Abstract. We develop a universal distributional calculus for regulated volumes of metrics that are singular along hypersurfaces. When the hypersurface is a conformal infinity we give simple integrated distribution expressions for the divergences and anomaly of the regulated volume functional valid for any choice of regulator. For closed hypersurfaces or conformally compact geometries, methods from a previously developed boundary calculus for conformally compact manifolds can be applied to give explicit holographic formulae for the divergences and anomaly expressed as hypersurface integrals over local quantities (the method also extends to non-closed hypersurfaces). The resulting anomaly does not depend on any particular choice of regulator, while the regulator dependence of the divergences is precisely captured by these formulæ. Conformal hypersurface invariants can be studied by demanding that the singular metric obey, smoothly and formally to a suitable order, a Yamabe type problem with boundary data along the conformal infinity. We prove that the volume anomaly for these singular Yamabe solutions is a conformally invariant integral of a local $Q$-curvature that generalizes the Branson $Q$-curvature by including data of the embedding. In each dimension this canonically defines a higher dimensional generalization of the Willmore energy/rigid string action. Recently Graham proved that the first variation of the volume anomaly recovers the density obstructing smooth solutions to this singular Yamabe problem; we give a new proof of this result employing our boundary calculus. Physical applications of our results include studies of quantum corrections to entanglement entropies.

Keywords: AdS/CFT, anomaly, calculus of variations, conformally compact, conformal geometry, entanglement entropy, hypersurfaces, renormalized volume, Willmore energy, Yamabe problem
1. Introduction

The problem of defining and computing volumes for manifolds with singular metrics

\[ ds^2 = \frac{dx^2 + h(x)}{x^2}, \]

has played a central role in the anti de Sitter/conformal field theory (AdS/CFT) correspondence as well as in conformal geometry [Ma98, AGMO00, FG02, GZ03]. Volumes of regions approaching the hypersurface/boundary \( \Sigma \) diverge at \( x = 0 \). However, by a suitable cut-off and renormalization, a renormalized volume functional can be defined that is invariant under conformal transformations of the boundary metric \( h \) up to a (conformally invariant) anomaly. An early and spectacular AdS/CFT success was the work of Henningson and Skenderis that identified this as the Weyl or trace anomaly of the boundary quantum field theory [HS98]. Significant mathematical progress was made when Fef-ferman and Graham [FG02] showed that for Poincaré–Einstein structures (Euclidean
signature, asymptotically AdS, Einstein manifolds), the renormalized volume anomaly recovered Branson’s $Q$-curvature \cite{Branson} for the boundary manifold. This is an important invariant of conformal geometries (see \cite{GJ, DM} and the reviews \cite{BG, CEOY}). The renormalized volume is usually obtained by computing a Fefferman–Graham coordinate expansion of a bulk metric tensor solving, to some order, a bulk problem with boundary data at a conformal infinity $\Sigma$. This expansion is inserted first in the metric determinant and, in turn, into a regulated volume integral. We shall present a general, simplifying and efficient approach to volume computations for singular metrics that, in contrast to previous studies, does not rely on solving any particular bulk problem.

Let $(M, g^o)$ be a Riemannian manifold whose metric $g^o$ is singular along an hypersurface $\Sigma$. For simplicity we take all structures to be oriented. Given a compact region $D$ such that $\partial D \cap \Sigma \neq \emptyset$, we define the regulated volume of $D$ as follows (see also the diagram in Display (3.3)).

**Definition 1.1.** Given $(M, g^o, D)$ as above, let $\varepsilon \geq 0$ and $\Sigma_\varepsilon$ be a smooth, one parameter family of oriented hypersurfaces such that

(i) $\Sigma_0 = \Sigma$, (ii) $\Sigma_\varepsilon > 0 \cap \Sigma = \emptyset$, and (iii) $\Sigma_\varepsilon > 0$ separates $D$ into a disjoint union $D = D_\varepsilon \cup (D \setminus D_\varepsilon)$, where $g^o$ is non-singular in $D_\varepsilon$.

Then the **regulated volume** of $D$ is defined to be

$$\text{Vol}_\varepsilon(D, \Sigma) := \int_{D_\varepsilon} \sqrt{\det g^{o}}.$$

Our methods can in principle be applied to quite general metric singularities, but we focus on the mathematically and physically central conformally compact case for which the hypersurface $\Sigma$ is a conformal infinity for the metric $g^o$. In this case the regulated volume may be expanded as a sum of divergences (poles in $\varepsilon$), an anomaly (a log $\varepsilon$ term) and the $\varepsilon$-independent renormalized volume plus $\mathcal{O}(\varepsilon)$ contributions. We give simple results for the divergences and anomaly in terms of integrals over Dirac-delta distributions, and their derivatives, depending on a defining function for the hypersurface. These results encode the precise dependence of the divergences on the choice of regulator $\Sigma_\varepsilon$, while the anomaly is independent of the regulator and is conformally invariant (in a suitable sense).

For applications, results for the anomaly and divergences given as hypersurface integrals over local quantities are required. Here it is propitious to assume that the hypersurface $\partial D \cap \Sigma$ is closed. We also indicate how to handle non-closed boundaries in the current work, but reserve a detailed treatment to a sequel article. The key tool for both cases is the boundary calculus for conformally compact manifolds developed in \cite{GW, GLW}. For conformally compact structures, we present exact and explicit formulas for both the divergences and the anomaly in the regulated volume. These are expressed as boundary integrals over local quantities and hold for any regulator and any conformally compact manifold.

Our results can be applied to study the conformal geometry of hypersurface embeddings. Quantities that depend only on the conformal embedding of the hypersurface $\Sigma$, can be found and studied by requiring that the metric $g^o$ solves a singular version of the Yamabe problem of finding conformally rescaled metrics with constant scalar curvature \cite{GW, GW2}. In fact, since a unique asymptotic solution to the singular Yamabe problem exists (at least up to the order required for the anomaly) for any conformally
compact structure, there is a corresponding canonical result for the anomaly which is given by an integral over a density that can be defined for any hypersurface in a Riemannian manifold; this gives a new $Q$-curvature that includes extrinsic curvature data. In particular, by construction, it only depends on the conformal data of how the hypersurface $\Sigma$ is embedded in the bulk.

Since we need not impose the bulk Einstein equation, our results apply to general bulk/boundary problems and thus extend an important aspect of the AdS/CFT program. A second motivation for our study is that this general setting allows us to study the extrinsic conformal geometry of the boundary geometry. Mathematically, our results are part of a general program to understand conformal hypersurface geometry [GW15] (see [CG15] for an overview), and to develop the calculus for integrated conformal hypersurface invariants begun in [CCHW15]. Indeed, we wish to initiate a new approach to geometric invariant theory based on holographic renormalization. This program is also of substantial physical interest: Soon after the original AdS/CFT duality was proposed, Graham and Witten showed how the renormalized volume method could be extended to bulk minimal surfaces in order to analyze holographic observables for boundary submanifolds [GW99]. This study produced conformal hypersurface invariants, the most notable of which, perhaps, is the Willmore energy for surfaces embedded in 3-manifolds. More recently, classes of these observables have been related to entanglement entropies of boundary field theories [RT06, AGS14, PRR15].

A key observation underlying our approach is that the metric in Equation (1.1) is determined by the pair
\[ g = dx^2 + h(x) \] and \( \sigma = x \),
where \((g, \sigma)\) are a non-singular bulk metric and function. However, we equally well could have chosen the pair \((\Omega^2 g, \Omega \sigma)\) where \(\Omega\) is any smooth, positive function of the bulk manifold. The equivalence
\[ g \sim \Omega^2 g \]
defines a conformal class of metrics \(c := [g] = [\Omega^2 g]\) and suggests that conformal, rather than Riemannian, geometry is the correct tool for simultaneously handling bulk and boundary geometries in an AdS/CFT setting. The equivalence \((g, \sigma) \sim (\Omega^2 g, \Omega \sigma)\) defines a bulk, weight one, conformal density \(\sigma := [g; \sigma] = [\Omega^2 g; \Omega \sigma]\). When the function \(\sigma\) has a suitable non-empty, nowhere dense zero locus, the data \((M, \sigma)\) is called an almost Riemannian geometry [Gov10] (note that the canonical equivalence class representative \([\sigma^{-2} g; 1]\) defines a singular Riemannian metric \(ds^2\) as in Equation (1.1)). When this zero locus \(\Sigma\) is a hypersurface or boundary component and the function \(\sigma\) is for it a defining function, then \(\Sigma\) is a conformal infinity for the singular metric \(g/\sigma^2\). When \(M\) is compact with boundary the zero locus of \(\sigma\), then \((M, \sigma)\) is said to be conformally compact. In fact, for our purposes, it suffices to work in a collar neighborhood of the boundary, therefore we shall say that \((M, \sigma)\) is conformally compact in any case where \(\Sigma\) is closed. Reformulating the renormalized volume problem in terms of almost Riemannian geometry brings to bear a potent boundary calculus of conformally compact manifolds that utilizes the bulk conformal structure [Gov10, GW14, GLW15].

One of our main results is that for any conformally compact manifold, the anomaly is given as an integral over the corresponding extrinsically coupled $Q$-curvature first introduced in [GW14]. When regulating a quantum field theory, a dimensionful scale must be introduced. A powerful way to handle dimensionful quantities is to use conformal densities. Physically, a dimensionful quantity, such as a length, will vary across spacetime
Renormalized Volume

if different choices of local unit systems are employed. For example, the invariant property of a length is its linear homogeneity under Weyl transformations. Hence to regulate renormalized volumes we introduce a nowhere vanishing, unit weight, bulk conformal density $\tau$ and cut off the bulk geometry at a regulating surface $\Sigma_\varepsilon$ determined by

$$\sigma/\tau = \varepsilon \in \mathbb{R}_+.$$ 

The renormalized volume anomaly is then given, in $d$ bulk dimensions, by a boundary/hypersurface integral

$$\mathcal{A} = \frac{1}{(d-1)!(d-2)!} \int_\Sigma Q^\sigma,$$

where $Q^\sigma = [g; Q]$ is an extrinsically coupled $Q$-curvature of $\Sigma$ which generalizes the standard Branson $Q$-curvature. When the singular metric is determined by the conformal hypersurface embedding through the singular Yamabe problem, it has a simple explicit formula

$$Q := (-L)^{d-1} \log \tau \bigg|_\Sigma.$$ 

Equally compact formulæ are available for the integrated, local coefficients of the $1/\varepsilon^k$ $(d-1 \geq k \geq 1)$ divergences in the regulated volume; these necessarily depend on the choice of regulator $\tau$ and are proportional to

$$\int_\Sigma L^{d-k-1} \left( \frac{1}{\tau^k} \right).$$

Details are given in Sections 3 and 4, but the main features of these results are as follows:

- The quantity $Q$ is a weight $1-d$ density and is invariant under simultaneous conformal rescalings $g \rightarrow \Omega^2 g$ and $\tau \rightarrow \Omega \tau$. Fixing a choice of regulator $\tau$ and transforming only the metric, the $Q$-curvature then has the famous linear shift property

$$Q \mapsto \Omega^{-d}(Q - P_{d-1} \log \Omega).$$

Here, $P_{d-1}$ is a so-called extrinsic conformal Laplacian power [GW15], which is a canonical extrinsically coupled analog of the conformally invariant GJMS operators of [GJMS92]. The quantity $P_{d-1} \log \Omega$ is a total divergence along $\Sigma$, and hence the $Q$-curvature integrates to an invariant of the (closed) boundary conformal manifold.

- The anomaly is in general non-vanishing. However, when the bulk geometry is Einstein, the extrinsic $Q$-curvature vanishes for odd dimensional $\Sigma$, while for even dimensional $\Sigma$ it reduces to the standard $Q$-curvature of the boundary conformal geometry.

- The operator $L$ is the so-called Laplace–Robin operator (see Section 2.3) determined by the conformal unit defining density $\sigma$ (see Section 4). Along the boundary $\Sigma$ it is a conformally invariant Robin-type (Dirichlet plus Neumann) operator that controls conformally invariant boundary data for conformal infinities, while in the bulk it is a Laplace-type operator that generates wave equations for matter fields [Gov07, GSW08, SW10, GLW15].

- The Laplace–Robin operator forms part of an $\mathfrak{sl}(2)$ solution generating algebra [GW13], this is the key technical tool for our computations.
• In dimension $d = 3$, the anomaly is a sum of the Euler characteristic for 2-manifolds and the rigid string action/Willmore energy for embedded surfaces (see Equation 4.10).

• The simplicity of the integrands appearing in the above formulæ for the anomaly and divergences is achieved by expressing these as local bulk quantities restricted to the hypersurface. This type of bulk boundary correspondence often carries the moniker “holography”, so expressions for hypersurface invariants given by the restriction of bulk quantities are termed holographic formulæ [GW14].

