r^{-1})''_{jk}\tilde{R}_{0jk0}
\]

\[
= \partial_r^2(\tilde{Ric}_{00}) + 4L^{jk}\partial_r(\tilde{R}_{0jk0}) - 2(3L^2 + \bar{G}, \bar{G}).
\]

Therefore, the relations

\[
\partial_r^2(\tilde{Ric}_{00}) = \bar{\nabla}_0^2(\tilde{Ric})_{00},
\]

\[
\partial_r(\tilde{R}_{0jk0}) = \bar{\nabla}_0(\bar{R})_{0jk0} + (L\bar{G} + \bar{G}L)_{jk}
\]

imply

\[
h^{jk}\partial_r^2(\tilde{R}_{0jk0}) = \bar{\nabla}_0^2(\tilde{Ric})_{00} + 4L^{jk}\bar{\nabla}_0(\bar{R})_{0jk0} + 8(L^2, \bar{G}) - 6(L^2, \bar{G}) - 2(\bar{G}, \bar{G}).
\] (6.6)

Now combining (6.5) and (6.6) proves the assertion. \(\square\)

**Example 6.6** Let \( n \geq 3 \) be general. Assume that \( g = r^2g_+ \) for a Poincaré–Einstein metric \( g_+ = r^{-2}(dr^2 + (h - \mathcal{P}r^2 + \mathcal{P}^2r^4/4)) \) with conformally flat conformal infinity \( h. \mathcal{P} \) is the Schouten tensor of \( h. r \) is the distance in the metric \( g \) from the hypersurface

\(\mathfrak{P} \text{ Springer} \)
\( r = 0 \). The formula for \( g \) shows that \( \text{tr}(h_{(4)}) = 1/4|P|^2 \). Comparing the coefficients of \( r \) and \( r^2 \) in the expansions of \( h_r \) shows that \( L = 0 \) and \( \bar{G} = P \). Hence the above formula reduces to

\[
12 \text{tr}(h_{(4)}) = -\bar{\nabla}_0^2(\text{Ric})_{00} + 4(P, P) = -\partial_r^2(\text{Ric})_{00} + 4(P, P).
\]

But [17, Lemma 6.11.2] shows that \( \bar{P} = -1/(2r)\partial_r(h_r) \). Hence \( \bar{P} = P - 1/2r^2P^2 \). It follows that \( \partial_r^2(\bar{P}) = -P^2 \). Therefore, \( \partial_r^2(\text{Ric}_{00}) = \partial_r^2(J) = |P|^2 \) (for \( r = 0 \)) using [17, Lemma 6.11.1]. Hence the right-hand side gives \( 3|P|^2 \), i.e., we reproduced the result \( 4 \text{tr}(h_{(4)}) = |P|^2 \). For general \( h \), the Poincaré–Einstein metric also involves the Bach tensor. But since the Bach tensor is trace-free, we still have \( \text{tr}(h_{(4)}) = 1/4|P|^2 \) and we get the same conclusion.

The above results imply the following formula for \( v_4 \).

**Lemma 6.7** It holds

\[
24v_4 = -\bar{\nabla}_0^2(\text{Ric})_{00} + 2L^{ij}\bar{\nabla}_0(\bar{R})_{0ij0} - 4nH\bar{\nabla}_0(\text{Ric})_{00} + 3(\text{Ric}_{00})^2 - 2(\bar{G}, \bar{G}) + 8nH(L, \bar{G}) - 8(L^2, \bar{G}) + 6|\bar{L}|^2\text{Ric}_{00} - 6n(n-1)H^2\text{Ric}_{00} + 24\sigma_4(L) \tag{6.7}
\]

or, equivalently,

\[
24v_4 = -\bar{\nabla}_0^2(\text{Ric})_{00} + 2L^{ij}\bar{\nabla}_0(\bar{R})_{0ij0} - (4n-2)H\bar{\nabla}_0(\text{Ric})_{00} + 3(\text{Ric}_{00})^2 - 2(\bar{G}, \bar{G}) + 8(n-2)H(\bar{L}, \bar{G}) - 8(\bar{L}^2, \bar{G}) - 2(n-1)(3n-4)H^2\text{Ric}_{00} + 6|\bar{L}|^2\text{Ric}_{00} + 24\sigma_4(L).
\]

In particular, for \( n = 3 \), we find

\[
24v_4 = -\bar{\nabla}_0^2(\text{Ric})_{00} + 2\bar{L}^{ij}\bar{\nabla}_0(\bar{R})_{0ij0} - 10H\bar{\nabla}_0(\text{Ric})_{00} + 3(\text{Ric}_{00})^2 - 2(\bar{G}, \bar{G}) + 8H(\bar{L}, \bar{G}) - 8(\bar{L}^2, \bar{G}) - 20H^2\text{Ric}_{00} + 6|\bar{L}|^2\text{Ric}_{00} \tag{6.8}
\]

using \( \sigma_4(L) = 0 \).

**Proof** This is a direct calculation. We omit the details. \( \square \)

The three terms in the first line of (6.7) coincide with the corresponding terms in the formula for \( v_4 \) in [1, Theorem 3.4]. However, the remaining terms in both formulas are expressed in different ways.

Note that Newton’s identity

\[
24\sigma_4(L) = \text{tr}(L)^4 - 6\text{tr}(L)^2|L|^2 + 3|L|^4 + 8\text{tr}(L)\text{tr}(L^3) - 6\text{tr}(L^4)
\]
gives
\[24\sigma_4(L) = n(n-1)(n-2)(n-3)H^4 - 6(n-2)(n-3)H|\hat{L}|^2 + 8(n-3)H \operatorname{tr}(\hat{L}^3) + 3(|\hat{L}|^4 - 2 \operatorname{tr}(\hat{L}^3)).\]

**Corollary 6.8** Let \( n = 3 \). Then \(|\hat{L}|^4 = 2 \operatorname{tr}(\hat{L}^4)\).

This result generalizes the fact that \( \operatorname{tr}(\hat{L}^3) = 0 \) for \( n = 2 \).

**Example 6.9** Assume that \( g = r^2 g_+ \) for a Poincaré–Einstein metric \( g_+ \) with conformal infinity \( h \) (as in Example 6.6). By \( L = 0 \), the formula (6.7) reads
\[24v_4 = -\bar{\nabla}_0^2 (\overline{\text{Ric}})_{00} + 3(\overline{\text{Ric}}_{00})^2 - 2(\bar{G}, \bar{G}).\]

As above, we obtain
\[24v_4 = -|P|^2 + 3J^2 - 2|P|^2\]
using the fact that \( \bar{G} = P \) implies \( \overline{\text{Ric}}_{00} = J \). This yields the well-known formula
\[v_4 = \frac{1}{8} (J^2 - |P|^2).\]

**6.3 Evaluation I**

Now we combine the formula (6.1) for \( B_3 \) with the results in Sect. 6.2. A calculation yields the following result.

**Lemma 6.10** \( 12B_3 \) equals the sum of
\begin{align*}
&\left(\bar{\nabla}_0^2 (\overline{\text{Ric}})_{00} - \frac{1}{2}\overline{\text{scal}}\right) + 5H \left(\bar{\nabla}_0 (\overline{\text{Ric}})_{00} - \frac{1}{2}\overline{\text{scal}}\right) + 2H \bar{\nabla}_0 (\overline{\text{Ric}})_{00} \\
&+ 2|\hat{G}|^2 - 2(\overline{\text{Ric}}_{00})^2 + 2\overline{\text{Ric}}_{00}J + 8H^2 \overline{\text{Ric}}_{00} - 12H^2 J + 6(dH, \overline{\text{Ric}}_0) + 2\Delta(\overline{\text{Ric}}_0), \quad (6.9) \\
&- 2\hat{L}^i j \bar{\nabla}_0 (\overline{R})_{0k,j0} - 2H (\hat{L}, \hat{G}) + 8(\hat{L}^2, \hat{G}) - 4|\hat{L}|^2 \overline{\text{Ric}}_{00} + 2|\hat{L}|^2 J \quad (6.10)
\end{align*}

and
\[\Delta(|\hat{L}|^2) + 6(\hat{L}, \text{Hess}(H)) + 6H \operatorname{tr}(\hat{L}^3) + |\hat{L}|^4 + 12|dH|^2. \quad (6.11)\]

Since the terms in (6.9) and (6.10) vanish for the flat metric, we immediately reproduced formula (4.10). For later reference, we formulate that result as

**Corollary 6.11** For a hypersurface \( M \) in the flat background \( \mathbb{R}^4 \), the obstruction \( B_3 \) is given by
\[\Delta(|\hat{L}|^2) + 6(\hat{L}, \text{Hess}(H)) + 6H \operatorname{tr}(\hat{L}^3) + |\hat{L}|^4 + 12|dH|^2. \quad (6.12)\]
We continue with the discussion of the curved case.

Next, we simplify the sum (6.9) using the second Bianchi identity. This step is analogous to the usage of the second Bianchi identity in Sect. 5.