• The above simple formulæ for the extrinsically coupled $Q$-curvature and divergences rely on the existence of asymptotic solutions to a singular version of the Yamabe problem. As already mentioned, there exist also extremely simple distributional formulæ for these quantities valid both for general singular metrics and for non-closed $\Sigma$; see Theorem 3.1. For conformally compact structures the local boundary integral expressions for these are given in Proposition 3.4 and Theorem 3.8.

Variational problems for $Q$-curvatures are also a subject of intense study. In particular, the metric variation of the Branson $Q$ curvature yields the Fefferman–Graham obstruction tensor [GH05]. This latter quantity determines whether log terms must be introduced when solving Einstein’s equations in a Fefferman–Graham expansion off a conformal infinity. For the extrinsically coupled $Q$-curvature, an analogous problem is to treat variations of the anomaly $A$ with respect to variations of the embedding of the hypersurface $\Sigma$. In [GGHW15], an efficient calculus for this type of variation was developed by writing boundary energy functionals holographically in terms of bulk integrals. This is also a key part of our extrinsic $Q$-curvature computation. Indeed the hypersurface variation of the anomaly plays the role of an obstruction to smoothly solving a bulk problem, but rather than Einstein’s equations, the relevant problem is the singular Yamabe problem. This problem was found to be obstructed in [ACF92] with the obstruction shown to be a non-trivial conformal invariant of embedded surfaces when $d = 3$.

Generally, the obstruction was shown to give a natural conformal hypersurface invariant and called the obstruction density in [GW15]. Low dimensional examples are known to be variational [GGHW15]. Very recently, Graham has proved that the obstruction density of [GW13, GW15] is the variation of the renormalized volume anomaly [Gra16]. In Section 4 we rederive this result within our framework.

Our results can be applied to the situation encountered in entanglement entropy studies where the relevant renormalized volume computation applies to the renormalized “area” of a minimal hypersurface in a (spatial) bulk geometry whose boundary is some (codimension two with respect to the spatial bulk geometry) closed hypersurface separating entangled spatial regions in a boundary quantum field theory. For that, one only needs to compute the induced metric along the minimal hypersurface and then treat the entangling hypersurface as the boundary for the minimal hypersurface. The Laplace–Robin operator characterization of volume divergences is extremely simple, but naturally will produce complicated formulæ in terms of both intrinsic and extrinsic curvatures when higher divergences in higher dimensions are considered. However, since quantum corrections to holographic entanglement entropies are of current topical interest (see for example [LM13, EW14]), we have converted our compact Laplace–Robin-type formulæ into integrated local curvature expressions for the first four divergences; see Equations (4.9) and (4.8) and Appendix B.
Many of our results were originally obtained using a tractor calculus approach [BEG94], and then rederived using conformal densities with a view to making the materially generally accessible. We refer the interested reader to our work [GW15] for further details in this direction.

1.1. Geometry conventions. All structures will be assumed to be smooth (\(i.e.\ C^\infty\)). We work with oriented manifolds \(M\) of dimension \(d\) and hypersurfaces in \(M\), meaning compatibly oriented, codimension 1 submanifolds embedded in \(M\). When the dimension \(d\) equals three or four, we often refer to the latter as surfaces and spaces, respectively, and we will refer interchangeably to the manifold \(M\) as the “bulk/ambient/host” manifold. (Note that the exterior derivative will be denoted by \(d\), to avoid confusion with the dimension \(d\).) When \(M\) is equipped with a Riemannian metric \(g\) (for simplicity we assume Euclidean signature), its Levi-Civita connection will be denoted by \(\nabla\) or \(\nabla_a\).

The corresponding Riemann curvature tensor \(R\) is

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

for arbitrary vector fields \(u, v\) and \(w\) (we drop the superscript indicating the dependence on the metric \(g\) on geometric quantities when this is clear by context). In an index notation, \(R\) is denoted by \(R_{abcd}\) and \(R(u, v)w = u^a v^b R_{abcd} w^d\). Cotangent and tangent spaces will be canonically identified using the metric tensor \(g_{ab}\), meaning that this will be used to raise and lower indices in the standard fashion.

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

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

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

\[
Ric_{bd} := R_{ab}^c d = (d - 2) P_{bd} + g_{bd} J, \quad J := P_a^a.
\]

The scalar curvature \(Sc = g^{ab} Ric_{ab}\), thus \(J = Sc/(2(d - 1))\). In two dimensions the Schouten tensor defined above is pure trace with \(J = \frac{1}{2}Sc\).

Given an embedded hypersurface \(\Sigma\), intrinsic analogs of the above geometric quantities will be decorated with bars, so for example, the induced metric is \(\bar{g}_{ab}\) and its Riemann tensor is \(\bar{R}_{abcd}\). The same indices are used for hypersurface tensors as for those in the host space \(M\) (remembering, of course, that the former are orthogonal to the unit normal vector). Equalities that hold only along the hypersurface \(\Sigma\) are denoted by \(\Sigma\).

We use \(|u| := \sqrt{u_a u^a} := \sqrt{u^2}\) to denote the length of a vector \(u\). Symmetrization over groups of indices is indicated by round brackets, and the notation \((\cdots)^o\) denotes the trace-free, symmetric part of a group of indices.

2. Mathematical background

2.1. Conformal densities. A conformal manifold is a \(d\)-manifold \(M\) equipped with a conformal class of metrics

\[
e := [g] = [\Omega^2 g],
\]

where \(\Omega := \exp(\pi)\) is any smooth, strictly-positive function. On a conformal manifold, a conformal density of weight \(w \in \mathbb{R}\) is an equivalence class of (metric, function) pairs defined by

\[
\tau := [g; \tau] = [\Omega^2 g; \Omega^w \tau].
\]
In the following we use density as a moniker for conformal density. A weight $w = 0$ density is a function on $M$, in which case we may denote $[g; f]$ by $f$. Equal weight densities $f = [g; f]$ and $h = [g; h]$ may be added according to $f + h = [g; f + h]$ yielding a density of the same weight, while multiplication $fh := [g; fh]$ yields a density with weight given by the sum of weights (here $f, h$ need not be equally weighted). The unit density is the weight 0 density $1 := [g; 1]$. Tensor-valued conformal densities can be defined analogously to their scalar counterparts. For example, if $f = [g; f]$ is a weight zero density then its conformal gradient

\[ \nabla a f := [g; \nabla a f], \]

defines a weight zero covector-valued density.

When $w = 1$ and the function $\tau$ is strictly positive, we call $\tau = [g; \tau]$ a true scale, or simply a “scale” (which dovetails nicely with its physical interpretation). A true scale canonically determines a Riemannian geometry $(M, g_{ab})$ via the equivalence class representative $\tau = [g^0; 1]$. Conversely, given a true scale $\tau$ and a density $f$, this canonically determines a function $f$ by expressing $f = [g^0, f]$. We will often perform computations involving densities in terms of such a function $f$ and term this “working in a scale”, which we will label either by specifying a given metric $g \in \mathcal{C}$ or a true scale $\tau$. In contexts where the choice of scale/metric is clear, we will use unbolded symbols for a scale”, which we will label either by specifying a given metric

\[ f := \begin{bmatrix} \tau \end{bmatrix} \]

defines a weight zero covector-valued density.

On occasion it will be useful to employ the weight operator $w$ defined acting on the conformal metric $g_{ab} := [g; g_{ab}]$ and its inverse $g^{ab} := [g; g^{ab}]$, a weight $w$ density $\tau$ and a weight $w$ log-density $\lambda$ by

\[ w g_{ab} = 2 g_{ab}, \quad w g^{ab} = -2 g^{ab}, \quad w \tau = w \tau, \quad w \lambda = w. \]

Note that the conformal metric and its natural inverse can be employed to perform index contractions for products of tensor densities.

The operator $\nabla_a$ is well-defined acting on log-densities, for example,

\[ \nabla_a \log \tau = [g; \sigma \nabla_a \log \tau - n_a] \]

is a unit weight density.

It is worth remarking that any dimensionful physical quantity can be regarded as a conformal density, since the transformation $g_{ab} \mapsto \Omega^2 g_{ab}$ amounts to a local choice of unit system while conformal weights then measure physical dimensions of observables.
2.2. Defining density. Given an embedded hypersurface $\Sigma \subset M$, a defining density $\sigma$ is a weight $w = 1$ density $\sigma = [g; \sigma]$ with zero locus

$$\mathcal{Z}(\sigma) := \{ P \in M | \sigma(P) = 0 \} = \Sigma,$$

and such that $d\sigma|_P \neq 0$, $\forall P \in \Sigma$ (so the function $\sigma$ is a defining function for $\Sigma$). For a given hypersurface, a defining density always exists, at least locally.

The $\mathcal{S}$-curvature of a conformal metric $c$ and defining density $\sigma$ is the weight $w = 0$ density (i.e., function) defined by

$$\mathcal{S} := \left[ g; g^{ab}(\nabla_a\sigma)(\nabla_b\sigma) - \frac{2\sigma}{d}(g^{ab}\nabla_a\nabla_b\sigma + \sigma J) \right].$$

Working in the scale $g_{ab}$, and denoting $n_a := \nabla_a\sigma$ and $\rho := -\frac{1}{2}(\Delta + J)\sigma$, the $\mathcal{S}$-curvature is given by the function $n_a^2 + 2\rho\sigma$.

2.3. The Laplace–Robin operator. Let $\sigma = [g; \sigma]$ be a weight 1 density. Then the corresponding Laplace–Robin operator $L$ maps weight $w$ scalar conformal densities to weight $w - 1$ conformal densities according to

$$Lf := \left[ g; (d + 2w - 2)(\nabla_n + w\rho)f - \sigma(\Delta + wJ)f \right].$$

Note that this a Laplacian-type operator that is degenerate along the zero locus of $\sigma$. In the case that $\sigma$ is a defining density, this restricts to a Robin-type (“Dirichlet plus Neumann”) operator along the corresponding hypersurface $\Sigma$.

The Laplace–Robin operator also maps weight $w$ log-densities to weight $-1$ densities via

$$L\lambda := \left[ g; (d - 2)(\nabla_n\lambda + w\rho) - \sigma(\Delta\lambda + wJ) \right].$$

The weight and Laplace–Robin operators obey the algebra

$$[w, L] = -L.$$

The multiplicative operators $sf := \sigma f$ and $Sf := \mathcal{S} f$, mapping weight $w$ densities to weight $w - 1$ and $w$ densities respectively, obey

$$[w, s] = s, \quad [w, S] = 0.$$

Importantly, for any conformal structure and defining density the following algebra holds \cite{GW14}

$$[L, s] = S \circ (d + 2w).$$

Thus, when the $\mathcal{S}$-curvature is non-vanishing, the operators $x := s$, $h := d + 2w$ and $y := -S^{-1}L$ obey the $\mathfrak{sl}(2)$ Lie algebra

$$[x, y] = h, \quad [h, x] = 2x, \quad [h, y] = -2y,$$

for reasons linked to its applications, we call this the solution generating algebra.

The algebra \cite{GW14} also holds upon replacing $y := -S^{-1}L$ by $y := -L \circ S^{-1}$. The difference between these two choices is encoded by the following lemma:

**Lemma 2.1.** Suppose the $\mathcal{S}$-curvature is nowhere vanishing, then acting on densities, the following operator identity holds:

$$[L, S^{-1}] = (L \mathcal{S}^{-1}) - 2(\nabla_a S^{-1}) g^{ab} \nabla_b \sigma.$$
Proof. Acting on a weight \( w \) density \( f := [g; f] \) and remembering that \( S = [g; S] \) has weight 0, we have

\[
[L, S^{-1}] f = [g; ((d + 2w - 2)(\nabla_n + w\rho) - \sigma(\Delta + wJ))(S^{-1} f) \\
- S^{-1}((d + 2w - 2)(\nabla_n + w\rho) - \sigma(\Delta + wJ)) f]
\]

\[
= [g; ((d - 2)(\nabla_n S^{-1}) - \sigma(\Delta S^{-1})) f - 2(\nabla^a S^{-1})(\sigma \nabla_a - n_a w)f]
\]

\[
= (L S^{-1}) f - 2(\nabla_a S^{-1}) g^{ab} \nabla_b f.
\]

\[\square\]

The Laplace–Robin operator also enjoys an integration by parts formula:

**Theorem 2.2.** Let \( f \) and \( g \) be densities of weight \( 1 - d - w \) and \( w \), respectively. Then \( L \) is formally self-adjoint and moreover

\[
f L g - (L f) g + \text{div } j = 0,
\]

where the weight \( 2 - d \) covector-valued density

\[
j_a = [g; \sigma (f \nabla_a g - (\nabla_a f) g) - (d + 2w - 1) n_a f g].
\]

Proof. The first equality follows simply from writing out the left hand side of the display in some scale \( g_{ab} \). Thereafter, it remains to verify that \( j_a \) is indeed a density of the quoted weight, which again follows from a direct computation. \[\square\]

Because the above result holds for generally curved conformal structures, we expect Theorem 2.2 to be of interest beyond our current context.

### 2.4. Conformal hypersurface invariants

Consider an embedded hypersurface described by a defining function \( \Sigma = Z(\sigma) \). A hypersurface preinvariant \( P(g, \sigma) \) amounts to a diffeomorphism invariant quantity built from \( \sigma \) and the metric such that

\[
P(g, \sigma)|_{\Sigma} = P(g, v\sigma)|_{\Sigma}
\]

for any positive function \( v \) (see [GW15] for a precise definition). A hypersurface invariant \( P(g_{ab}, \Sigma) \) is the restriction of a hypersurface preinvariant to \( \Sigma \); per its definition, this depends only on the Riemannian embedding of the hypersurface \( \Sigma \), and in particular not on the choice of a defining function. Key examples include the unit normal

\[(2.8) \quad \hat{n}_a := \frac{\nabla_a \sigma}{|\nabla \sigma|}|_{\Sigma}, \]

the first fundamental form

\[(2.9) \quad I_{ab} := \left(g_{ab} - \frac{(\nabla_a \sigma)(\nabla_b \sigma)}{|\nabla \sigma|^2}\right)|_{\Sigma}, \]

the mean curvature

\[(2.9) \quad H := \frac{1}{d - 1} \nabla^a \left(\frac{\nabla_a \sigma}{|\nabla \sigma|}\right)|_{\Sigma}, \]

and the second fundamental form

\[(2.9) \quad II_{ab} := \left(\nabla_a - \frac{(\nabla_a \sigma)(\nabla^c \sigma)}{|\nabla \sigma|^2}\nabla_c\right)\left(\frac{\nabla_b \sigma}{|\nabla \sigma|}\right)|_{\Sigma}. \]

Hypersurface invariants obey various non-trivial identities, the most of important of which include the identification of the intrinsic hypersurface metric \( g_{ab} \) with the first
fundamental form, and the Gauß equation expressing the difference between ambient 
and hypersurface curvatures in terms of the second fundamental form:

\[(2.10) \quad I_{ab} = \bar{g}_{ab}, \quad R_{abcd}|\Sigma = \bar{R}_{abcd} - 2\Pi_{a[c}I_{d]b} \].

Here and throughout, we use a superscript \(\top\) to denote orthogonal projection onto 
hypersurface-tangential directions. Note that \(I_{ab}^{\top} = I_{ab}\) and \(\Pi_{a[b}^{\top} = \Pi_{ab}\). Indeed, us-
ing that the projected tangent bundle \(T^\top M|\Sigma\) and the hypersurface tangent bundle \(T\Sigma\) 
are isomorphic, we may use the same indices to label host space and hypersurface tensors.

We will need the following technical result for the mean curvature:

**Lemma 2.3.** Let \((g, \sigma)\) be a metric and a defining function for a hypersurface \(\Sigma\) such 
that the corresponding \(S\)-curvature obeys

\[(2.11) \quad S = [g; 1 + \mathcal{O}(\sigma^2)] \).

Then along \(\Sigma\)

\[
\rho := -\frac{\Delta g \sigma + Jg \sigma}{d} \equiv -H.
\]

**Proof.** This result was originally obtained in [Gov10, Section 3.1] for the case \(S = 1\) and 
the proof proceeds along similar lines to that given there. Starting with the preinvariant 
on the right hand side of Equation (2.9) we have

\[\nabla^a \left( \frac{\nabla a \sigma}{|\nabla \sigma|} \right) = \frac{\Delta \sigma}{|\nabla \sigma|} + \nabla_n (|\nabla \sigma|^{-1}),\]

where \(n_a := \nabla a \sigma\). Comparing Equations (2.3) and (2.11) yields \(|\nabla \sigma|^2 + 2\rho \sigma = 1 + \mathcal{O}(\sigma^2)\), 
so that along \(\Sigma\) it follows that \(|\nabla \sigma| = 1\), \(\Delta \sigma = -d \rho\) and

\[
\nabla_n (|\nabla \sigma|^{-1}) \equiv \rho.
\]

Thus

\[\nabla^a \left( \frac{\nabla a \sigma}{|\nabla \sigma|} \right) \equiv -(d-1) \rho.\]

When \(P(\Omega^2 g, \Sigma) = \Omega^w P(g, \Sigma)\), the equivalence class of hypersurface invariants

\[P := [g; P(g, \Sigma)] = [\Omega^2 g; \Omega^w P(g, \Sigma)]\]

defines a conformal hypersurface invariant. Important standard examples include the weight \(w = 1\) unit normal density and weight \(w = 2\) first fundamental form density

\[\hat{n}_a := [g; \hat{n}_a] \quad \text{and} \quad I_{ab} := [g; I_{ab}],\]

as well as the (weight \(w = 1\)) trace-free second fundamental form density

\[\hat{\Pi}_{ab} := [g; \Pi_{ab} - H I_{ab}].\]

We define the weight \(w = -2\) density

\[K := \hat{\Pi}_{ab} \hat{\Pi}^{ab}.\]

For rigid surfaces, this gives a measure of the energy density due to bending. It also 
appears as the Lagrangian density for a rigid string [PSG]; hence we call \(K\) the rigidity 
density. As a simple consequence of the Gauß Equation (2.10), in ambient dimension \(d \geq 3\), the rigidity density can be reexpressed in terms of Riemann and mean curvatures:

\[(2.12) \quad K = (d-2) \left( [g; 2(J - P_{ab} \hat{n}^a \hat{n}^b - \bar{J}) + (d-1)H^2] \right).\]
We shall also need the weight \( w = 0 \) Fialkow tensor defined in dimensions \( d > 3 \) by [Gra03, Sta05]

\[
\mathcal{F}_{ab} := \left[ g; P_{ab} - \bar{P}_{ab} + H\hat{H}_{ab} + \frac{1}{2} \bar{g}_{ab} H^2 \right]
\]

\[
= \frac{1}{d-3} \left( \hat{H}_{ac} \hat{H}_{cb} - \frac{1}{2(d-2)} I_{ab} K - W_{cabd} \hat{n}^c \hat{n}^d \right).
\]

The second line above follows from a standard application of the Gauß equations (see [Vya13, GW15]); we have used conformal invariance of the Weyl tensor \( W_{abcd} \) to define the weight \( 2 \) density \( W_{abcd} := [g; W_{abcd}] \). Finally, in dimension \( d = 4 \), the hypersurface Bach tensor density of weight \(-1\) is defined by [GGHW15]

\[
B_{ab} := [g; \left( \hat{n}^c C_{c(\alpha\beta)} \right)^\top + HW_{c\alpha\beta} \hat{n}^c \hat{n}^d - \bar{\nabla}^c (\hat{n}^d W_{d(\alpha\beta)c})^\top] \quad \text{.}
\]

In the above, \( C_{abc} \) is the ambient Cotton tensor. Continued to dimensions greater than four, for almost Einstein structures, the first term on the right hand side above is linked to the ambient Bach tensor [Gov10, GLW15].

2.5. Extrinsic conformal Laplacian powers and BGG operators. Given a hypersurface \( \Sigma \) and a corresponding defining density \( \sigma \), a smooth operator \( \mathcal{O} \), whose domain is densities on \( M \), is said to be tangential if

\[
\mathcal{O} \circ s = s \circ \tilde{\mathcal{O}}
\]

for some other smooth operator \( \tilde{\mathcal{O}} \). Tangential operators are useful since they can be used to define and efficiently treat operators on hypersurface densities \( \bar{f} \) via

\[
\tilde{\mathcal{O}} \bar{f} := \left( \mathcal{O} f \right) |_{\Sigma}
\]

where \( f \) is any smooth extension of \( \bar{f} \) to \( M \).

A key point for us is that nontrivial tangential operators can be constructed using the solution generating algebra (2.7) by employing the standard \( \mathfrak{sl}(2) \) enveloping algebra identity

\[
[y^k, x] = -ky^{k-1}(h - k + 1).
\]

This implies that the operator

\[
P_{k}^\sigma := (-S^{-1} L)^k
\]

is tangential when acting on densities of weight \( k - \frac{d+1}{2} \). In general this operator depends on the choice of defining density \( \sigma \). However, in Section 4 we present a canonical defining density \( \bar{\sigma} \) obtained by solving a singular version of the Yamabe problem, this yields extrinsic conformal Laplacian powers

\[
P_k := P_k^\bar{\sigma},
\]

determined entirely by the data \((M, c, \Sigma)\) (for orders \( k \geq d \) the above definition must be slightly modified, see [GW15] for details). The simplest example is when \( k = 2 \). In this case \( P_2 \) is an extrinsic generalization of the hypersurface Yamabe operator

\[
P_2 [g; \bar{f}] = \left[ g; \left\{ \Delta + \left(1 - \frac{d-1}{2}\right) \left( \bar{\nabla}^c - \frac{K}{2(d-2)} \right) \right\} \bar{f} \right].
\]

Here \( K := \hat{H}_{ab} \hat{H}^{ab} \) is the rigidity density. For \( k \) even, the operators \( P_k \) have leading term proportional to the Laplacian power \( \Delta_k^2 \), and are therefore extrinsic analogs of GJMS operators.
A second class of non-trivial hypersurface operators is linked to the BGG construction of [CSS01]. The very general BGG technology provides sequences of conformally invariant operators associated to finite dimensional irreducible representations of the conformal group. Specializing to hypersurfaces, the first BGG operator associated to the defining (or vector) representation acts on weight one densities and therefore also conformal hypersurface invariants $\bar{f}$ according to

$$L_{ab} \bar{f} = [\bar{g} ; (\bar{\nabla}_{(a} \nabla_{b)} + \bar{P}_{(ab)}) \bar{f}] , \quad d \geq 4 .$$

In hypersurface dimension two, the above (intrinsically defined) operator is unavailable. However, in that case, there exists an extrinsic hypersurface BGG operator [GGHW15]. We will need the formal adjoint of this operator which maps rank 2, weight $-3$ symmetric, trace-free, conformal hypersurface tensor densities $X^{ab} : = [\bar{g} ; X^{ab}]$ to a conformal hypersurface density of weight $-3$ according to (2.14)

$$L^*_{ab} X^{ab} = [g ; \bar{\nabla}_a \bar{\nabla}_b X^{ab} + \bar{P}_{ab} X_{ab} + H \bar{H}_a X^{ab}] .$$

2.6. Integrated densities. Recall that a weight $-d$ density $f : = [g ; f]$ can be invariantly integrated over a conformal $d$-manifold $M$ or some region $D \subset M$ since the volume element $dV^g$ of $g_{ab} \in c$ defines a weight $d$, measure-valued density $dV := [g ; dV^g]$, because $dV^{\Omega^2 g} = \Omega^d dV^g$. Hence, we may define the conformally invariant integral over $f$ by

$$\int_D f := \int_D dV^g f .$$

Similarly, for hypersurface conformal invariants, the induced metric $\bar{g}_{ab} = I_{ab}$ defines an “area” element $dA^\bar{g}$ (i.e. the volume form of $\bar{g}$ along the hypersurface $\Sigma$). From this we may build the weight $d - 1$ density $dA := [\bar{g} ; dA^\bar{g}]$. Thus, for any weight $1 - d$, scalar, conformal hypersurface invariant $P : = [g ; P(g, \Sigma)]$ we define

$$\int_\Sigma P := \int_\Sigma dA^\bar{g} P .$$

2.7. The Dirac-delta density. We now describe of the main ideas of our approach: We will employ the Dirac delta function to express hypersurface integrals as bulk integrals. Given a defining function $s$ for a hypersurface $\Sigma$ and $\bar{f} : = f|_\Sigma$ with $f \in C^\infty M$, we may then rewrite the integral of $\bar{f}$ as a bulk integral according to (see, for example [GGHW15] or [OF03])

$$\int_\Sigma dA^\bar{g} \bar{f} = \int_{\bar{D}} dV^\bar{g} \delta(s) |\nabla s| f ,$$

where $\bar{D} \supset \text{supp}(\bar{f}) \subset \Sigma$ is some region in $M$ that includes the support of $\bar{f}$.