Let \( \tilde{G} \equiv \tilde{\text{Ric}} - \frac{1}{2} \text{scal} g \) be the Einstein tensor of \( g \). The second Bianchi identity implies \( 2\delta^g(\tilde{\text{Ric}}) = d\text{scal} \). Hence

\[
\tilde{\nabla}_0(\tilde{\text{Ric}})(\partial_0, \partial_0) = \delta^g(\tilde{\text{Ric}})(\partial_0, \partial_0) - g^{ij} \tilde{\nabla}_{\partial_i}(\tilde{\text{Ric}})(\partial_j, \partial_0)
\]

\[
= \frac{1}{2} (d\text{scal}, \partial_0) - g^{ij} \partial_i(\tilde{\text{Ric}}(\partial_j, \partial_0)) + g^{ij} \tilde{\text{Ric}}(\tilde{\nabla}_{\partial_i}(\partial_j), \partial_0) + g^{ij} \tilde{\text{Ric}}(\partial_j, \tilde{\nabla}_{\partial_i}(\partial_0))
\]

\[
= \frac{1}{2} (d\text{scal}, \partial_0) - h^r_{ij} \partial_i(\tilde{\text{Ric}}(\partial_j, \partial_0)) + h^r_{ij} \tilde{\text{Ric}}(\tilde{\nabla}^{h_r}_{\partial_i}(\partial_j))
\]

\[
- (L_r)_{ij} \partial_0, \partial_0) + h^r_{ij} \tilde{\text{Ric}}(\partial_j, \tilde{\nabla}_{\partial_i}(\partial_0))
\]

\[
= \frac{1}{2} (d\text{scal}, \partial_0) - \delta^{h_r}(\tilde{\text{Ric}}_0) - nH_r \tilde{\text{Ric}}_{00} + h^r_{ij} \tilde{\text{Ric}}(\partial_j, \tilde{\nabla}_{\partial_i}(\partial_0)),
\]

on any level surface of \( r \). Here \( \delta^{h_r} \) denotes the divergence operator for the induced metric on the level surfaces of \( r \). Similarly, \( L_r \) and \( H_r \) are the second fundamental form and the mean curvature of these level surfaces. Therefore, using \( \tilde{\nabla}_{\partial_i}(\partial_0) = (L_r)_{ia} h^r_{ak} \partial_k \), we obtain

\[
\tilde{\nabla}_0(\tilde{G})_{00} = -\delta^{h_r}(\tilde{\text{Ric}}_0) - nH_r \tilde{\text{Ric}}_{00} + h^r_{ij} h^r_{ak} (L_r)_{ia} \tilde{\text{Ric}}_{jk},
\]

i.e., we have proved the relation

\[
\tilde{\nabla}_0(\tilde{G})_{00} = -\delta^{h_r}(\tilde{\text{Ric}}_0) - nH_r \tilde{\text{Ric}}_{00} + (L_r, \tilde{\text{Ric}})_{hr}
\]

(6.13)

on any level surface of \( r \). Differentiating the identity (6.13) (for \( n = 3 \)) with respect to \( r \) at \( r = 0 \) gives a formula for the term

\[
\tilde{\nabla}_0^2(\tilde{\text{Ric}})_{00} - \frac{1}{2} \text{scal}'' = \tilde{\nabla}_0^2(\tilde{G})_{00} = \partial_r(\tilde{\nabla}_0(\tilde{G})_{00})
\]

for \( r = 0 \). For that purpose, we use the variation formulas

\[
3H' = -|L|^2 - \tilde{\text{Ric}}_{00},
\]

\[
L' = L^2 - \tilde{G}
\]

(6.14)

for the variation of these quantities under the normal exponential map. Here we denote the derivative in \( r \) by a prime. We recall that in normal geodesic coordinates the metric \( g \) takes the form \( dr^2 + h_r \) with \( h_r = h + 2rL + \cdots \). Moreover, let \( \delta' \equiv (d/dr)|_0(\delta^{h_r}) \). Then

\[
\delta'(\omega) = -2(L, \nabla(\omega))_h - 2(\delta(L), \omega)_h + 3(dH, \omega)_h
\]

(6.15)
for \( \omega \in \Omega^1(M^3) \) [5, (1.185)]. Note that the latter identity fits with the variation formula (6.2). Now differentiating (6.13) for \( n = 3 \) implies

\[
\tilde{\nabla}_0^2 (\tilde{G})_{00} = -\delta' (\tilde{\text{Ric}}_0) - \delta (\partial_r (\tilde{\text{Ric}}_0)) - 3H \tilde{\text{Ric}}_0 - 3H \tilde{\nabla}_0 (\tilde{\text{Ric}})_0
\]
\[
+ (L', \tilde{\text{Ric}}) + L_{ij} \partial_r (\tilde{\text{Ric}}_{ij}) - 4(L^2, \tilde{\text{Ric}}),
\]

where \( L' = (d/dr)_{0}(L_r) \). Hence

\[
\tilde{\nabla}_0^2 (\tilde{G})_{00} = 2(L, \nabla (\tilde{\text{Ric}}_0)) + 2(\delta (L), \tilde{\text{Ric}}_0) - 3(dH, \tilde{\text{Ric}}_0)
\]
\[
- \delta (\tilde{\nabla}_0 (\tilde{\text{Ric}})_0) - \delta (L \tilde{\text{Ric}}_0) + |L|^2 \tilde{\text{Ric}}_0 + (\tilde{\text{Ric}}_0)^2 - 3H \tilde{\nabla}_0 (\tilde{\text{Ric}})_0
\]
\[
- 3(L^2, \tilde{\text{Ric}}) - (\tilde{g}, \tilde{\text{Ric}}) + (L, \tilde{\nabla}_0 (\tilde{\text{Ric}})) + 2(L^2, \tilde{\text{Ric}})
\]

(6.16)

at \( r = 0 \). Here we used the relations

\[
\tilde{\nabla}_0 (\tilde{\text{Ric}}_0) = \partial_r (\tilde{\text{Ric}}_{00}) - (L \tilde{\text{Ric}})_0,
\]
\[
\tilde{\nabla}_0 (\tilde{\text{Ric}})_{ij} = \partial_r (\tilde{\text{Ric}}_{ij}) - (L \tilde{\text{Ric}} + \tilde{\text{Ric}}L)_{ij}.
\]

Now separating the trace-free part of \( L \) in some terms we obtain

\[
\tilde{\nabla}_0^2 (\tilde{G})_{00} = 2(L, \nabla (\tilde{\text{Ric}}_0)) + 2H \delta (\tilde{\text{Ric}}_0) + 2(\delta (L), \tilde{\text{Ric}}_0) - (dH, \tilde{\text{Ric}}_0)
\]
\[
- \delta (\tilde{\nabla}_0 (\tilde{\text{Ric}})_0) - \delta (L \tilde{\text{Ric}}_0) + |L|^2 \tilde{\text{Ric}}_0 + (\tilde{\text{Ric}}_0)^2 - 3H \tilde{\nabla}_0 \tilde{\text{Ric}}_0
\]
\[
- (L^2, \tilde{\text{Ric}}) - (\tilde{g}, \tilde{\text{Ric}}) + (L, \tilde{\nabla}_0 (\tilde{\text{Ric}})) + H \text{scal}' - H \tilde{\nabla}_0 (\tilde{\text{Ric}})_0.
\]

This leads to the following result.

**Lemma 6.12** Let \( n = 3 \). Then

\[
\tilde{\nabla}_0^2 (\tilde{G})_{00} = -4H \tilde{\nabla}_0 (\tilde{\text{Ric}})_0 + H \text{scal}'
\]
\[
+ 2(L, \nabla (\tilde{\text{Ric}}_0)) - \delta (\tilde{\nabla}_0 (\tilde{\text{Ric}})_0) + (L, \tilde{\nabla}_0 (\tilde{\text{Ric}}))
\]
\[
+ H \delta (\tilde{\text{Ric}}_0) - 2(dH, \tilde{\text{Ric}}_0) + 2(\delta (L), \tilde{\text{Ric}}_0) - \delta (L \tilde{\text{Ric}}_0)
\]
\[
+ |L|^2 \tilde{\text{Ric}}_0 - (L^2, \tilde{\text{Ric}}) + (\tilde{\text{Ric}}_0)^2 - (\tilde{g}, \tilde{\text{Ric}}).
\]

Lemma 6.12 enables us to replace second-order normal derivatives in Lemma 6.10 by first-order normal and tangential derivatives. More precisely, it follows that (6.9) equals

\[
3H \tilde{\nabla}_0 (\tilde{G})_{00} + 2(L, \nabla (\tilde{\text{Ric}}_0)) - \delta (\tilde{\nabla}_0 (\tilde{\text{Ric}})_0) + (L, \tilde{\nabla}_0 (\tilde{\text{Ric}}))
\]
\[
+ H \delta (\tilde{\text{Ric}}_0) + 4(dH, \tilde{\text{Ric}}_0) + 2(\delta (L), \tilde{\text{Ric}}_0) - \delta (L \tilde{\text{Ric}}_0)
\]
\[
+ |L|^2 \tilde{\text{Ric}}_0 - (L^2, \tilde{\text{Ric}}) + (\tilde{\text{Ric}}_0)^2 - (\tilde{g}, \tilde{\text{Ric}})
\]
\[
+ 2|\tilde{g}|^2 - 2(\tilde{\text{Ric}}_0)^2 + 2\tilde{\text{Ric}}_0 \tilde{J} + 2\Delta (\tilde{\text{P}}_0) + 8H^2 \tilde{\text{Ric}}_0 - 12H^2 \tilde{J}.
\]
Now a second application of the second Bianchi identity \((6.13)\) enables us to replace the first-order normal derivative of the Einstein tensor in this formula by tangential derivatives. Hence \((6.9)\) equals the sum
\[
-3H\delta(Rc_0) - 9H^2Rc_{00} + 3H(L, Rc) \\
+ 2(\hat{L}, \nabla(Rc_0)) - \delta(\hat{V}_0(Rc_0)) + (\hat{L}, \hat{V}_0(Rc)) \\
+ H\delta(Rc_0) + 4(dH, Rc_0) + 2(\delta(\hat{L}), Rc_0) - \delta((\hat{L}Rc_0) \\
+ |L|^2Rc_{00} - (L^2, Rc) + (Rc_{00})^2 - (\hat{G}, Rc) \\
+ 2|\hat{G}|^2 - 2(Rc_{00})^2 + 2Rc_{00}\hat{J} + 2\Delta(\hat{P}_0) + 8H^2Rc_{00} - 12H^2\hat{J}.
\]
A slight reordering and simplification of this sum shows that the sum \((6.9)\) equals
\[
-\delta(\hat{V}_0(Rc_0)) - 2H\delta(Rc_0) + 4(dH, Rc_0) \\
+ (\hat{L}, \nabla(Rc)) + 2(\hat{L}, \nabla(Rc_0)) + 2(\delta(\hat{L}), Rc_0) - \delta((\hat{L}Rc_0) \\
+ |L|^2Rc_{00} - (L^2, Rc) + 3H(L, Rc) \\
- (Rc_{00})^2 - (\hat{G}, Rc) + 2|\hat{G}|^2 + 2Rc_{00}\hat{J} + 2\Delta(\hat{P}_0) - H^2Rc_{00} - 12H^2\hat{J}.
\]
\[(6.17)\]