Given a metric $g$ the function $f$ determines a weight $1 - d$ density $[g ; f] = : f$, and the above display can be expressed as an integral over densities. This is particularly important for us when the hypersurface is given in terms of a defining density $\sigma : = [g ; \sigma]$. Then we may use the the distributional identity (valid for non-vanishing $\Omega$; see Section 2.8 below)

$$\delta(\Omega \sigma) = \Omega^{-1} \delta(\sigma)$$

to infer that

$$\delta := [g ; \delta(\sigma)]$$
is a weight \( w = -1 \) (distribution-valued) density. Since, in a scale \( g_{ab} \), we have that \( \sigma \) is a defining function, it follows that the \( S \)-curvature of \( \sigma \) obeys
\[
S = |\nabla \sigma|^2 \quad \text{along } \Sigma.
\]

Hence
\[
(2.16) \quad \int_D \delta \sqrt{S} f = \int_D dV^g \delta(\sigma) \sqrt{S} f = \int_{\Sigma} \bar{f},
\]
where \( \bar{f} = [\bar{g}_{ab}; f|\Sigma] \). We will often drop the bar notation when using this formula. This identity allows efficient handling of integrated conformal hypersurface invariants. Note that this does not require using an extension \( f \) of \( \bar{f} \) which is a hypersurface preinvariant, but for variational problems it will be useful to do so.

### 2.8. Distributional identities.

Standard distributional identities (on \( \mathbb{R} \)) for the Dirac delta and Heaviside step function such as
\[
\theta'(x) = \delta(x), \quad x\delta(x) = 0, \quad x\delta'(x) = -\delta(x) \quad \text{and} \quad x\delta^{(n)}(x) = -n\delta^{(n-1)}(x), \quad n \in \mathbb{Z} \geq 1,
\]
and their consequences will play a crucial role in our derivation of volume anomalies and divergences. Such identities hold when integrating against suitable test functions. Some care is required to justify their use, but the details are essentially the same in each case. Therefore we explain the key ideas here and suppress the details when presenting the computations below.

We wish to apply distributional identities to the situation where the variable \( x \in \mathbb{R} \) is replaced by a defining function \( \sigma \) for a hypersurface \( \Sigma \) embedded in a manifold \( M \); in particular we will be dealing with the distribution \( \delta(\sigma) \) and derivatives thereof. In our computations we assume that the hypersurface \( \Sigma \) is closed (compact without boundary) and that in a neighborhood of \( \Sigma \) the bulk manifold \( M \) is a product \( \Sigma \times I \subset M \) where \( I \) is some small open interval about \( 0 \). Moreover, we assume that the defining function \( \sigma \) pulls back to the standard coordinate \( x \) on \( I \). In particular, in what follows, we assume that bulk integrals are over regions contained in \( \Sigma \times I \) and so can be treated by Fubini’s theorem.

Then to treat distributional computations in detail, we introduce a fixed, smooth, cutoff function \( \chi \) taking the value 1 on the neighborhood \( \Sigma \times I' \), for some open interval \( I' \subset I \). Thus, integrals involving the distributions \( \theta(\sigma) \) or \( \delta(\sigma) \) and their derivatives are defined by the expressions given below but with the insertion of the test function \( \chi \). It is then easily verified that these integrals have their intended meaning and we leave the details of the distributional calculations to the reader.

The results we obtain this way are local terms integrated along the hypersurface \( \Sigma \). Hence, they apply beyond the situation where \( \Sigma \) is closed, to more general settings as depicted in Diagram (3.3) and applied in the example computation given in Section A.1.

### 3. Renormalized volume

#### 3.1. Conformal infinity.

Let \((M, c, \Sigma)\) denote a conformal manifold \((M, c)\) equipped with an embedded, oriented, hypersurface or boundary component \( \Sigma \). Given this data and some choice of defining density \( \sigma \) for \( \Sigma \) (see Section 2.2), then on the manifold \( \hat{M} := M \setminus \Sigma \) we may extract a canonical metric \( g^o \) such that on one side of \( \Sigma \)
\[
\sigma = [g^o; 1].
\]
The metric $g^o$ is then singular along $\Sigma$ and the hypersurface $\Sigma$ is a conformal infinity of $g^o$. The metric $g^o$ may be used to compute volumes of bounded domains $\hat{D} \subset \hat{M}$ via

$$\text{Vol}(\hat{D}; \sigma) = \int_{\hat{D}} \text{d}V_{g^o} \sigma,$$

where $\text{d}V_{g^o}$ is the volume form of the metric $g^o$. Rewriting the above display in terms of a general equivalence class representative $[g; \sigma]$ we have

$$(3.1) \quad \text{Vol}(\hat{D}; \sigma) = \int_{\hat{D}} \frac{\text{d}V_g}{\sigma^d} \sigma = \int_{\hat{D}} \frac{1}{\sigma^d},$$

which at the same time manifests the conformal invariance of $\text{Vol}(\hat{D}; \sigma)$ (as a functional of $(c, \sigma)$) while emphasizing that it would be singular for regions intersecting the hypersurface $\Sigma$.

3.2. The regulated volume. We now wish to study bounded regions $D$ for which the intersection $\partial D \cap \Sigma$ is non-vanishing and admits a finite collar neighborhood contained in $D$, as depicted in the first diagram below. In that case the analog of the expression $(3.1)$ is divergent. Therefore, working on the side of $\Sigma$ where $\sigma$ is positive, we regulate this expression by inserting a cut-off

$$\theta(\sigma/\tau - \varepsilon),$$

where $\theta : \mathbb{R} \to \{0, 1\}$ is the Heaviside step function (with support $\mathbb{R}_{\geq 0}$) and $\tau = [g; \tau]$ is any true scale. The freedom to choose different regulators is captured by the choice of the true scale $\tau$. Given $\tau$, we define the corresponding regulated volume $\text{Vol}_\varepsilon$ by

$$(3.2) \quad \text{Vol}_\varepsilon(D, \Sigma) := \int_{D} \theta_\varepsilon \frac{\text{d}V_g}{\sigma^d} \sigma = \int_{D} \frac{\text{d}V_g \theta(\sigma/\tau - \varepsilon)}{\sigma^d}.$$

Here we have used the weight 0 density $\theta_\varepsilon := [g; \theta(\sigma/\tau - \varepsilon)]$. By construction this definition agrees with Definition 1.1 with $\Sigma_\varepsilon$ determined by the zero locus of the function $\sigma/\tau - \varepsilon$. The above integral computes the volume of the darker shaded region $D_\varepsilon$ depicted in the second diagram displayed below:

$$(3.3)$$

A technical remark will be important when dealing with surface terms in Section 3.5: The regulated volume is unchanged if we extend the region of integration $D$ beyond the hypersurface $\Sigma$ to a new, compact, region $\tilde{D}$ as depicted below. We assume this is always possible; for the case $\Sigma = \partial M$ we choose an extension to enable this.
Since we are ultimately interested in the dependence of the regulated volume on the hypersurface embedding, in the following we will write $\Sigma$ for the intersection $\Sigma \cap D$. Alternatively, one can consider the conformally compact setting common in applications where $\Sigma = \partial M$ and $D = M$. In the case where $M$ has a puct structure and $\Sigma$ is compact as discussed in Section 2.8 the last diagram above is replaced by:

In all cases, the regulated volume is given by

\begin{equation}
(3.4) \quad \Vol_\varepsilon(D, \Sigma) := \int_{D} \frac{\theta_{\varepsilon}}{\sigma^d}.
\end{equation}

3.3. \textbf{The $\varepsilon$ expansion.} Our strategy will be to show that the regulated volume is a Laurent series plus a logarithm in $\varepsilon$. Except for the constant term, the coefficient of each term will be a hypersurface integral over $\Sigma$. For our purposes the standard distributional identity

\[
\frac{d\theta(\sigma/\tau - \varepsilon)}{d\varepsilon} = -\delta(\sigma/\tau - \varepsilon)
\]

is key to studying the analyticity properties of the regulated volume $\Vol_\varepsilon$ as a function of $\varepsilon$. By the meaning of this identity this implies

\[
\frac{d\Vol_\varepsilon}{d\varepsilon} = - \int_{D} \frac{dV^g}{\sigma^d} \delta(\sigma/\tau - \varepsilon) = -\varepsilon^{-d} \int_{D} \frac{dV^g}{\tau^d} \delta(\sigma/\tau - \varepsilon).
\]
We now need to analyze the integral
\[ I(\varepsilon) := \int_D \frac{dV_g}{\tau^d} \delta(\sigma/\tau - \varepsilon). \]

To that end, consider the function \( s := \sigma/\tau \). Since \( f = \tau^{-d}/|\nabla s| \) is smooth in a neighborhood including \( \Sigma \), we may rewrite this expression as a hypersurface integral by employing the delta function identity (2.15):
\[ I(\varepsilon) = \int_{\Sigma_\varepsilon} dA^g (\tau^{-d}/|\nabla s|)|_{\Sigma_\varepsilon}. \]

We have assumed \( D \) such that \( \Sigma_\varepsilon \) is bounded. Since all functions in the integral are smooth, the hypersurface integral \( I(\varepsilon) \) depends smoothly on \( \varepsilon \) and, for small enough \( \varepsilon > 0 \), may be written as a Taylor series with error term. Hence it follows that the regulated volume is the sum of Laurent series terms about \( \varepsilon = 0 \), plus a \( \log \) term:
\[ (3.5) \quad \text{Vol}_\varepsilon = \sum_{k \in \{d-1, \ldots, 1\}} \frac{v_k}{\varepsilon^k} + \text{Vol}_\text{ren} + A \log \varepsilon + \varepsilon R(\varepsilon), \]
where \( \mathcal{R}(\varepsilon) \) is smooth. The \( \varepsilon \) independent part of this series \( \text{Vol}_\text{ren} := v_0 \) defines the renormalized volume and the \( \log \varepsilon \) coefficient \( A \) is the anomaly. Computing \( A \) in full generality and understanding its link to extrinsically coupled \( Q \)-curvatures is a main goal of our work.

3.4. Expansion coefficients. To extract the anomaly we employ the formula
\[ A = \frac{1}{(d-1)!} \frac{d^{d-1}}{d\varepsilon^{d-1}} \left( \varepsilon^d \frac{d\text{Vol}_k}{d\varepsilon} \right) \bigg|_{\varepsilon=0} = -\frac{1}{(d-1)!} \frac{d^{d-1}I(\varepsilon)}{d\varepsilon^{d-1}} \bigg|_{\varepsilon=0}, \]
where
\[ I(\varepsilon) = \int_D \frac{dV_g}{\tau^{d-1}} \delta(\sigma - \varepsilon\tau). \]
This gives a simple formula for the anomaly
\[ (3.6) \quad A = \frac{(-1)^d}{(d-1)!} \int_D \delta^{(d-1)}. \]

Here \( \delta^{(k)}(x) := \frac{d^k\delta(x)}{dx^k} \) and
\[ \delta^{(k)} := [g ; \delta^{(k)}(\sigma)] \]
is a weight \(-k - 1\) distribution-valued density. Importantl, Equation (3.6) shows that the anomaly \( \mathcal{A} \) is independent of the choice of regulating scale \( \tau \).

It is also not difficult to generate similar formulæ for the coefficients \( u_{k \neq 0} \) (and \( k \leq d-1 \)) by noting \( u_{k \neq 0} = \frac{1}{(d-1-k)!k} \frac{d^{d-1-k}I(\varepsilon)}{d\varepsilon^{d-1-k}} \bigg|_{\varepsilon=0} \) so that
\[ (3.7) \quad u_{k \neq 0} = \frac{(-1)^{d-k-1}}{(d-1-k)!k} \int_D \frac{\delta^{(d-1-k)}}{\tau^k}. \]

As expected, these coefficients do depend on the regulating scale \( \tau \). We gather together the results established above in the following theorem:
Theorem 3.1. The regulated volume $\text{Vol}_\epsilon := \text{Vol}_\epsilon(D, \Sigma)$ as defined in Equation (3.4) depends on $\epsilon$ according to

$$\text{Vol}_\epsilon = \frac{1}{d-1} \frac{1}{\epsilon^{d-1}} \int_D \frac{\delta}{\tau^{d-1}} - \frac{1}{d-2} \frac{1}{\epsilon^{d-2}} \int_D \frac{\delta'}{\tau^{d-2}} + \frac{1}{2(d-3)} \frac{1}{\epsilon^{d-3}} \int_D \frac{\delta''}{\tau^{d-3}} + \cdots + \frac{(-1)^{d-2}}{(d-2)!} \frac{1}{\epsilon^{d-2}} \int_D \frac{\delta^{(d-2)}}{\tau} + \frac{(-1)^d}{(d-1)!} \log \epsilon \int_D \delta^{(d-1)} + \text{Vol}_{\text{ren}} + \epsilon \mathcal{R}(\epsilon),$$

where the renormalized volume $\text{Vol}_{\text{ren}}$ is independent of $\epsilon$ and $\mathcal{R}(\epsilon)$ is smooth.

3.5. Holographic formulæ. The following technical result for powers of the Laplace–Robin operator acting on $\delta$ is the key tool for generating a holographic formula for the anomaly $A$.