We continue by further simplifying the sum \((6.17)\). First of all, we observe

**Lemma 6.13** Let \(n = 3\). Then
\[-(Rc_{00})^2 - (\hat{G}, Rc) + 2|\hat{G}|^2 + 2Rc_{00}\hat{J} = 2(\hat{P}, \hat{V}) + 2|\hat{V}|^2.\]

**Proof** We recall that \(\hat{G}_{ij} = \hat{P}_{ij} + \hat{P}_{00}h_{ij} + \hat{V}_{ij}\). Therefore, we get \(Rc_{ij} = 2\hat{P}_{ij} + \hat{J}h_{ij} = 2\hat{G}_{ij} - 2\hat{V}_{ij} - (2\hat{P}_{00} - \hat{J})h_{ij}\). Thus \((\hat{G}, Rc) = 2(\hat{G}, \hat{G}) - 2(\hat{G}, \hat{V}) - (2\hat{P}_{00} - \hat{J})Rc_{00}\). This relation implies
\[2|\hat{G}|^2 - (\hat{G}, Rc) = (2\hat{P}_{00} - \hat{J})Rc_{00} + 2(\hat{G}, \hat{V}) = (Rc_{00})^2 - 2Rc_{00}\hat{J} + 2(\hat{P}, \hat{V}) + 2|\hat{V}|^2.\]

The proof is complete. \(\square\)

Next, we have the following identities.

**Lemma 6.14** Let \(n = 3\). Then
\[|L|^2Rc_{00} - (L^2, Rc) = |\hat{L}|^2Rc_{00} - (\hat{L}^2, Rc) - 2H(\hat{L}, Rc) + 4H^2Rc_{00} - 6H^2\hat{J},\]
and
\[(L, Rc) = (\hat{L}, Rc) + 6H\hat{J} - H\hat{Rc}_{00}.\]

**Proof** The assertions follow by direct calculation. \(\square\)
By Lemmas 6.13 and 6.14, the last two lines of (6.17) simplify to
\[ |\hat{L}|^2 \overline{\text{Ric}}_{00} - (\hat{L}^2, \overline{\text{Ric}}) + H(\hat{L}, \overline{\text{Ric}}) + 2\Delta(\overline{P}_{00}) + 2(\overline{P}, \overline{\nabla}) + 2|\overline{\nabla}|^2. \]

Therefore, (6.9) equals
\[
-\delta(\overline{\nabla}_0(\overline{\text{Ric}})_{00}) - 2H\delta(\overline{\text{Ric}}_{00}) + 6(dH, \overline{\text{Ric}}_{00}) + 2\Delta(\overline{P}_{00}), (\hat{L}, \overline{\nabla}_0(\overline{\text{Ric}})_{00}) (6.18)
\]
\[
-2\hat{L}^{ij}\overline{\nabla}_0(\overline{\text{Ric}})_{0ij0} + 2(\hat{L}, \overline{\nabla}(\overline{\text{Ric}}_{00})) + 2\delta(\hat{L}, \overline{\text{Ric}}_{00})
\]
\[
-\delta((\hat{L}\overline{\text{Ric}})_{00}) - 3|\hat{L}|^2\overline{\text{Ric}}_{00} - (\hat{L}^2, \overline{\text{Ric}}) + H(\hat{L}, \overline{\text{Ric}}), (6.19)
\]
\[
-2H(\hat{L}, \tilde{\mathcal{G}}) + 8(\hat{L}^2, \tilde{\mathcal{G}}) + 2|\hat{L}|^2\hat{J}, (6.20)
\]
\[
2(\overline{P}, \overline{\nabla}) + 2|\overline{\nabla}|^2 (6.21)
\]

and the flat terms
\[ 6(\hat{L}, \text{Hess}(H)) + \Delta(|\hat{L}|^2) + 6H \text{tr}(\hat{L}^3) + |\hat{L}|^4 + 12|dH|^2. \]

(6.22)

Note that the first term in (6.18) contains a normal derivative of \( \overline{\text{Ric}} \). Likewise the first two terms in (6.19) contain normal derivatives of the curvature of \( g \). All other terms in (6.18)–(6.22) live on \( M \). The mixed terms in (6.19) and (6.20) involve the curvature of \( g \) and \( L \). Finally, the terms in (6.21) involve the Weyl tensor, and the terms in (6.22) are completely determined by \( L \).

**Example 6.16** If the background metric \( g \) is Einstein, i.e., if \( \overline{\text{Ric}} = \lambda g \), then
\[
12\mathcal{B}_3 = -2\hat{L}^{ij}\overline{\nabla}_0(\overline{\nabla})_{0ij0} - 2H(\hat{L}, \overline{\nabla}) + 8(\hat{L}^2, \overline{\nabla}) + 2|\overline{\nabla}|^2
\]
\[
+ 6(\hat{L}, \text{Hess}(H)) + \Delta(|\hat{L}|^2) + 6H \text{tr}(\hat{L}^3) + |\hat{L}|^4 + 12|dH|^2.
\]

Of course, if in addition \( \overline{\mathcal{W}} = 0 \), then this formula reduces to Corollary 6.11.

**Proof** The assumption implies \( \hat{J} = \frac{2}{3}\lambda, \overline{\mathcal{P}} = \frac{1}{6}\lambda g, \tilde{\mathcal{G}} = \frac{1}{3}\lambda h + \overline{\nabla} \) and \( |\tilde{\mathcal{G}}|^2 = \frac{1}{3}\lambda^2 + |\overline{\nabla}|^2 \). Furthermore, the terms in (6.18) and the terms in the first line of (6.19) except the second one vanish. The remaining terms in (6.19)–(6.21) read
\[
-3\lambda|\hat{L}|^2 - \lambda|\hat{L}|^2 - 2H(\hat{L}, \overline{\nabla}) + \frac{8}{3}\lambda|\hat{L}|^2 + 8(\hat{L}^2, \overline{\nabla}) + \frac{4}{3}\lambda|\hat{L}|^2 + 2|\overline{\nabla}|^2.
\]

Simplification proves the claim. □
6.4 Evaluation II

We further simplify Lemma 6.15. The following result shows that, up to some contributions of the Weyl tensor, the first two terms in (6.19) cancel and that the last term of (6.19) cancels against the first term of (6.20).

**Lemma 6.17** Let \( n = 3 \). Then it holds

\[
\langle \hat{L}, \tilde{\nabla}_0(\tilde{\text{Ric}}) \rangle + 2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{W})_{0ij0} = 2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{R})_{0ij0},
\]

\[
\langle \hat{L}, \text{Ric} \rangle + 2(\hat{L}, \tilde{W}) = 2(\hat{L}, \tilde{G}).
\]

**Proof** By the Kulkarni–Nomizu decomposition \( R = -P \otimes g + W \), we have

\[
\tilde{G}_{ij} = \tilde{R}_{0ij0} = \tilde{p}_{ij} + \tilde{p}_{00}(h_r)_{ij} + \tilde{W}_{0ij0}.
\]

Hence using

\[
\tilde{\nabla}_0(\tilde{R})_{0ij0} = \partial_0(\tilde{R}_{0ij0}) - \tilde{R}(\partial_0, \tilde{\nabla}_0(\partial_i), \partial_j, \partial_0) - \tilde{R}(\partial_0, \partial_i, \tilde{\nabla}_0(\partial_j), \partial_0)
\]

and similarly for \( \tilde{W} \) as well as \( \tilde{\nabla}_0(\partial_i) = L^k_i \partial_k \) we find

\[
\tilde{\nabla}_0(\tilde{R})_{0ij0} - \tilde{\nabla}_0(\tilde{W})_{0ij0} = \partial_0(\tilde{p}_{ij}) + \partial_0(\tilde{p}_{00})h_{ij} + \tilde{p}_{00}h'_{ij}
\]

\[
- \tilde{p}(\tilde{\nabla}_0(\partial_i), \partial_j) - \tilde{p}(\partial_i, \tilde{\nabla}_0(\partial_j))
\]

\[
- \tilde{p}_{00}h(\tilde{\nabla}_0(\partial_i), \partial_j) - \tilde{p}_{00}h(\partial_i, \tilde{\nabla}_0(\partial_j))
\]

\[
= \tilde{\nabla}_0(\tilde{p})_{ij} + \partial_0(\tilde{p}_{00})h_{ij} + 2\tilde{p}_{00}L_{ij} - 2\tilde{p}_{00}L_{ij}
\]

\[
= \tilde{\nabla}_0(\tilde{p})_{ij} + \partial_0(\tilde{p}_{00})h_{ij}
\]

for \( r = 0 \). Therefore,

\[
2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{R})_{0ij0} = 2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{p})_{ij} + 2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{W})_{0ij0} = \hat{L}^{ij}\tilde{\nabla}_0(\tilde{\text{Ric}})_{ij} + 2\hat{L}^{ij}\tilde{\nabla}_0(\tilde{W})_{0ij0}.
\]

This proves the first identity. The second identity follows from the decomposition \( \tilde{G} = \tilde{P} + \tilde{p}_{00}h + \tilde{W} \). \( \square \)

Next, we evaluate the first term of (6.18).