Proposition 3.2. Let $Z_{d-1} \ni j \leq d-1$ and suppose the $\mathcal{S}$-curvature is nowhere vanishing. Then

$$(S^{-1}L)^j \delta = (d-j-1) \cdots (d-3)(d-2) \delta^{(j)}.$$ \(\square\)

Proof. The proof is by induction. Consider first the base case $j = 1$. We choose some scale $g$ and then compute

$$L \delta(\sigma) = (d-4)(\nabla_n - \rho)\delta(\sigma) - \sigma(\Delta - J)\delta(\sigma).$$

Using the distributional identities (see Section 2.8) and chain rule we have

$$x \delta(x) = 0, \quad x \delta'(x) = -\delta(x),$$

and $\nabla_n \delta(\sigma) = n^a(\nabla_a \sigma)\delta(\sigma) = n^2 \delta'(\sigma) = (S - 2\rho \sigma)\delta'(\sigma)$, so that (suppressing the $\sigma$ dependence of the delta functions)

$$L \delta = (d-4)S \delta' + (d-4)\rho \delta + [\Delta, \sigma] \delta.$$

But $[\Delta, \sigma] = 2\nabla_n + (\nabla \cdot n)$ and $\nabla \cdot n = -d\rho - J\sigma$ so $L \delta = (d-2)S \delta'$ whence

$$S^{-1}L \delta = (d-2) \delta'.$$

For the induction step we use the further identity

$$(3.8) \quad x \delta^{(j)}(x) = -j \delta^{(j-1)}(x), \quad j \in Z_{d-1},$$

to compute (again in some choice of scale)

$$L \delta^{(j-1)} = (d-2j-2)(\nabla_n - j\rho) \delta^{(j-1)} - \sigma(\Delta - J) \delta^{(j-1)}$$

$$= (d-2j)(\nabla_n - (j+1)\rho) \delta^{(j-1)} + (j-1)(\Delta - (j-1)J) \delta^{(j-2)}.$$\(\square\)

We shall need the following related result:

Proposition 3.3. Let $f$ be a weight zero density. Then

$$L(f \delta^{(d-2)}) = (L f) \delta^{(d-2)}.$$\(\square\)

In particular $L \delta^{(d-2)} = 0.$
Proof. Were the operator $L$ to obey the Leibniz rule, the result would be a direct consequence of Equation (3.9) for $j = d - 1$. Thus it suffices to verify that the non-Leibniz terms in $L(f \delta^{(d-2)})$ vanish. This is a straightforward computation that requires only the methods used in the proof of the preceding lemma. □

3.5.1. Divergences. We now apply the above Proposition 3.2 and the formal self-adjoint property of the Laplace–Robin operator given in Theorem 2.2 to translate the regulated volume expansion coefficients as given in Equation (3.7), into explicit, geometric, boundary integrals. Firstly, computing the coefficient of the leading divergence requires only the integrated delta function identity (2.16), which leads to the holographic formula

\[ v_{d-1} = \frac{1}{d-1} \int_{\Sigma} \left( \frac{1}{\sqrt{S} \tau^{d-1}} \right) \Sigma. \]

For the remaining divergences, we use Proposition 3.2 to rewrite the differentiated delta function densities $\delta^{(j)}$ as powers of the Laplace–Robin operator acting on the undifferentiated delta density $\delta$ and then integrate these by parts onto the power of the regulator $\tau$ using Theorem 2.2, and finally perform the delta integration according to Equation (2.16). At this point we consider the case that $\Sigma$ is closed. Then, the compactly supported test function $\chi$ introduced in Section 2.8 ensures that the surface terms generated by the total divergence term $\text{div} \ j^a$ of the integration by parts Theorem 2.2, do not contribute.

We record the result of this computation in the following proposition:

Proposition 3.4. Let $\Sigma$ be a closed hypersurface. Then the divergences $v_k$ in Equation (3.7) are given by

\[ v_k \in \{ d - 1, \ldots, 1 \} = \frac{(k - 1)!}{(d - 2)! (d - k - 1)! k} \int_{\Sigma} \frac{1}{\sqrt{S} (\tau^{d-1})^{d-k-1}} \frac{1}{\tau^k}. \]

Remark 3.5. In a setting where one is given a distinguished defining density $\sigma$ smoothly determined to all orders (for example this not the case for the singular Yamabe problem dealt with in Theorem 4.1), working in a choice of scale, it is possible to determine the coefficients of finite terms $v_k \leq -1$ generated by the error term $\varepsilon R(\varepsilon)$ in Equation (3.5), in terms of boundary integrals by using the relation

\[ S \delta^{(j)}(\sigma) = (\nabla_n - 2j \rho) \delta^{(j-1)}(\sigma) \]

to successively remove derivatives from the delta function in Equation (3.7).

Remark 3.6. When the hypersurface $\Sigma$ has boundary there are surface terms which can be computed using the result quoted in the theorem for the current $j^a$. We reserve that computation for a future work.

3.5.2. The anomaly. We now compute the anomaly. For that, according to Equation (3.6), we need to compute $d - 1$ derivatives of the delta function $\delta(\sigma)$. However, Proposition 3.2 is no longer of immediate assistance, since this is the critical case where

\[ (S^{-1} L)^{d-1} \delta = 0. \]

The main idea to resolve this problem is to strategically introduce a logarithm of a true scale. Indeed even though Equation (3.6) does not involve the regulating scale $\tau$, by reintroducing some true scale $\tau$ (which need not coincide with the regulating scale, but for efficiency we lose no generality by recycling this quantity, as the final result for $A$ is independent of any such choice) we can write a holographic formula for the anomaly. The following lemma is key:
Lemma 3.7. Let Σ be a closed hypersurface and τ be a weight one density, and suppose the \( \mathcal{S} \)-curvature is nowhere vanishing, then

\[
(3.12) \quad \int_D \delta^{(d-1)} = -\int_D \delta^{(d-2)} (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla_b^\tau) \log \tau.
\]

Proof. First note that \( \log \tau \) is a weight one log density as described in Section 2.1. Let us work in the scale \( \tau = [g; 1] \). From Equations (2.5) and (2.2), and using Equation (3.8) we have

\[
\delta^{(d-2)} (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla_b^\tau) \log \tau
\]

\[
= \left[ g : \delta^{(d-2)} S^{-1} ((d-2) \rho - \sigma J) + \delta^{(d-2)} \nabla_n S^{-1} \right]
\]

\[
= \left[ g : (d-2) S^{-1} (\rho \delta^{(d-2)} + J \delta^{(d-3)}) + \delta^{(d-2)} \nabla_n S^{-1} \right]
\]

\[
= \left[ g : -\frac{d-2}{d} S^{-1} (- (\nabla n) \delta^{(d-2)} + 2J (d-1) \delta^{(d-3)}) + \delta^{(d-2)} \nabla_n S^{-1} \right].
\]

We now concentrate on the divergence of the normal vector term:

\[
\int_D dV g S^{-1} (\nabla n) \delta^{(d-2)} = -\int_D dV g (S^{-1} n^2 \delta^{(d-1)} + \delta^{(d-2)} \nabla_n S^{-1})
\]

\[
= -\int_D dV g (1 - 2 \rho \sigma S^{-1}) \delta^{(d-1)} + \delta^{(d-2)} \nabla_n S^{-1})
\]

\[
= -\int_D dV g \delta^{(d-1)} - \int_D dV g (2(d-1) \nabla_n S^{-1} \rho + (\nabla_n S^{-1})) \delta^{(d-2)}
\]

\[
= \frac{d}{d-2} \int_D dV g (\delta^{(d-1)} + (\nabla_n S^{-1}) \delta^{(d-2)}) + 2(d-1) \int_D dV g S^{-1} J \delta^{(d-3)}.
\]

Because we are in the case where \( \Sigma \) is closed, the integrands have no support along \( \partial \tilde{D} \). Hence, in the first line of the above computation, there no surface terms generated by an integration by parts. Combining the above two displays gives the quoted result. \( \Box \)

Computing the anomaly is now simple: Proposition 3.2 can now be used to handle the differentiated delta-density \( \delta^{(d-2)} \) appearing on the right hand side of (3.12), and thereafter, following the same method employed for the computation of the divergences, one applies the integration by parts result of Theorem 2.2. We record the result in the following theorem:

Theorem 3.8. Suppose the \( \mathcal{S} \)-curvature is nowhere vanishing, and \( \Sigma \) is closed, then the anomaly is given by

\[
(3.13) \quad A = \frac{1}{(d-1)! (d-2)!} \int_\Sigma Q^\sigma,
\]

where

\[
(3.14) \quad Q^\sigma := -\frac{1}{\sqrt{S}} (- L S^{-1})^{d-2} \circ (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla_b^\tau) \log \tau \bigg|_{\Sigma}.
\]

Remark 3.9. The non-vanishing requirement on the \( \mathcal{S} \)-curvature results in no essential loss of generality since there must exist a neighborhood of \( \Sigma \) where \( \mathcal{S} \neq 0 \) by virtue of the definition of a defining density in Section 2.2. *
The quantity $Q^\sigma$ is a weight $1-d$ density along $\Sigma$. Moreover it matches the holographic formula for the Branson $Q$-curvature in the special case of Poincaré–Einstein structures given in [GW14, Theorem 4.7] since in that case $S = 1$.

The integral of $Q$-curvature is a conformal invariant. The analogous result for the integral of $Q^\sigma$ holds here: According to Equation (3.6), the anomaly $A$ does not depend on the choice of regulator $\tau$, so nor does $\int_\Sigma Q^\sigma$ by virtue of the above theorem; but changing the choice of true scale $\tau$ amounts to changing the choice of metric $g \in c$. It is also interesting to construct a direct version of this argument. For that we study the behavior of $Q^\sigma$ upon replacing the scale $\tau$ by $\exp(\varphi)\tau$ where $\varphi$ is any smooth weight 0 density. Since $\log \tau$ then becomes $\varphi + \log \tau$, the corresponding change in $Q^\sigma$ is given by

$$Q^\sigma \mapsto Q^\sigma + \tilde{P}^\sigma \varphi$$

where the operator $\tilde{P}^\sigma$ is given by

$$\tilde{P}^\sigma := \frac{1}{\sqrt{S}} (-S^{-1})^{d-2} \circ (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla_b^\sigma).$$

For Poincaré–Einstein structures the above reproduces the holographic formula for the GJMS conformal Laplacian powers presented in [GW14]. For general scales $\sigma$, it amounts to a version of the tangential operator appearing in Equation (2.13) modified precisely so that $\int_\Sigma \tilde{P}^\sigma \varphi = 0$, which implies that that $\int_\Sigma Q^\sigma$ is conformally invariant. To prove this, we use that

$$\int_\Sigma \tilde{P}^\sigma \varphi = \int_D \delta \sqrt{S} \tilde{P}^\sigma \varphi \propto \int_D \delta^{(d-2)} (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla_b^\sigma) \varphi.$$

The last expression above follows from Proposition 3.2. From Theorem 2.2 and Proposition 3.3 we see that the first term on the right hand side above equals $\int_D \delta^{(d-2)} \varphi L S^{-1}$. Therefore we must compute the final term of the above display:

$$\int_D \delta^{(d-2)} (\nabla_a S^{-1}) g^{ab} \nabla_b^\sigma \varphi = - \int_D dV g \varphi \nabla_a (\sigma (\nabla^a S^{-1}) \delta^{(d-2)})$$

$$= \int_D dV g \delta^{(d-2)} \varphi ((d - 2) \nabla_a S^{-1} - \sigma \Delta S^{-1}) = \int_D \delta^{(d-2)} \varphi L S^{-1}.$$

For the first equality above we made a choice of scale and used that we are in the case that $\Sigma$ is closed to integrate the operator $\nabla^\sigma$ by parts without incurring surface terms. The second equality relied on the identity (3.8) and the final result follows from Equation (2.4). We have therefore proved the following result twice:

**Proposition 3.10.** Let $\Sigma$ be a closed hypersurface with defining function $\sigma$. Then $\int_\Sigma Q^\sigma$ is a conformal hypersurface invariant depending only on the data of the conformal embedding and the defining density $\sigma$.

### 3.6. Asymptotically hyperbolic spaces.

To illustrate our method’s efficacy we compute, in terms of standard Riemannian quantities, the anomaly for an almost hyperbolic 3-manifold: Given any conformally compact manifold with boundary $\Sigma$, there is a conformally related singular metric $g^\sigma$ with the property that the scalar curvature $S_{g^\sigma}$ is non-singular and approaches the strictly negative constant $-d(d - 1)$ along $\Sigma$. In this case $(M, g^\sigma)$ is said to be *asymptotically hyperbolic* (AH) and

$$g^\sigma = \frac{g}{\sigma^2}.$$
where $g$ is a smooth metric on the manifold with boundary $\overline{M}$ and $\sigma$ is a defining function for $\Sigma = \partial \overline{M}$ such that

\begin{equation}
|d\sigma|^g|_{\Sigma} = 1. \tag{3.15}
\end{equation}

Observe that the $S$-curvature of $\sigma = [g; \sigma]$ then obeys

\begin{equation}
S|_{\Sigma} = 1, \tag{3.16}
\end{equation}

which may also be taken as the definition of asymptotic hyperbolicity.