**Lemma 6.18** In general dimensions, it holds

\[
\delta(\tilde{\nabla}_0(\text{Ric})).c = \frac{1}{2} \Delta(\text{scal}) - n\delta(H\text{Ric})_0 - \delta((L\text{Ric})_0) - \delta(\text{Ric}). (6.23)
\]

**Proof** The result follows from the second Bianchi identity. Combining the identity

\[
\tilde{\nabla}_0(\text{Ric})(\partial_0, \partial_a) = \delta^g(\text{Ric})(\partial_a) - h^{ij}\tilde{\nabla}_0(\text{Ric})(\partial_j, \partial_a)
\]

on \( M \) with \( 2\delta^g(\text{Ric}^g) = d \text{scal}^g \), we obtain

\[
\delta(\tilde{\nabla}_0(\text{Ric})).c = \frac{1}{2} \Delta(\text{scal}) - n\delta(H\text{Ric})_0 - \delta((L\text{Ric})_0) - \delta(\text{Ric}).
\]
\[\bar{\nabla}_0 (\text{Ric}) (\partial_0, \partial_a) = \frac{1}{2} \langle d \text{scal}, \partial_a \rangle - h^{ij} \partial_i (\text{Ric} (\partial_j, \partial_a))
\]
\[+ h^{ij} \text{Ric} (\bar{\nabla}_a (\partial_j), \partial_a) + h^{ij} \text{Ric} (\partial_j, \bar{\nabla}_a (\partial_a))
\]
\[= \frac{1}{2} \langle d \text{scal}, \partial_a \rangle - h^{ij} \partial_i (\text{Ric} (\partial_j, \partial_a))
\]
\[+ h^{ij} \text{Ric} (\partial_j, \bar{\nabla}_a (\partial_a) - L_{ia} \partial_0)
\]
\[= \frac{1}{2} \langle d \text{scal}, \partial_a \rangle - \delta^h (\text{Ric}) (\partial_a) - h H \text{Ric} (\partial_0, \partial_a) - h^{ij} L_{ia} \text{Ric} (\partial_j, \partial_0).
\]

Now we apply \(\delta = \delta^h\) to this identity of 1-forms on \(M\). We obtain
\[
\delta (\bar{\nabla}_0 (\text{Ric})_0) = \frac{1}{2} \Delta (\text{scal}) - \delta \delta (\text{Ric}) - n \delta (H \text{Ric}_0) - \delta ((L \text{Ric})_0).
\]

The proof is complete. \(\square\)

In order to apply Lemma 6.18, we combine it with the following formula for the last term on the right-hand side of (6.23).

Lemma 6.19 Let \(n = 3\). Then
\[
\delta \delta (\text{Ric}) = 2 \Delta (J) + \Delta (\bar{J}) - \Delta (H^2) - 2 \Delta \delta (H \bar{L}) + 2 \delta \delta (\bar{L}^2) - \frac{1}{2} \Delta (|\bar{L}|^2) + 2 \delta \delta (\bar{W}).
\]

Proof First, we note that
\[
\delta \delta (\text{Ric}) = 2 \delta \delta (\bar{P}) + \delta \delta (\bar{J} H) = 2 \delta \delta (\bar{P}) + \Delta (\bar{J}).
\]

Now we utilize the identity (3.7). It follows that
\[
2 \delta \delta (\bar{P}) = 2 \delta \delta (P) - 2 \delta \delta (H \bar{L}) - \Delta (H^2) + 2 \delta \delta (\bar{L}^2) - \frac{1}{2} \Delta (|\bar{L}|^2) + 2 \delta \delta (\bar{W}).
\]

Combining these results with \(\delta (P) = dJ\) proves the assertion. \(\square\)

Now, combining Lemmas 6.18 and 6.19 with the Gauss identity
\[
\bar{J} - J = \bar{P}_{00} + 1/4 |\bar{L}|^2 - 3/2 H^2,
\]
gives
\[
\delta (\bar{\nabla}_0 (\text{Ric})_0) = 2 \Delta (\bar{J} - J) - 3 \delta (H \text{Ric}_0) - \delta ((L \text{Ric})_0)
\]
\[+ \Delta (H^2) + 2 \delta \delta (H \bar{L}) - 2 \delta \delta (\bar{L}^2) - \frac{1}{2} \Delta (|\bar{L}|^2) - 2 \delta \delta (\bar{W})
\]
\[= 2 \Delta (\bar{P}_{00}) + \Delta (|\bar{L}|^2) - 2 \Delta (H^2) - 3 \delta (H \text{Ric}_0) - \delta ((L \text{Ric})_0)
\]
\[+ 2 \delta \delta (H \bar{L}) - 2 \delta \delta (\bar{L}^2) - 2 \delta \delta (\bar{W}).
\]
This result shows that (6.18) equals
\[
- \Delta (|L|^2) - 2\delta \delta (H L) + 2\delta \delta (\hat{L}^2) + 2\Delta (H^2) + \delta (H \hat{\text{Ric}}_0) + \delta ((L \hat{\text{Ric}})_0) + 6(d H, \hat{\text{Ric}}_0) + 2\delta \delta (\hat{W}).
\] (6.25)

**Remark 6.20** The identity (6.24) shows that
\[
\Delta (|L|^2) - 2\delta \delta (\hat{L}^2) + 2\delta \delta (H \hat{L}) - 2\Delta (H^2) = 0
\]
for a flat background. This relation also is a consequence of the difference formula (3.18) and the identity
\[
\delta \delta (H \hat{L}) = (\hat{L}, \text{Hess}(H)) + 4|d H|^2 + 2 H \Delta (H),
\] (6.26)
which is a consequence of Lemma 6.21 and the Codazzi–Mainardi equation \(\delta (\hat{L}) = 2d H\) for a flat background. More generally, if \(g\) is Einstein, i.e., if \(\hat{\text{Ric}} = \lambda g\), then \(\hat{\text{Ric}}_0 = 0\) and the identity (6.24) implies
\[
\Delta (|L|^2) - 2\delta \delta (\hat{L}^2) + 2\delta \delta (H \hat{L}) - 2\Delta (H^2) - 2\delta \delta (\hat{W}) = 0.
\]
By combination with the Codazzi–Mainardi relation \(\delta (\hat{L}) = 2d H\), Lemmas 3.14 and 6.21, we conclude the interesting identity
\[
-2\hat{L}^{ij} \nabla^k \hat{W}_{kij0} + |\hat{W}_0|^2 - 2\delta \delta (\hat{W}) = 0.
\]

**Lemma 6.21** In general dimensions, it holds
\[
\delta \delta (H \hat{L}) = (\hat{L}, \text{Hess}(H)) + 2(d H, \delta (\hat{L})) + H \delta \delta (\hat{L}).
\]

**Proof** The identity is obvious. \(\square\)

Now we combine formula (6.25) with (6.19)–(6.22). Note that the term \(\delta ((L \hat{\text{Ric}})_0)\) in (6.25) sums up with the fifth term in (6.19) to \(\delta (H \hat{\text{Ric}}_0)\) and that the term \(-\Delta (|L|^2)\) in (6.25) cancels with the term \(\Delta (|\hat{L}|^2)\) in (6.22). We also use Lemma 6.21.

By Lemmas 6.17–6.21, the formula in Lemma 6.15 turns into the sum of
\[
2\Delta (H^2) + 2\delta (H \hat{\text{Ric}}_0) \overset{!}{=} 2\delta (H \delta (\hat{L})) = 2 H \delta \delta (\hat{L}) + 2, (d H, \delta (\hat{L}))
\] (6.27)
(by Codazzi–Mainardi \(\hat{\text{Ric}}_0 = \delta (\hat{L}) - 2d H\),
\[
6(d H, \hat{\text{Ric}}_0), -2\delta \delta (H \hat{L}) + 2\delta \delta (\hat{L}^2) + 2(\hat{L}, \nabla (\hat{\text{Ric}}_0)) + 2(\delta (\hat{L}), \hat{\text{Ric}}_0) - 3|\hat{L}|^2 \hat{\text{Ric}}_{00} - (\hat{L}^2, \hat{\text{Ric}})
\] \(\overset{!}{=} -2(\hat{L}, \text{Hess}(H)) - 4(d H, \delta (\hat{L})) + 2(\delta (\hat{L}), \hat{\text{Ric}}_0) - 2 H \delta \delta (\hat{L}) + 2 \delta \delta (\hat{L}^2)
\] + 2(\hat{L}, \nabla (\hat{\text{Ric}}_0)) - 3|\hat{L}|^2 \hat{\text{Ric}}_{00} - (\hat{L}^2, \hat{\text{Ric}}),
\] (6.28)
(by Lemma 6.21),

\[
8(\hat{L}^2, \hat{\mathcal{G}}) + 2|\hat{\mathcal{L}}|^2 \hat{\mathcal{J}} = 8(\hat{L}^2, \hat{\mathcal{P}}) + 8|\hat{\mathcal{L}}|^2 \hat{\mathcal{P}}_{00} + 2|\hat{\mathcal{L}}|^2 \hat{\mathcal{J}} + 8(\hat{L}^2, \hat{\mathcal{W}})
\]

(by \(\hat{\mathcal{G}} = \hat{\mathcal{P}} + \hat{\mathcal{P}}_{00}h + \hat{\mathcal{W}}\))

\[
= 4(\hat{L}^2, \hat{\text{Ric}}) - 2|\hat{\mathcal{L}}|^2 \hat{\mathcal{J}} + 8|\hat{\mathcal{L}}|^2 \hat{\mathcal{P}}_{00} + 8(\hat{L}^2, \hat{\mathcal{W}})
\]

\[
\frac{1}{4} = 4(\hat{L}^2, \hat{\text{Ric}}) - 6|\hat{\mathcal{L}}|^2 \hat{\mathcal{J}} + 4|\hat{\mathcal{L}}|^2 \hat{\text{Ric}}_{00} + 8(\hat{L}^2, \hat{\mathcal{W}}),
\]

\[
2(\hat{P}, \hat{\mathcal{W}}) + 2|\hat{\mathcal{W}}|^2 + 2\delta(\hat{\mathcal{W}}) - 2\hat{L}_{ij} \hat{\nabla}_0(\hat{\mathcal{W}})_{0ij0} - 2H(\hat{L}, \hat{\mathcal{W}}) = 8(\hat{\mathcal{L}}^2, \hat{\mathcal{W}})
\]

(6.29)

and

\[
6(\hat{\mathcal{L}}, \text{Hess}(H)) + 6H \text{tr}(\hat{\mathcal{L}}^3) + |\hat{\mathcal{L}}|^4 + 12|dH|^2.
\]

Note that the contributions \(2H\delta(\hat{\mathcal{L}})\) in (6.27) and (6.28) cancel.

By Codazzi–Mainardi, we find

\[
(\delta(\hat{\mathcal{L}}), \hat{\text{Ric}}_{0}) - (\delta(\hat{\mathcal{L}}), dH) = |\delta(\hat{\mathcal{L}})|^2 - 3(\delta(\hat{\mathcal{L}}), dH).
\]

Hence

\[
2(dH, \delta(\hat{\mathcal{L}})) - 4(dH, \delta(\hat{\mathcal{L}})) + 6(dH, \hat{\text{Ric}}_{0}) + 2(\delta(\hat{\mathcal{L}}), \hat{\text{Ric}}_{0}) = 2|\delta(\hat{\mathcal{L}})|^2 - 12|dH|^2.
\]

Thus, we have proved

**Proposition 6.22** 12\(\mathcal{B}_3\) equals the sum of

\[
2\delta(\hat{\mathcal{L}}^2) + 2|\delta(\hat{\mathcal{L}})|^2,
\]

\[
2(\hat{\mathcal{L}}, \nabla(\hat{\text{Ric}}_{0}))+ |\hat{\mathcal{L}}|^2 \hat{\text{Ric}}_{00} + 3(\hat{\mathcal{L}}^2, \hat{\text{Ric}}) - 6|\hat{\mathcal{L}}|^2 \hat{\mathcal{J}},
\]

(6.30)

the Weyl-curvature terms

\[
2(\hat{P}, \hat{\mathcal{W}}) + 2|\hat{\mathcal{W}}|^2 + 2\delta(\hat{\mathcal{W}}) - 2\hat{L}_{ij} \hat{\nabla}_0(\hat{\mathcal{W}})_{0ij0} - 2H(\hat{L}, \hat{\mathcal{W}}) + 8(\hat{\mathcal{L}}^2, \hat{\mathcal{W}})
\]

(6.31)

and

\[
4(\hat{\mathcal{L}}, \text{Hess}(H)) + 6H \text{tr}(\hat{\mathcal{L}}^3) + |\hat{\mathcal{L}}|^4.
\]

(6.32)

(6.33)

Note that there is no Laplace term in that formula.
6.5 Proof of the Main Result: Equivalences

Proposition 6.22 has the disadvantage that the conformal invariance of \( B_3 \) is not obvious. Therefore, it is natural to reformulate the results in a way which makes the conformal invariance transparent. For this purpose, we relate Proposition 6.22 to the formula

\[
12B_3 = 6D(( \tilde{L}^2 )_o) + 2|\tilde{L}|^4 + \star
= 6\delta\delta(\tilde{L}^2) - 2\Delta(|\tilde{L}|^2) + 6(\tilde{L}^2, P) - 2|\tilde{L}|^2 J + 2|\tilde{L}|^4 + \star
\]

(6.34)
in [8, Proposition 1.1], where

\[
\star \stackrel{\text{def}}{=} 2D(\bar{W}) + 4|\bar{W}|^2 + 2|\bar{W}_0|^2 - 2(\bar{L}, B) + 14(\bar{L}^2, \bar{W}) - 2\bar{L}^{ab}\bar{L}^{cd}\bar{W}_{cabd}.
\]

(6.35)

Here \( B \) is a certain conformally invariant symmetric bilinear form of weight \(-1\) which will be defined in (6.43). Here we took into account that in [8], the signs of the components of the curvature tensor and the Weyl tensor are opposite to ours. All terms in (6.35) are conformally invariant. The difference of both formulas is

\[
2(\Delta(|\tilde{L}|^2) - 2\delta\delta(\tilde{L}^2)) + 2|\delta(\tilde{L})|^2
+ 4(\tilde{L}, \mathrm{Hess}(H)) + 6H \mathrm{tr}(\tilde{L}^3) - |\tilde{L}|^4
+ 2(\tilde{L}, \nabla(\text{Ric}_0)) + |\tilde{L}|^2\text{Ric}_0 + 3(\tilde{L}^2, \text{Ric}) - 6|\tilde{L}|^2 J - 6(\tilde{L}^2, P) + 2|\tilde{L}|^2 J
+ 2(\bar{P}, \bar{W}) + 2|\bar{W}|^2 + 2\delta\delta(\bar{W}) - 2\tilde{L}^{ij}\bar{\nabla}_0(\bar{W})_{0ij0} - 2H(\tilde{L}, \bar{W}) + 8(\tilde{L}^2, \bar{W}) - \star.
\]

(6.36)

Lemma 6.23 The sum (6.36) vanishes.

In other words, Proposition 6.22 is equivalent to [8, Proposition 1.1]. The proof of this result will also establish the equivalence to Theorem 1.

Remark 6.24 Lemma 6.23 holds for a flat background metric. In this case \( \star = 0 \). In fact, the identity (3.7) implies

\[
6(\tilde{L}^2, P) - 2|\tilde{L}|^2 = 6H \mathrm{tr}(\tilde{L}^3) - |\tilde{L}|^4.
\]

(6.37)

By \( \delta(\tilde{L}) = 2dH \) (Codazzi–Mainardi), the sum (6.36) equals

\[
2(\Delta(|\tilde{L}|^2) - 2\delta\delta(\tilde{L}^2)) + 8|dH|^2
+ 4(\tilde{L}, \mathrm{Hess}(H)) + 6H \mathrm{tr}(\tilde{L}^3) - |\tilde{L}|^4 - 6H \mathrm{tr}(\tilde{L}^3) + |\tilde{L}|^4
= 2(\Delta(|\tilde{L}|^2) - 2\delta\delta(\tilde{L}^2)) + 8|dH|^2 + 4(\tilde{L}, \mathrm{Hess}(H)).
\]

The identity (3.18) shows that this sum vanishes.

\[\text{ Springer}\]
A key role in the argument in Remark 6.24 is played by the formula (3.18) for the divergence term $\Delta(|\hat{L}|^2) - 2\delta \delta(\hat{L}^2)$. Lemma 3.14 extends this result to general backgrounds. We also need the following curved analog of (6.37).

**Lemma 6.25** If $n = 3$, then it holds

$$6(\hat{L}^2, P) - 2|\hat{L}|^2 J = 6H \tr(\hat{L}^3) - |\hat{L}|^4 + 6(\hat{L}^2, \hat{P}) - 2|\hat{L}|^2 \bar{P} + 2|\hat{L}|^2 \bar{P}_{00} - 6(\hat{L}^2, \bar{W}).$$

**Proof** The identity (3.7) yields

$$t^* \hat{P} - P = \hat{L}^2 - \frac{1}{4} \hat{L}^2 h - H \hat{L} - \frac{1}{2} H^2 h + \bar{W}.$$

Taking the trace yields the Gauss identity

$$\bar{J} - \bar{P}_{00} - J = |\hat{L}|^2 - \frac{3}{4} |\hat{L}|^2 - \frac{3}{2} H^2 = \frac{1}{4} |\hat{L}|^2 - \frac{3}{2} H^2$$

(see (2.1)). These relations imply the assertion. \qed

Now, by Lemma 6.25, (6.36) simplifies to

$$2(\Delta(|\hat{L}|^2) - 2\delta \delta(\hat{L}^2)) + 2|\delta(\hat{L})|^2 + 4(\hat{L}, \text{Hess}(H))$$

$$+ 2(\hat{L}, \nabla(\overline{\text{Ric}}_0)) + |\hat{L}|^2 \overline{\text{Ric}}_{00} + 3(\hat{L}^2, \overline{\text{Ric}}) - 4|\hat{L}|^2 \bar{J} - 6(\hat{L}^2, \hat{P}) - 2|\hat{L}|^2 \bar{P}_{00}$$

$$+ 2(\hat{P}, \overline{W}) + 2|\overline{W}|^2 + 2\delta \delta(\overline{W}) - 2\hat{L}^i \overline{\nabla}_0(W)_{0i,j} - 2H(\hat{L}, \overline{W}) + 14(\hat{L}^2, \overline{W}) - \ast. \ (6.38)$$