For a given fixed AH singular metric $g^o$, it is possible to find conformal representatives for the defining density $\sigma = [g; \sigma]$ such that the defining function obeys the unit length condition \[3.15\] not only along $\Sigma$, but also in some collar neighborhood thereof. Using this defining function as a coordinate $x$, there exist further coordinates such that the singular metric takes the Graham–Lee normal form \[GL91\]

\[ g^o = \frac{dx^2 + h(x)}{x^2}. \]

Clearly the $S$-curvature is left unchanged.

It is also possible via a normal coordinate construction to instead fix $g$ and find a new AH singular metric with defining function obeying \[3.15\] in a neighborhood of $\Sigma$ (see for example \[Wal84\] or \[GW14, Proposition 2.5\] for an explicit asymptotic construction). The $S$-curvature then still obeys the AH condition \[3.16\] but is changed away from $\Sigma$.

In the following example both situations are covered: We assume that the defining density $\sigma = [g; \sigma]$ obeys the AH condition \[3.16\], and $n = \nabla \sigma$ obeys $|n|^g = 1$ in some neighborhood of $\Sigma$ in which we now work. In $d = 3$ dimensions the $S$-curvature of $\sigma$ is then given by

\[ S = [g; 1 + 2\rho \sigma], \]

where $\rho = -\frac{1}{3}(\Delta \sigma + J \sigma)$. Now we consider the weight one density $\tau = [g; 1]$ determined by $g$ and a weight zero density $f = [g; e^\varphi]$ so that $f \tau$ may be viewed as an arbitrary true scale. We want to compute $Q^\sigma$ as given in Equation \[3.14\]:

\[ -\frac{1}{\sqrt{S}} (-LS^{-1})^{d-2} \circ (S^{-1} \circ L - (\nabla_a S^{-1}) g^{ab} \nabla^b \log(g^o)) \log(f \tau) \bigg|_{\Sigma} \]

\[ = \left[ g; -(\nabla_n - \rho)(S^{-2}(S \nabla_n \varphi + \rho - \sigma \Delta \varphi - \sigma J + (\nabla^a \log S)(\sigma \nabla_a \varphi - n_a))) \right] \bigg|_{\Sigma} \]

\[ = \left[ g; -(\nabla_n - 5\rho)(S \nabla_n \varphi + \rho - \nabla_n \log S) + \Delta \varphi - (\nabla^a \log S) \nabla_a \varphi + J \right] \bigg|_{\Sigma} \]

\[ = \left[ g; \Delta \varphi - \nabla_n \rho + 5\rho^2 + (\nabla_n^2 - 5\rho \nabla_n) \log S + J \right] \bigg|_{\Sigma}. \]

In the above we used that $|n| = 1$ implies that $(\Delta \varphi + 3\rho \nabla_n \varphi - \nabla_n^2) \big|_{\Sigma} = \Delta \varphi$. Thus we see that $Q^\sigma$ depends on $\varphi$ only through the hypersurface total divergence $\Delta \varphi$ so that, in concordance with Proposition \[3.10\] its integral along $\Sigma$ is independent of the choice of regulator $f \tau$. We still wish to express the remaining terms as curvatures:

\[ -\nabla_n \rho + 5\rho^2 + (\nabla_n^2 - 5\rho \nabla_n) \log S + J \overset{\Sigma}{=} 3\nabla_n \rho - 9\rho^2 + J \overset{\Sigma}{=} K + P_{\hat{n}} - H^2 + J. \]

Here we used that $|n| = 1$ implies that $\nabla_a n_b|_{\Sigma} = \Pi_{ab}, \rho|_{\Sigma} = -\frac{3}{2}H$ and $\nabla_n \rho|_{\Sigma} = H^2 + \frac{1}{2}(K + P_{\hat{n}})$. Using the hypersurface identity $J = J + P_{\hat{n}} - H^2 + \frac{1}{2}K$ we have the general result for the anomaly in almost hyperbolic 3-space

\[ A = \frac{1}{2} \int_{\Sigma} Q^\sigma = \int_{\Sigma} dA^g \left( J - \frac{K}{2} \right) + \int_{\Sigma} dA^g (P_{\hat{n}} + K - H^2). \]
The rigidity density $K$ is a conformal hypersurface invariant and the integral over $\bar J$ is proportional to the Euler characteristic of $\Sigma$, so the first term is an invariant of the conformal embedding. In fact, the integrand of the second term equals $\frac{3}{4}((\nabla^2 n S - 3 (\nabla n S)^2)\big|_{\Sigma}$. Thus imposing a condition $S = 1 + O(\sigma^3)$, the anomaly would then be an invariant of the conformal embedding $\Sigma \hookrightarrow (M, c)$. This further motivates the singular Yamabe problem studied in the next section.

4. THE SINGULAR YAMABE PROBLEM

The volume $\text{Vol}(\hat D; \sigma)$ defined in Equation (3.1) depends on the choice of defining density $\sigma$, or equivalently the bulk metric $g^0$. When given only the conformal embedding $\Sigma \hookrightarrow (M, c)$, there is a canonical choice of defining density (determined up to the order required to compute a renormalized version of the volume integral). The divergences simplify considerably in that setting, and the anomaly is an invariant of the conformal embedding [Gra16]. Indeed, the singular Yamabe problem underlies a general program for the study of conformal hypersurface invariants [GW13, GW14].

On a compact manifold, every metric is conformal to a metric of constant scalar curvature. On closed manifolds, the problem of finding a conformal rescaling $\Omega$ such that $Sc_{\Omega}^2 g$ is constant is called the Yamabe problem. We term the analogous problem for conformally compact manifolds the singular Yamabe problem (cf. [Maz91]). This is formulated simply in terms of the $S$-curvature:

Firstly consider an arbitrarily chosen defining density $\sigma_0 = [g; \sigma_0]$. Then since $d\sigma_0$ is non-vanishing along $\Sigma$, its $S$-curvature is positive in a neighborhood of $\Sigma$. Hence, at least in this neighborhood of $\Sigma$, the new defining density $\bar \sigma = \sigma_0 / \sqrt{S(\sigma_0)}$ is well-defined and its $S$-curvature obeys the AH condition

$$S|_{\Sigma} = 1.$$  

In the following discussion, let us assume that the chosen defining density $\sigma$ obeys the unit property in the above display. Now suppose it were also possible to choose $\sigma$ such that the unit property held throughout $M$, namely

$$1 =: [g; 1] = S = [g; S].$$

Then in the interior $\hat M$, evaluating $S$ in the scale $g^0$ (so that $\sigma = 1$) we would have

$$1 = -2 e^u,$$

corresponding to an interior metric with constant negative scalar curvature

$$Sc^g = -d(d - 1).$$

Hence the singular Yamabe problem amounts to finding smooth defining densities such that

$$S = 1.$$  

In general smooth solutions to the singular Yamabe problem do not exist [ACF92]. However, approximate solutions to sufficiently high orders to define a renormalized volume do exist, as encapsulated by the following theorem (based in part on [ACF92]):

**Theorem 4.1 (GW15).** Given a defining density $\sigma_0$, there exists an improved defining density

$$(4.1) \quad \bar \sigma = \sigma (1 + \alpha_1 \sigma + \cdots + \alpha_{d-1} \sigma^{d-1}),$$

where $\sigma = \sigma_0 / \sqrt{S(\sigma_0)}$ in a neighborhood of $\Sigma$, and $\alpha_k$ are smooth densities, such that the $S$-curvature of $\bar \sigma$ obeys

$$(4.2) \quad S = 1 + \sigma^d B.$$
Moreover, the weight $w = -d$ density $B(\sigma_0)$ is a preinvariant for a conformal hypersurface invariant
\[
B := B|_{\Sigma},
\]
which depends only on the data of the conformal embedding $\Sigma \hookrightarrow (M, c)$.

The density $\bar{\sigma}$ of the theorem is unique up to terms $\sigma^{d+1}\alpha$, where $\alpha$ is a smooth weight $-d$ density, and $\bar{\sigma}$ is termed a conformal unit defining density. Since the density $B$ obstructs smooth solutions to the singular Yamabe problem, it is called the obstruction density. For surfaces embedded in conformally Euclidean 3-space, in a Euclidean scale $3B$ equals the Willmore invariant
\[
(4.3) \quad \bar{\Delta} H + 2H(H^2 - \kappa),
\]
where $\kappa = \bar{S}e/2$ is the Gauß curvature. It follows that the above quantity, which appears as one side of the Willmore equation, is invariant under rigid conformal motions, a fact which is well known.

4.1. Divergences. It is not difficult to generate general formulæ for the divergences in the regulated volume (3.2) for singular metrics solving the singular Yamabe problem. We focus on the case where $\Sigma$ is closed throughout this section. Computations are simplified by working in the scale $\tau$. For the leading divergence of Equation (3.10), this yields the hypersurface integral
\[
(4.4) \quad v_{d-1} = \frac{1}{d - 1} \int_{\Sigma} dA^\bar{g}.
\]
In a Poincaré–Einstein setting this behavior of the leading divergence is well known, see for example [Gra00].

By virtue of Equation (4.2), the subleading divergences (3.11) become
\[
(4.5) \quad v_{k \in \{d-1, \ldots, 1\}} = \frac{(k - 1)!}{(d - 2)! (d - k - 1)! k} \int_{\Sigma} (-L)^{d-k-1} \frac{1}{\tau^k},
\]
and it is not difficult to develop explicit formulæ for the first few values of $k$: Using Equation (2.4) we compute
\[
L \tau^{2-d} \equiv \{g; (d-2)^2 \rho\},
\]
where again $\tau = [g; 1]$. Thus, using Lemma 2.3 it follows that in this scale the coefficient of the next-to-leading order (nlo) divergence is
\[
(4.6) \quad v_{d-2} = \int_{\Sigma} dA^\bar{g} H.
\]
To compute the next-to-next-to-leading order (nnlo) divergence we must calculate $L^2 \tau^{3-d}|_{\Sigma}$. The geometric data required for this computation is given in [GW14, Lemma 7.9]. In the scale $\tau = [g; 1]$, using Equation (2.12), we then find
\[
(4.7) \quad L^2 \tau^{3-d} \equiv -(d-2)(d-3) \left( g; J + (d-4) \left( P^{ab} \tilde{n}_a \tilde{n}_b - (d-2) H^2 + \frac{K}{d-2} \right) \right).
\]
Thus, in this scale, the coefficient of the nnlo divergence is
\[
(4.8) \quad v_{d-3} = -\frac{1}{2(d-3)} \int_{\Sigma} dA^\bar{g} \left\{ J + (d-4) \left( P^{ab} \tilde{n}_a \tilde{n}_b - (d-2) H^2 + \frac{K}{d-2} \right) \right\}.
\]
The computation of the next-to-next-to-next-to-leading (nnnlo) divergence is somewhat more involved and has been relegated to Appendix B.
To summarise, given the data of a compact hypersurface embedded in a Riemannian manifold \((M, g)\) and the corresponding choice of true scale \(\tau := [g; 1]\), the regulated volume for a conformal unit defining density is given by

\[
\text{Vol}_\varepsilon(D, \Sigma) = \frac{1}{d-1} \int_\Sigma \frac{dA^\theta}{\varepsilon^{d-1}} + \frac{1}{d-2} \int_\Sigma \frac{dA^\theta H}{\varepsilon^{d-2}} + \cdots + A \log \varepsilon + \text{Vol}_{\text{ren}} + \mathcal{O}(\varepsilon).
\]

Formulae for the \(1/\varepsilon^{d-3}\) and \(1/\varepsilon^{d-4}\) divergences can be found in Equation (4.8) and Appendix B.

4.2. The anomaly. We can also generate explicit results for the anomaly in the singular Yamabe setting. These are of particular interest, since they generate integrated conformal invariants depending only on the conformal embedding.

To begin with note that Theorem (3.8) simplifies considerably for defining densities satisfying Equation (4.2). In this case \(Q\) is independent of \(\Sigma\) and given by \((-L)^{d-1} \log \tau \big|_\Sigma\).

Thus, for closed \(\Sigma\), the anomaly is given by

\[
A = \frac{1}{(d-1)!(d-2)!} \int_\Sigma (-L)^{d-1} \log \tau \big|_\Sigma.
\]

We now develop the above formula for embedded surfaces and spaces.

4.2.1. Surfaces embedded in 3-manifolds. To compute the log term in the \(\varepsilon\) expansion of the regulated volume when the host space is three dimensional we need to compute the square of the Laplace–Robin operator acting on a log-density. An explicit formula for the square of the Laplace–Robin operator of a conformal unit density acting on general densities (and tractors) is known (see for example [GW15, Lemma 7.9]) and is given by

\[
L^2 \log \tau \equiv \left[ g; \frac{\bar{J}}{2} \right].
\]

Orchestrating the above with our results for the leading and subleading divergences in Equations (3.10) and (4.6), the regulated volume in the scale \(\tau\) is given by

\[
\text{Vol}_\varepsilon(D, \Sigma) = \int_\Sigma \frac{dA^\theta}{\varepsilon^2} + \frac{\log \varepsilon}{2} \int_\Sigma dA^\theta \left( \frac{\bar{J}}{2} - K \right) + \text{Vol}_{\text{ren}} + \mathcal{O}(\varepsilon).
\]

Thus, remembering that the Gauss curvature equals \(\bar{J}\), we see that the anomaly for closed hypersurfaces and singular metrics defined by a conformal unit defining density is

\[
A = \pi \chi - \frac{1}{4} \int_\Sigma K,
\]

where the Euler characteristic \(\chi\) of \(\Sigma\) is clearly conformally invariant and the rigidity density is a local conformal hypersurface invariant. Hence \(A\) depends only on the conformal embedding. Of course, the integral of intrinsic scalar curvature does not contribute to the functional gradient of \(A\) so that for Euclidean ambient spaces, Equation (2.12) shows that the only remaining variational term is the integral of mean curvature-squared, or in other words the classical Willmore energy functional.

4.2.2. Spaces embedded in 4-manifolds. Here we need the square of the Laplace–Robin operator acting on \(1/\tau\) and its cube acting on a log-density. The former is given in Equation (4.7) and for \(d = 4\) yields

\[
L^2 \frac{1}{\tau \Sigma} \equiv [g; -2J].
\]
The cubic computation is more involved although significantly simplified by calculating in the \( \tau \) scale. First we use the definition of the Laplace–Robin operator in Equa-
tions \([2.4], (2.5)\) and find along the hypersurface
\[
L^3 \log \tau \overset{\Sigma}{=} [g; (2\nabla_n \circ \bar{\sigma} (\Delta - J))(2\rho - \bar{\sigma} J)] \overset{\Sigma}{=} [g; 2(\Delta - J)(2\rho - \bar{\sigma} J)].
\]
The second equality above used that for a conformal unit defining density \( \nabla_n \bar{\sigma} \overset{\Sigma}{=} 1 \). Furthermore, along \( \Sigma \) we also have the operator identities (see \([GW15]\))
\[
(4.11) \quad \Delta \circ \bar{\sigma} \overset{\Sigma}{=} 2\nabla_n + d H \text{ and } \Delta \overset{\Sigma}{=} \Delta + \nabla_n^2 + (d - 2)H\nabla_n.
\]
Hence
\[
L^3 \log \tau \overset{\Sigma}{=} [g; -4 \Delta H + 4 \nabla_n^2 \rho + 8H\nabla_n \rho - 4(\nabla_n + H)J].
\]
The quantities appearing above have been computed in \([GW15]\) Lemmas 6.6 & 6.8, in particular
\[
(4.12) \quad \nabla_n \rho \overset{\Sigma}{=} P_{ab} n^a n^b + \frac{K}{d - 2},
\]
and
\[
(4.13) \quad \nabla_n^2 \rho \overset{\Sigma}{=} (\nabla_n + H) \nabla_n \rho \overset{\Sigma}{=} \frac{1}{(d - 2)(d - 3)} \left( \nabla^a \nabla^b \bar{H}_{ab} + (d - 2)(d - 4)\tilde{H}^{ab} \tilde{P}_{ab} \right)
- \frac{d - 2}{d - 3} \tilde{H}^{ab} \tilde{F}_{ab} - \nabla^a (P_{ab} n^b) - H(4 - 2)P_{ab} n^a n^b + K).
\]
Also, we have the hypersurface identity
\[
(4.14) \quad \bar{\Delta}H = \frac{1}{d - 2} \bar{\nabla}^a \bar{\nabla}^b \bar{H}_{ab} - \bar{\nabla}^a (P_{ab} n^b)^\top.
\]
Orchestrating the above gives
\[
L^3 \log \tau \overset{\Sigma}{=} [g; -4 \bar{\nabla}^a \bar{\nabla}^b \bar{H}_{ab} - 8 \bar{H}^{ab} \bar{F}_{ab}].
\]
Up to the leading divergence (and so non-variational) term, this matches the higher Willmore energy density found for embedded spaces in \([GGHW15]\).

A useful check of our result is the linear shift property of the \( Q \)-curvature discussed in the introduction: For that, notice that under a conformal transformation \( g \mapsto \Omega^2 g \), we have
\[
\nabla^a \nabla^b \bar{H}_{ab} \mapsto \Omega^{-3} \left[ (\nabla^a \nabla^b \hat{\bar{H}}_{ab}) + 2(\hat{\bar{H}}^{ab} \nabla_a \nabla_b + (\nabla_a \hat{\bar{H}}^{ab} \nabla_b) \log \Omega) \right],
\]
which implies the correct shift transformation:
\[
Q := 4 \left( \nabla^a \nabla^b \hat{\bar{H}}_{ab} + 2 \hat{\bar{H}}^{ab} \bar{F}_{ab} \right) \mapsto \Omega^{-3} \left( Q - P_3 \log \Omega \right),
\]
where the third order extrinsic conformal “Laplacian power” \( P_3 \) acts on weight zero, scalar densities in host dimension \( d = 4 \) according to
\[
P_3 := -8 \bar{H}^{ab} \nabla_a \nabla_b - 8 (\nabla_a \hat{\bar{H}}^{ab} \nabla_b) = -8 \nabla_a \circ \hat{\bar{H}}^{ab} \circ \nabla_b,
\]
see \([GW15]\) Proposition 8.5. Like the standard, even dimension parity GJMS Laplacian powers of \([GJMS92]\), the above operator is formally self adjoint and annihilates constant functions. In using the term Laplacian power for odd dimensional hypersurfaces, we view the trace-free second fundamental form as a metric-like tensor.
Altogether, the regulated volume in the scale $\tau$ reads

\[ \text{Vol}_\varepsilon(D, \Sigma) = \frac{\int_{\Sigma} dA^\beta}{3\varepsilon^3} + \frac{\int_{\Sigma} dA^\beta H}{\varepsilon^2} - \frac{\int_{\Sigma} dA^\beta J}{2\varepsilon} + \frac{1}{3} \log \varepsilon \int_{\Sigma} dA^\beta \left( \tilde{\nabla}^a \tilde{\nabla}^b \tilde{H}_{ab} + 2\tilde{H}^{ab} \mathcal{F}_{ab} \right) + \text{Vol}_{\text{ren}} + \mathcal{O}(\varepsilon). \]

(4.15)

5. The functional gradient

We now use our boundary calculus to compute the variation of the anomaly. This confirms the result of [Gra16] that the functional gradient of the anomaly $A$, for singular metrics determined by a conformal unit defining density, is the obstruction density $B$. More precisely:

\[ \frac{\delta A}{\delta \Sigma} = \frac{d(d-2)}{2} B, \]

where $\delta A/\delta \Sigma$ denotes the functional gradient with respect to variations of the embedding of the hypersurface $\Sigma$.

In [GGHW15], a holographic approach for variations of embeddings was developed and exploited for computations of higher Willmore energy variations. This method is well adapted to the current situation where our starting point is the bulk integral expression in Equation (3.4) for the regulated volume. The main idea of the method is as follows: Given a functional $E(\Sigma) = \int_{\Sigma} P$ where $P$ is a hypersurface invariant, we first express $\Sigma$ as the zero locus of a defining function $\sigma_0$ and $P$ as the restriction of a preinvariant $\mathcal{P}$. As explained in Section 2.7, we can then express $E(\Sigma)$ as a bulk integral

\[ E[\sigma_0] = \int_{\mathcal{D}} dV^g \delta(\sigma) \sqrt{S} \mathcal{P}, \]

where $S$ is the $S$-curvature of $\sigma_0 = [g; \sigma_0]$ in a scale $g$. Then the embedding can be varied by functionally varying the defining function $\sigma_0$. For that we introduce a smooth one-parameter family of hypersurfaces $\Sigma_t$ such $\Sigma_0 = \Sigma$ and $\Sigma_t = \Sigma$ outside some compactly supported region. We also define the variational operator $\delta(\cdot) := \frac{d}{dt}\big|_{t=0}$. The functional gradient is then defined by

\[ \delta E[\sigma_0] = \int_{\Sigma} dA^\beta \delta \sigma_0 \frac{\delta A}{\delta \Sigma}, \]

where $\delta \sigma_0$ is the hypersurface invariant defined by the preinvariant $\delta \sigma_0/|\nabla \sigma_0|$ (this is the variational analog of the preinvariant formula for the unit normal in Equation (2.8)).

For conformal hypersurface invariants defined in terms of the jets of a conformal unit defining density, there is one further useful simplification afforded by the holographic variational calculus. Namely, the uniqueness property of conformal unit defining densities (i.e., $\hat{\sigma}(\sigma_0)$ see [GW15 Theorem 4.5]) ensures that the integrand $Q[\hat{\sigma}(\sigma_0)]$ of the anomaly is a preinvariant. Since the functional derivative $\delta \hat{\sigma}(\sigma_0)/\delta \sigma_0$ along $\Sigma$ is given by $\delta \sigma_0/|\nabla \sigma_0|$ (this follows directly from the functional dependence $\hat{\sigma}(\sigma_0)$ implied by the expansion in Equation (4.11)), we have

\[ \delta \hat{\sigma} = \frac{\delta \sigma_0}{|\nabla \sigma_0|} = \delta \sigma_0. \]
Hence the functional gradient can be computed by functionally varying \( \bar{\sigma} \). Our strategy, therefore, is to consider the one parameter family of regulated volume integrals
\[
\text{Vol}_\epsilon(D, \Sigma_t) = \text{Vol}_\epsilon(D, \bar{\sigma}_t) = \int_D \frac{dV}{\bar{\sigma}_t^d} \theta(\bar{\sigma}_t/\tau - \epsilon)
\]
corresponding to conformal unit densities \( \bar{\sigma}_t \) of hypersurfaces \( \Sigma_t \). Then, since we have already shown that \( \text{Vol}_\epsilon \) is the sum of a Laurent series in \( \epsilon \) plus \( \log \epsilon \) times the anomaly, we need only compute the \( \log \epsilon \) contribution to \( \delta = \frac{d}{dt} |_{t=0} \) of the above expression.

5.1. Varying the defining density. The variation of the regulated volume breaks into two terms
\[
\delta \text{Vol}_\epsilon(D, \Sigma) = -d \int_D dV_g \frac{\delta \bar{\sigma}}{\bar{\sigma}^{d+1}} \theta(\bar{\sigma}/\tau - \epsilon) + \int_D dV_g \frac{\delta \bar{\sigma}}{\bar{\sigma}} \delta(\bar{\sigma}/\tau - \epsilon).
\]
By performing the delta function integration, the second term can be rewritten as \( \epsilon^{-d} \) multiplying a hypersurface integral:
\[
\frac{1}{\epsilon^d} \int_{\Sigma_t} dA_{\bar{\sigma}} \frac{\delta \bar{\sigma}}{\bar{\sigma}^{d+1}}.
\]
Since this hypersurface integral depends smoothly on \( \epsilon \) and is well-defined at \( \epsilon = 0 \), the above display yields some Laurent series in \( \epsilon \) and does not produce a \( \log \epsilon \) contribution. Hence we must focus on the first term in the functional gradient above. For this we will need a pair of lemmas.

**Lemma 5.1.** Let \( \bar{\sigma}_t \) be a smooth one parameter family of conformal unit defining densities with \( \bar{\sigma}_0 = \bar{\sigma} \). Then the variation \( \delta \bar{\sigma} \) obeys
\[
L \delta \bar{\sigma} = \frac{1}{2} \bar{\sigma}^{d-1} \left( \mathcal{B} \delta \bar{\sigma} + \frac{1}{d} \bar{\sigma} \delta \mathcal{B} \right).
\]
**Proof.** The key is to vary the defining relation for a conformal unit defining density
\[
S_t = 1 + \bar{\sigma}_t^d \mathcal{B}_t.
\]
The variation of the \( S \)-curvature is easily computed
\[
\delta S = \left[ g ; \ 2 g^{ab} (\nabla_a \bar{\sigma}) \nabla_b \delta \bar{\sigma} - \frac{2 \delta \bar{\sigma}}{d} (\Delta + J) \bar{\sigma} - \frac{2 \bar{\sigma}}{d} (\Delta + J) \delta \bar{\sigma} \right]
\]
\[
= \left[ g ; 2 \left( \nabla^a + \rho - \frac{\bar{\sigma}}{d} (\Delta + J) \right) \delta \bar{\sigma} \right] = \frac{2}{d} L \delta \bar{\sigma},
\]
while the variation of the right hand side is \( d \bar{\sigma}^{d-1} \mathcal{B} \delta \bar{\sigma} + \bar{\sigma}^d \delta \mathcal{B} \).