But

$$|\hat{L}|^2 \overline{\text{Ric}}_{00} + 3(\hat{L}^2, \overline{\text{Ric}}) - 4|\hat{L}|^2 \bar{J} - 6(\hat{L}^2, \hat{P}) - 2|\hat{L}|^2 \bar{P}_{00} = 0,$$

i.e., the second last line of (6.38) reduces to $2(\hat{L}, \nabla(\overline{\text{Ric}}_0))$. Therefore, (6.36) further simplifies to

$$2(\Delta(|\hat{L}|^2) - 2\delta \delta(\hat{L}^2)) + 2|\delta(\hat{L})|^2 + 4(\hat{L}, \text{Hess}(H)) + 2(\hat{L}, \nabla(\overline{\text{Ric}}_0))$$

$$+ 2(\hat{P}, \overline{W}) + 2|\overline{W}|^2 + 2\delta \delta(\overline{W}) - 2\hat{L}^i \overline{\nabla}_0(W)_{0i,j} - 2H(\hat{L}, \overline{W}) + 14(\hat{L}^2, \overline{W}) - \ast.$$

Now, by Lemma 3.14, this sum equals

$$4\hat{L}^i \overline{\text{V}}^k \overline{W}_{ikj0} + 2|\overline{W}_{0i}|^2$$

$$+ 2(\hat{P}, \overline{W}) + 2|\overline{W}|^2 + 2\delta \delta(\overline{W}) - 2\hat{L}^i \overline{\nabla}_0(W)_{0i,j} - 2H(\hat{L}, \overline{W}) + 14(\hat{L}^2, \overline{W}) - \ast. \ (6.39)$$

Now we apply the identity

$$(\hat{P}, \overline{W}) = (P, \overline{W}) + (\hat{L}^2, \overline{W}) - H(\hat{L}, \overline{W}) + |\overline{W}|^2$$
(see (3.7)). Hence the sum (6.39) equals
\[
2\delta\delta(\mathcal{W}) + 2(P, \mathcal{W}) - 2\hat{L}^{ij} \hat{\nabla}_0(\mathcal{W})_{0ij0} - 4H(\hat{L}, \mathcal{W}) \\
+ 16(\hat{L}^2, \mathcal{W}) + 4|\mathcal{W}|^2 + 2|\mathcal{W}_0|^2 + 4\hat{L}^{ij} \nabla^k W_{ikj0} - \star.
\]

Therefore, Lemma 6.23 holds true iff
\[
\star = 2D(\mathcal{W}) - 2\hat{L}^{ij} \hat{\nabla}_0(\mathcal{W})_{0ij0} + 4\hat{L}^{ij} \nabla^k W_{ikj0} \\
- 4H(\hat{L}, \mathcal{W}) + 16(\hat{L}^2, \mathcal{W}) + 4|\mathcal{W}|^2 + 2|\mathcal{W}_0|^2. \tag{6.40}
\]

Equivalently, Lemma 6.23 holds true iff
\[
-2(\hat{L}, B) + 14(\hat{L}^2, \mathcal{W}) - 2\hat{L}^{ij} \hat{\nabla}^{kl} \mathcal{W}_{kijl} \\
= -2\hat{L}^{ij} \hat{\nabla}_0(\mathcal{W})_{0ij0} + 4\hat{L}^{ij} \nabla^k W_{ikj0} - 4H(\hat{L}, \mathcal{W}) + 16(\hat{L}^2, \mathcal{W}). \tag{6.41}
\]

It remains to prove (6.41). As a preparation, we observe

**Lemma 6.26** Let \( n = 3 \). Then
\[
\hat{L}^{ij} \hat{\nabla}^k W_{ikj0} = \hat{L}^{ij} \nabla^k W_{ikj0} + (\hat{L}^2, \mathcal{W}) - 3H(\hat{L}, \mathcal{W}) + \hat{L}^{ij} \hat{\nabla}^{kl} \mathcal{W}_{kijl}.
\]

**Proof** By \( \hat{\nabla}_i(\partial_j) = \nabla_i(\partial_j) - L_{ij} \partial_0 \) and \( \hat{\nabla}_k(\partial_0) = L^m_k \partial_m \), we find
\[
\hat{\nabla}^k W_{ikj0} = \nabla^k W_{ikj0} - L^{kl} \mathcal{W}_{kijl} + L^k_0 \mathcal{W}_{0k0j0} + 3H \mathcal{W}_0 W_{ij0} + L^k_0 \mathcal{W}_{ik00} \\
= \nabla^k W_{ikj0} + L^{kl} \mathcal{W}_{kijl} + L^k_0 \mathcal{W}_{0k0j0} - 3H \mathcal{W}_0 W_{ij0} \\
= \nabla^k W_{ikj0} + \hat{L}^{kl} \mathcal{W}_{kijl} - H \mathcal{W}_0 W_{ij0} + \hat{L}_0^k \mathcal{W}_{0k0j0} + H \mathcal{W}_0 W_{ij0} - 3H \mathcal{W}_0 W_{ij0} \\
= \nabla^k W_{ikj0} + \hat{L}^{kl} \mathcal{W}_{kijl} + \hat{L}_0^k \mathcal{W}_{0k0j0} - 3H \mathcal{W}_0 W_{ij0}.
\]

The assertion follows by contraction with \( \hat{L}^{ij} \).

**Lemma 6.27** It holds
\[
(\hat{L}, B) = \hat{L}^{ij} \hat{\nabla}_0(\mathcal{W})_{0ij0} + 2H(\hat{L}, \mathcal{W}) \\
-2\hat{L}^{ij} \nabla^k W_{jki0} - (\hat{L}^2, \mathcal{W}) - \hat{L}^{ij} \hat{\nabla}^{kl} \mathcal{W}_{kijl}. \tag{6.42}
\]

**Proof** We first restate the definition of \( B \) in our conventions\(^5\):
\[
B_{ij} = \hat{C}_{0(ij)} - H \mathcal{W}_{ij} + \nabla^k \mathcal{W}_{0(ijk)} \\
= \hat{\nabla}^k (\mathcal{W})_{0(ij)} - H \mathcal{W}_{ij} + \nabla^k \mathcal{W}_{0(ijk)}. \tag{6.43}
\]

\(^5\) We recall that our signs of the components of \( \mathcal{W} \) are opposite.
where
\[ C_{ijk} \overset{\text{def}}{=} \nabla_l (W)_{ijkl} \]
is the Cotton tensor (in dimension \( n = 4 \)). We emphasize that, in the definition (6.43) of \( B \), the index \( k \) in the first sum runs over the tangential and the normal vectors. \((ij)\) denotes symmetrization. We first verify that the symmetric tensor \( B \) satisfies the conformal transformation law \( e^{\varphi} \hat{B} = B \). For this purpose, we note that the well-known conformal transformation law
\[ e^{\varphi} \hat{C}_{ijk} = C_{ijk} + W_{ijkl} \partial_0(\varphi), \]
implies that in general dimensions \( \dim(M) = n \)
\[ e^{-2\varphi} \hat{W}_{ijkl} = \hat{W}_{ijkl} + (n - 4) \hat{W}_{ijkl} \partial_0(\varphi) - \hat{W}_{ijkl} \partial_0(\varphi). \]
Finally, let \( \hat{\partial}_0 = \partial_0 = e^{-\varphi} \partial_0 \). We calculate
\[ \hat{\nabla}^k \hat{W}_{0ijk} = g^k (e^{\varphi} \hat{W}_{0ijk}) - e^{\varphi} \hat{W} (\partial_0, \hat{\nabla}^k (\partial_i), \partial_j, \partial_k) - e^{\varphi} \hat{W} (\partial_0, \partial_i, \hat{\nabla}^k (\partial_j), \partial_k) - e^{\varphi} \hat{W} (\partial_0, \partial_i, \partial_j, \hat{\nabla}^k (\partial_k)). \]
Now the general transformation law
\[ \hat{\nabla}_i (\partial_j) = \nabla_i (\partial_j) + \partial_i (\varphi) \partial_j + \partial_j (\varphi) \partial_i - g_{ij} \partial_0, \]
implies that in general dimensions \( \dim(M) = n \)
\[ e^{-\varphi} \hat{\nabla}^k \hat{W}_{0ijk} = \nabla^k \hat{W}_{0ijk} + (n - 4) \hat{W}_{0ijk} \partial_0(\varphi) - \hat{W}_{0ijk} \partial_0(\varphi). \]
Hence for \( n = 3 \) we find
\[ e^{-\varphi} \hat{\nabla}^k \hat{W}_{0(ijk)k} = \nabla^k \hat{W}_{0(ijk)k} - \hat{W}_{0(ijk)k} \partial_0(\varphi). \]
Therefore,
\[ e^{\varphi} \hat{B}_{ij} = B_{ij} + \hat{W}_{0(ij)} \partial_0(\varphi) + \hat{W}_{ij} \partial_0(\varphi) - \hat{W}_{ij} \partial_0(\varphi) - \hat{W}_{0(ij)} \partial_0(\varphi) = B_{ij}. \]

\(^6\) That identity corrects [8, (2.10)].

\( \otimes \) Springer
Now the definition of $B$ gives

$$ (\hat{L}, B) \overset{\text{def}}{=} \hat{L}^{ij} \hat{\nabla}^{k}(\bar{W})_{0ijk} - H(\hat{L}, \bar{W}) + \hat{L}^{ij} \nabla^{k} \bar{W}_{0ij} $$

$$ = -\hat{L}^{ij} \hat{\nabla}^{k}(\bar{W})^{t}_{jki0} + \hat{L}^{ij} \hat{\nabla}^{0}(\bar{W})^{t}_{0ij0} - H(\hat{L}, \bar{W}) - \hat{L}^{ij} \nabla^{k} \bar{W}_{jki0}, $$

where the superscript $t$ in the first sum indicates that indices are only tangential. Now Lemma 6.26 yields

$$ (\hat{L}, B) = \hat{L}^{ij} \hat{\nabla}^{0}(\bar{W})_{0jki0} + 2H(\hat{L}, \bar{W}) - 2\hat{L}^{ij} \nabla^{k} \bar{W}_{jki0} - (\hat{L}^{2}, \bar{W}) - \hat{L}^{ij} \hat{\nabla}^{k} \bar{W}_{jkl}. $$

The proof of (6.42) is complete. \qed

Lemma 6.27 shows that

$$ -2(\hat{L}, B) = -2\hat{L}^{ij} \hat{\nabla}^{0}(\bar{W})_{0ij0} - 4H(\hat{L}, \bar{W}) $$

$$ + 4\hat{L}^{ij} \nabla^{k} \bar{W}_{jki0} + 2(\hat{L}^{2}, \bar{W}) + 2\hat{L}^{ij} \hat{\nabla}^{k} \bar{W}_{jkl}. $$

Hence

$$ -2(\hat{L}, B) + 14(\hat{L}^{2}, \bar{W}) - 2\hat{L}^{ij} \hat{\nabla}^{k} \bar{W}_{jkl} $$

$$ = 16(\hat{L}^{2}, \bar{W}) - 2\hat{\nabla}^{0}(\bar{W})_{0ij0} - 4H\bar{W}_{ij} + 4\hat{L}^{ij} \nabla^{k} \bar{W}_{jki0} $$

(note the cancellation!). This proves (6.41) and hence Lemma 6.23.

Now, in order to finish the Proof of Theorem 1, it suffices to combine (6.34) with (6.40).

**Remark 6.28** The formula for $B_3$ in the published version of [8] reads

$$ 12B_3 = 4D((\hat{L}^{2})_{o}) + 2D(\hat{F}) - 2(\hat{L}, B) + |\hat{L}|^4 + 4(\hat{F}, \hat{F}) + 2(\hat{\nabla}^{0}(\hat{L}^{2}), \bar{W}) + 2|\bar{W}_{0}|^2. $$

By $\hat{F} = (\hat{L}^{2})_{o} + \bar{W}$, this formula is equivalent to

$$ 12B_3 = 6D((\hat{L}^{2})_{o}) + 2D(\bar{W}) - 2(\hat{L}, B) + |\hat{L}|^4 + 2|\bar{W}_{0}|^2 $$

$$ + 2((\hat{L}^{2})_{o} + \bar{W}, \hat{L}^{2}) + 4((\hat{L}^{2})_{o} + \bar{W}, \hat{L}^{2} - \frac{1}{4}|\hat{L}|^2 h + \bar{W}). $$

The second line simplifies to

$$ |\hat{L}|^4 + 10(\hat{L}^{2}, \bar{W}) + 4|\bar{W}|^2. $$

If follows that the resulting formula for $12B_3$ differs from (6.34) and (6.35).

Finally, we note that for a conformally flat background, Theorem 1 states that

$$ 6B_3 = 3D((\hat{L}^{2})_{o}) + |\hat{L}|^4 = 3\delta\delta((\hat{L}^{2})_{o}) + 3((\hat{L}^{2})_{o}, P) + |\hat{L}|^4. $$
Lemma 3.13 implies that this formula is equivalent to
\[ 6B_3 = \Delta(|\hat{L}|^2) - |\nabla \hat{L}|^2 + 3/2|\delta(\hat{L})|^2 - 2J|\hat{L}|^2 + |\hat{L}|^4 \] (6.44)
(as also stated in [11, Proposition 2.10]).

7 Variational Aspects

Let \( \iota : M^3 \hookrightarrow X^4 \) be an embedding. In this section, we prove that the conformally invariant equation \( B_3 = 0 \) is the Euler–Lagrange equation of the conformally invariant functional
\[ W_3(\iota) \overset{\text{def}}{=} \int_{\iota(M)} (\text{tr}(\hat{L}^3) + (\hat{L}, \bar{\nabla})) \, d\text{vol} \] (7.1)
under normal variations of the embedding \( \iota \). Let \( u \in C^\infty (M) \) and \( \partial_0 \) be a unit normal field of \( M \). We set \( \iota_t(m) = \exp\left( tu(m)\partial_0 \right) \), where \( \exp \) is the exponential map. Then \( \iota_0 = \iota \) and \( \iota_t \) is a variation of \( M \) with variation field \( u\partial_0 \). Let \( M_t = \iota_t(M) \). Let \( W_3(\iota_t) \) be the analogous functional for \( \iota_t \) and define
\[ \text{var}(W_3)[u] \overset{\text{def}}{=} (d/dt)|_0(W_3(\iota_t)). \]

**Theorem 2** It holds
\[ -\text{var}(W_3)[u] = 6 \int_M uB_3 \, d\text{vol}. \]

This result reproves [8, Proposition 1.2]. Our arguments differ from those in the reference (see the comments after the proof).

**Proof** We first note that the variation of \( \int_M \text{tr}(\hat{L}^3) \, d\text{vol} \) has been determined in [20, Lemma 13.9.1] for conformally flat backgrounds. The given arguments easily extend to the general case and yield
\[ -\text{var} \left( \int_M \text{tr}(\hat{L}^3) \, d\text{vol}_h \right)[u] = 3 \int_M u \left( \delta\delta((\hat{L}^2)_o) + (\hat{L}_o, (\hat{L}_o)^2) + 2(\hat{L}_o, \bar{\nabla}) + \frac{1}{3} |\hat{L}|^4 \right) \, d\text{vol}_h \]
\[ = \int_M u \left( 3\mathcal{D}(\hat{L}_o) + 6(\hat{L}_o, \bar{\nabla}) + |\hat{L}|^4 \right) \, d\text{vol}_h. \]

In the second part of the proof, we determine the variation of \( \int_M (\hat{L}, \bar{\nabla}) \, d\text{vol}_h \). We write the integrand as \( h^{ai}h^{bj} \hat{L}_{ab} \bar{\nabla}_{ij} \) and apply the well-known variation formulas [4, Theorem 3-15], [16, Theorem 3.2]
\[ \text{var}(h)[u] = 2uL, \]
\[ \text{var}(L)[u] = -\text{Hess}(u) + uL^2 - u\bar{\nabla}, \]
\[ 3\text{var}(H)[u] = -\Delta(u) - u|L|^2 - uRic_{00} \]

and

\[ \text{var}(dvol_h)[u] = 3uHdvol_h. \]

It follows that the variation of \( \int_M (\hat{L}, \hat{W})dvol_h \) is given by the integral of the sum of

\[ -4u(\hat{L}^2, \hat{W}) - 4uH(\hat{L}, \hat{W}) \quad \text{(by variation of the metric)}, \quad (7.2) \]

\[ (\text{var}(\hat{L})[u], \hat{W}) = \hat{W}^{ij}(\text{var}(L)_{ij} - H\text{var}(h)_{ij}) \]

\[ = \hat{W}^{ij}(-\text{Hess}_{ij}(u) + u(L^2)_{ij} - u\check{g}_{ij}) - 2uH\hat{W}^{ij}L_{ij} \]

\[ = -(\text{Hess}(u), \hat{W}) + u(\hat{L}^2, \hat{W}) - u(\check{g}, \hat{W}) \quad (7.3) \]

(by variation of \( L \) and the metric),

\[ 3uH(\hat{L}, \hat{W}) \quad \text{(by variation of the volume form)} \]

(7.4)

and

\[ (\hat{L}, \text{var}(\hat{W})[u]) = \hat{L}^{ij}(d/dt)|_0 \hat{W}(N_t, \iota_{\tau_\ast}(\partial_i), \iota_{\tau_\ast}(\partial_j), N_t), \]

where \( N_t \) is the unit normal vector field of \( M_t \) that restricts to \( \partial_0 \) on \( M_0 \). In the following, we also identify \( \iota_{\tau_\ast}(\partial_i) \) with \( \partial_i \). Now we calculate

\[ \text{var}(\hat{W})_{ij}[u] = (d/dt)|_0 \hat{W}(N_t, \iota_{\tau_\ast}(\partial_i), \iota_{\tau_\ast}(\partial_j), N_t) \]

\[ = \nabla_{\iota_{\tau_\ast}(\partial_i)}(\hat{W})_{0j} + \hat{W}(\nabla_{\iota_{\tau_\ast}(\partial_i)}(N_t), \partial_j, \partial_0) + \hat{W}(\partial_0, \partial_j, \partial_0, (\nabla_{\iota_{\tau_\ast}(\partial_i)}(N_t))_0) 
\]

\[ + \hat{W}(\partial_0, \nabla_{\iota_{\tau_\ast}(\partial_i)}(\iota_{\tau_\ast}(\partial_j))_0, \partial_0, \partial_0) + \hat{W}(\partial_0, \partial_0, \partial_j, \partial_0) \]

By \( \nabla_{\iota_{\tau_\ast}(\partial_i)}(\iota_{\tau_\ast}(\partial_j))_0 = \nabla_{\iota_{\tau_\ast}(\partial_j)}(\iota_{\tau_\ast}(\partial_i)) = \nabla_{\partial_j}(u\partial_0) = \partial_j(u\partial_0) + u\nabla_{\partial_j}(\partial_0) = \partial_j(u\partial_0) + uL_k^i\partial_k \) and similarly for \( \nabla_{\iota_{\tau_\ast}(\partial_i)}(\iota_{\tau_\ast}(\partial_j))_0 \), we obtain

\[ \text{var}(\hat{W})_{ij}[u] = u\nabla_{\partial_0}(\hat{W})_{0i} + u(L_k^i\hat{W}_{0kj0} + L_k^j\hat{W}_{0ik0}) - \hat{W}_{\text{grad}(u)i}j0 - \hat{W}_{0i}\text{grad}(u) \]

(by variation of the normal vector field. Hence

\[ (\hat{L}, \text{var}(\hat{W})[u]) = u\hat{L}^{ij}\nabla_0(\hat{W})_{0i}j0 + uL^i_j(\hat{L}^k\hat{W}_{0kj0} + L^k_j\hat{W}_{0ik0}) - 2\hat{L}^{ij}\hat{W}_{\text{grad}(u)i}j0 \]

\[ = u\hat{L}^{ij}\nabla_0(\hat{W})_{0i}j0 + 2u(\hat{L}^2, \hat{W}) + 2uH(\hat{L}, \hat{W}) - 2\hat{L}^{ij}\hat{W}_{\text{grad}(u)i}j0. \quad (7.5) \]
Now using partial integration, we obtain

\[
\text{var} \left( \int_M (\vec{L}, \vec{\mathcal{W}}) d\text{vol}_h \right) [u] = \int_M u \left[ -\delta \mathcal{A}(\vec{\mathcal{W}}) - (\vec{L}^2, \vec{\mathcal{W}}) + H(\vec{L}, \vec{\mathcal{W}}) - (\vec{G}, \vec{\mathcal{W}}) + \hat{L}^{ij} \vec{\nabla}_0 (\vec{\mathcal{W}})_{0ij0} \right] d\text{vol}_h \\
- 2 \int_M \hat{L}^{ij} \vec{W}_{\text{grad}(u)ij0} d\text{vol}_h.
\]

Since

\[
(\vec{G}, \vec{\mathcal{W}}) = (\vec{P}, \vec{\mathcal{W}}) + (\vec{\mathcal{W}}, \vec{\mathcal{W}}) = (P, \mathcal{W}) - H(\vec{L}, \vec{\mathcal{W}}) + (\vec{L}^2, \vec{\mathcal{W}}) + 2|\mathcal{W}|^2
\]

by (3.7), we get

\[
\text{var} \left( \int_M (\vec{L}, \vec{\mathcal{W}}) d\text{vol}_h \right) [u] = \int_M u \left[ -\mathcal{D}(\vec{\mathcal{W}}) + 2H(\vec{L}, \vec{\mathcal{W}}) - 2(\vec{L}^2, \vec{\mathcal{W}}) - 2|\mathcal{W}|^2 + \hat{L}^{ij} \vec{\nabla}_0 (\vec{\mathcal{W}})_{0ij0} \right] d\text{vol}_h \\
- 2 \int_M (du, \hat{L}^{ij} \vec{W}_{ij0}) d\text{vol}_h.
\]

By partial integration, we find

\[
2 \int_M (du, \hat{L}^{ij} \vec{W}_{ij0}) d\text{vol}_h = -2 \int_M u \delta(\hat{L}^{ij} \vec{W}_{ij0}) d\text{vol}_h = -2 \int_M u \nabla^k (\hat{L}^{ij} \vec{W}_{kij0}) d\text{vol}_h \\
= -2 \int_M u \hat{L}^{ij} \nabla^k \vec{W}_{kij0} d\text{vol}_h + \int_M u |\vec{W}_0|^2 d\text{vol}_h
\]

using the trace-free Codazzi–Mainardi equation (3.9) (similarly as on page 11). Summarizing these results proves the claim. \(\square\)

Graham’s theorem [13, Theorem 3.1] and [20, (3.8)] imply that the variation of \(\int v_3 d\text{vol}\) equals \(4 \int uB_3 d\text{vol}\). Here the singular Yamabe renormalized volume coefficient \(v_3\) (as defined in [13]) satisfies

\[
12 \int_M v_3 d\text{vol} = -\int_M Q_3 d\text{vol} = -8 \int_M (\text{tr}(\hat{L}^3) + (\hat{L}, \vec{\mathcal{W}})) d\text{vol} = -8\mathcal{W}_3,
\]

where \(Q_3\) is the extrinsic \(Q\)-curvature (see [20, Example 13.10.2 and (13.10.7)]). In other words, the variation of \(\mathcal{W}_3\) equals \(-6 \int uB_3 d\text{vol}\). This shows that Theorem 2 fits with Graham’s theorem. On the other hand, [8, Proposition 1.2] states that the variation of \(\mathcal{W}_3\) equals \(6 \int uB_3 d\text{vol}\). The discrepancy of the sign is due to the altered definition of variations.

\(\square \) Springer
References

1. Abbena, E., Gray, A., Vanhecke, L.: Steiner’s formula for the volume of a parallel hypersurface in a Riemannian manifold. Ann. Sci. Norm. Sup. Pisa 8(3), 473–493 (1981)
2. Albin, P.: Poincaré-Lovelock metrics on conformally compact manifolds. Adv. Math. 367, 107108 (2020)
3. Andersson, L., Chruściel, P., Friedrich, H.: On the regularity of solutions to the Yamabe equation and the existence of smooth hyperboloidal initial data for Einstein’s field equations. Commun. Math. Phys. 149, 587–612 (1992)
4. Andrews, B.: Contraction of convex hypersurfaces in Riemannian spaces. J. Diff. Geom. 39, 407–431 (1994)
5. Besse, A.: Einstein Manifolds, Ergebnisse der Mathematik und ihrer Grenzgebiete, vol. 10. Springer, New York (1987)
6. Fefferman, C., Graham, C. R.: The Ambient Metric, Vol. 178. Princeton University Press (2012). arXiv:0710.0919
7. Fialkow, A.: Conformal differential geometry of a subspace. Trans. Am. Math. Soc. 56(2), 309–433 (1944)
8. Giaros, M., Gover, R., Halbasch, M., Waldron, A.: Singular Yamabe problem Willmore energies. J. Geom. Phys. 138, 168–193 (2019). arXiv:1508.01838v1
9. Gover, R.: Almost Einstein and Poincaré-Einstein manifolds in Riemannian signature. J. Geom. Phys. 60, 182–204 (2010). arXiv:0803.3510v1
10. Gover, R., Waldron, A.: Generalising the Willmore equation: submanifold conformal invariants from a boundary Yamabe problem. arXiv:1407.6742v1
11. Gover, R., Waldron, A.: Conformal hypersurface geometry via a boundary Loewner-Nirenberg-Yamabe problem, Commun. in Analysis and Geometry (to appear). arXiv:1506.02723v3
12. Gover, R., Waldron, A.: Renormalized volume. Commun. Math. Phys. 354(3), 1205–1244 (2017)
13. Graham, C.R.: Volume renormalization for singular Yamabe metrics. Proc. Am. Math. Soc. 145, 1781–1792 (2017). arXiv:1606.00069
14. Gover, R., Waldron, A.: Chern-Gauss-Bonnet formula for singular Yamabe metrics in dimension four. arXiv:1902.01562
15. Gray, A.: Tubes, Progress in Mathematics, vol. 221. Birkhäuser, Basel (2004)
16. Huisken, G., Polden, A.: Geometric evolution equations for hypersurfaces. In: Hildebrand, S., Struwe, M. (eds.) Calculus of Variations and Geometric Evolution Problems. Lecture Notes in Mathematics 1713, pp. 45–84. Springer, Berlin (1999)
17. Juhl, A.: Families of Conformally Covariant Differential Operators, Q-Curvature and Holography. Progress in Mathematics, vol. 275. Birkhäuser, Basel (2009)
18. Juhl, A.: Explicit formulas for GJMS-operators and Q-curvatures. Geom. Funct. Anal. 23(4), 278–1370 (2013). arXiv:1108.0273
19. Juhl, A., Ørsted, B.: Shift operators, residue families and degenerate Laplacians. Pac. J. Math. 308(1), 103–160 (2020). arXiv:1806.02556
20. Juhl, A., Ørsted, B.: Residue families, singular Yamabe problems and extrinsic conformal Laplacians. arXiv:2101.09027v1
21. Polyakov, A.: Fine structure of strings. Nucl. Phys. B 268, 406–412 (1986)
22. Schoen, R., Simon, L., Yau, S.-T.: Curvature estimates for minimal hypersurfaces. Acta Math. 134, 276–288 (1975)
23. Simons, J.: Minimal varieties in Riemannian manifolds. Ann. Math. 88(1), 62–105 (1968)
24. Soloduchin, S.N.: Boundary terms of conformal anomaly. Phys. Lett. B 752, 13–134 (2016)
25. Stafford, R.: Tractor Calculus and Invariants for Conformal Sub-Manifolds, Master’s thesis, University of Auckland, New Zealand (2005)
26. Vyatkin, Y.: Manufacturing Conformal Invariants of Hypersurfaces, PhD thesis, University of Auckland (2013)
27. Willmore, T.J.: Riemannian Geometry. Oxford Science Publications, Oxford (1993)

Publisher’s Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.