Because \( \delta \bar{\sigma} \) is a weight 1 density, it is not difficult to verify (see [GW14, Lemma 3.1]) that the algebra \( (2.6) \) implies that
\[
L \left( \frac{\delta \bar{\sigma}}{\bar{\sigma}^{d+1}} \right) = \frac{1}{2} \frac{\delta \bar{\sigma}}{\bar{\sigma}} \frac{\delta \mathcal{B}}{\bar{\sigma}^{d+1}},
\]
whence via Lemma 5.1 we have
\[
(5.2) \quad L \left( \frac{\delta \bar{\sigma}}{\bar{\sigma}^{d+1}} \right) = \frac{d^2}{2 \bar{\sigma}^2} \left( \mathcal{B} \delta \bar{\sigma} + \frac{1}{d} \bar{\sigma} \delta \mathcal{B} \right).
\]
The second lemma relates the left hand side of the above display to \( \delta \bar{\sigma}/\bar{\sigma}^{d+1} \).
Lemma 5.2. Let \( f \) be a weight \(-d\) density. Then (for any defining density \( \sigma \)),
\[
\mathcal{S} f = \frac{\sigma}{d} L f + \left[ g; \nabla_c j^c \right],
\]
where \( j^c = \frac{1}{d}(\sigma \nabla^c(\sigma f) + (d-1)\sigma(\nabla^c \sigma) f) \).

Proof. Firstly, since \((d+2w)f = -df\), the algebra \((2.6)\) implies
\[
\sigma L f = d \mathcal{S} f + L(\sigma f).
\]
Then Theorem 2.2 applied to densities 1 and \( \sigma f \) yields
\[
L(\sigma f) + \left[ g; \nabla_c (\sigma \nabla^c(\sigma f) + (d-1)\sigma n^c f) \right] = 0.
\]
Here we used the identity \( L 1 = 0 \).

For the case of a conformal unit defining density and \( f = \delta \bar{\sigma}/\bar{\sigma}^{d+1} \), applying this lemma to Equation \((5.2)\) and subsequently using Equation \((4.2)\) gives
\[
(5.3)
\]
\[
\frac{\delta \bar{\sigma}}{\bar{\sigma}^{d+1}} = \frac{d-2}{2} \mathcal{B} \frac{\delta \bar{\sigma}}{\bar{\sigma}} + \frac{1}{2} \delta \mathcal{B} + \left[ g; \nabla_c j^c \right],
\]
where
\[
\frac{\delta \sigma}{\bar{\sigma} d+1} = \frac{1}{d} \left( \bar{\sigma} \nabla^c \left( \delta \sigma \right) + (d-1) \frac{n^c \delta \sigma}{\bar{\sigma}^d} \right).
\]
The first term on the right hand side of \((5.3)\) will be responsible for the \( \log \varepsilon \) contribution. Before studying it in detail, we first establish that the other two terms can only produce Laurent series contributions: The obstruction density and therefore its variation are regular along \( \Sigma \) while the \( \mathcal{S} \)-curvature is unity there. Hence the second term on the right hand side of Equation \((5.3)\) can only produce terms analytic in \( \varepsilon \). For the total divergence term we employ Green’s theorem, \( \int_{D_{\varepsilon}} dV^g \nabla_a j^a = \int_{\partial D_{\varepsilon}} dA^{b\alpha} \partial_{D_{\varepsilon}} \nabla_a j^a \) where \( \partial_{D_{\varepsilon}} \nabla_a j^a \) is the unit outward normal. We thus find a contribution to the variation proportional to
\[
\int_{\Sigma_{\varepsilon}} dA^{b\alpha} \partial_{D_{\varepsilon}} \nabla_a j^a \left( \bar{\sigma} \nabla^c \left( \delta \sigma \right) + (d-1) \left( \nabla^c \delta \sigma \right) \frac{\delta \bar{\sigma}}{\bar{\sigma}^d} \right),
\]
where we have dropped the contribution from the surface term integrated over \( \partial D_{\varepsilon} \setminus \Sigma_{\varepsilon} \) as this term is not responsible for a \( \log \varepsilon \) contribution. In the above display the outward unit normal vector to \( \Sigma_{\varepsilon} \) is given by
\[
\partial_{D_{\varepsilon}} \nabla_a j^a = -\nabla_a \left( \bar{\sigma} \nabla^c \left( \delta \sigma \right) + (d-1) \left( \nabla^c \delta \sigma \right) \frac{\delta \bar{\sigma}}{\bar{\sigma}^d} \right)_{\Sigma_{\varepsilon}},
\]
because \( \bar{\sigma}/\tau - \varepsilon \) is a defining function for \( \Sigma_{\varepsilon} \). Since \( n_a \) is well-defined along \( \Sigma \), it follows that \( n_a \) is regular around \( \varepsilon = 0 \). Furthermore, along \( \Sigma_{\varepsilon} \) we have
\[
\partial_{D_{\varepsilon}} \nabla^c \left( \delta \sigma \right) + (d-1) \left( \nabla^c \delta \sigma \right) \frac{\delta \bar{\sigma}}{\bar{\sigma}^d} = -\frac{1}{\varepsilon^d} \frac{n^c \delta \bar{\sigma} - \varepsilon \tau \nabla^c \delta \bar{\sigma}}{\tau^d}.
\]
Since \( \delta \bar{\sigma} \) and \( n^c \) are regular as \( \varepsilon \) approaches zero and \( \tau \) is a true scale, the above is a Laurent series in \( \varepsilon \). This establishes that the total divergence term of \((5.3)\) yields a Laurent series in \( \varepsilon \) but no \( \log \varepsilon \) term.

It now remains only to study the contribution to the variation given by
\[
-\frac{d(d-2)}{2} \int_{D_{\varepsilon}} \mathcal{B} \frac{\delta \bar{\sigma}}{\bar{\sigma}}.
\]
As discussed in Section 2.8, we can employ \( \bar{\sigma} \) as a coordinate in a collar neighborhood of \( \Sigma \). Ignoring a finite contribution, it will be sufficient to restrict the above integral to this collar. Since \( |\nabla \bar{\sigma}| = 1 \) along \( \Sigma \) for any scale \( g \), the volume form can be written as

\[
dV^g = d\bar{\sigma} \, dA(\bar{\sigma})
\]

where \( dA(\bar{\sigma}) \) is a measure for constant \( \bar{\sigma} \) hypersurfaces \( \Sigma_a \). Then by Fubini’s theorem the collar restriction of integral displayed above is (in some scale \( g \) where \( B = [g; B] \))

\[
-\frac{d(d-2)}{2} \int_{\varepsilon}^* \frac{d\bar{\sigma}}{\bar{\sigma}} \int_{\Sigma_3} dA(\bar{\sigma}) \, \delta\bar{\sigma} \, B,
\]

where \( \ast \) indicates our choice of collar neighborhood. Noting that \( dA|_\Sigma = dA(0) = dA^g \), and using that the obstruction density is non-singular along \( \Sigma \) it follows that the behavior of this integral is

\[
-\frac{d(d-2)}{2} \log(1/\varepsilon) \int_{\Sigma} dA^g \, \delta\bar{\sigma} \, B + O(\varepsilon^0).
\]

Remembering that \( \delta\Sigma \equiv \delta\sigma_0 \), we can read off the variation of the anomaly from the above display. Thus we find that the functional gradient of the regulated volume is a Laurent series plus the desired log term:

\[
\text{Laurent}(\varepsilon) + \frac{d(d-2)}{2} \log \varepsilon \, B.
\]

Equation (5.1) for the functional gradient of the anomaly follows accordingly.

5.2. Examples. Let \( (M, g) \) be a Riemannian \( d \)-manifold. Since we are given a metric \( g \) as data, we may define a true scale \( \tau = [g; 1] \). Now suppose we are further given a hypersurface \( \Sigma \) as the zero locus of some function \( \sigma_0 : M \rightarrow \mathbb{R} \). As explained in Section 3.6, we may improve this to a unit defining function meaning that \( |\nabla \sigma| = 1 \) also away from \( \Sigma \). This yields a corresponding defining density for \( \Sigma \)

\[
\sigma = [g; \sigma],
\]

which, for our renormalized volume computation, we wish to further improve to a conformal unit defining density \( \bar{\sigma} \). A closed form algorithm for this was given in [GW15]. In dimension \( d = 3 \) (see [CGHW15] for explicit expressions in dimensions \( d = 4, 5 \)) the algorithm gives \( \bar{\sigma} = [g; \bar{\sigma}] \) where (here \( n := \nabla \sigma \) rather than \( \nabla \bar{\sigma} \))

\[
\bar{\sigma} = \sigma \left( 1 + \frac{\sigma^2}{4} \nabla.n + \frac{\sigma^4}{12} \left[ 2 (\nabla.n)^2 + \nabla.n \nabla.n + 4 J \right] \right).
\]

An elementary computation shows that the \( S \)-curvature of the above conformal unit defining scale \( \bar{\sigma} \) is

\[
S = 1 - \frac{\sigma^3}{12} \left[ g; 2 \Delta \nabla.n + 2 \nabla^2_n \nabla.n + 8 (\nabla.n) \nabla.n + 3 (\nabla.n)^3 + 8 \nabla.n J + 8 \nabla.n J \right].
\]

Then a simple calculation based on the above formula [GW13]—or a general holographic formula, or a general recursion (see [GW15])—gives the obstruction density for surfaces in terms of the extrinsic BGG operator of Equation (2.14)

\[
-3B = L_{ab} \hat{H}^{ab}.
\]

A formula for the generally conformally curved surface obstruction density was first found in [ACF92] (see also [Vya13] for a related result); this reduces to the Euclidean result (1.3) when the host metric is conformally flat. The two-dimensional obstruction density \( B \) is well known to be the functional gradient of the Willmore energy...
\[-\frac{1}{6} \oint_\Sigma K = -\frac{1}{6} \oint_\Sigma \tilde{H}_{ab} \tilde{H}^{ab}.\] Since the Euler characteristic does not contribute to the functional gradient, this establishes that the variation of the anomaly \(A\) in Equation (4.10) is given by \(\frac{3}{2} B\) in accordance with Equation (5.1).

In dimension \(d = 4\), the obstruction density \(B\) was computed explicitly in [GGHW15] by using the holographic formula of [GW15, Theorem 8.11]:

\[B = \frac{1}{6} L^{ab} \left( 2 \tilde{H}^{(a(b)c)} + \mathcal{F}^{(ab)c} \right) - \tilde{H}^{ab} B_{ab} + \frac{1}{2} K^2 + \mathcal{F}^{(ab)c} \tilde{H}^{bc} + 2 \mathcal{F}_{ab} + (\hat{n}^d W_{dabc})^\top \hat{n}^e W_{eabc}.\]

This density was proved to be the functional gradient of \(\frac{1}{6} \oint_\Sigma \tilde{H}_{ab} \tilde{H}^{ab}\) (see [GGHW15, Proposition 1.2]). For compactly supported variations, the double divergence term in the three dimensional extrinsic \(Q\)-curvature formula (4.15) does not contribute to the functional gradient. Hence the variation of the \(d = 4\) anomaly \(A\) is precisely \(4B\), which once again agrees with Equation (5.1).

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**Appendix A. Explicit metrics**

Given an explicit metric and hypersurface

\[ ds^2 = g, \quad \Sigma = Z(\sigma), \]

and a choice of scale \(\tau = [g; \tau]\), with the aid of computer software (see for example [LMP01]) it is not difficult to calculate the divergences and anomaly for the regulated volume for a singular metric determined by a asymptotic solution to the singular Yamabe as described in Theorem 4.1. These are given by our formula:

\[
\text{Vol}_\varepsilon = \sum_{k=1}^{d-1} \frac{(k-1)!}{(d-k-1)!(d-2)!k} \frac{1}{\varepsilon^k} + \oint_\Sigma (-L)^{d-1} \log \tau \frac{1}{(d-1)!(d-2)!} \log \varepsilon + \mathcal{O}(\varepsilon^0). \tag{A.1}
\]

The divergences will in general depend on the choice of true scale \(\tau\) while the anomaly given by the coefficient of the logarithm is a conformal invariant. Given \(g\), a natural choice for the scale is \(\tau = [g; 1]\). We will compute the above formula in that scale for explicit four and five dimensional hypersurfaces \(\Sigma\).

**A.1. The Kasner metric.** The Kasner metric models spatially inhomogeneous expanding cosmologies; see for example [LL51, Chapter 14]. Consider the following metric and hypersurface:

\[
\text{Vol}_\varepsilon = \sum_{k=1}^{d-1} \frac{(k-1)!}{(d-k-1)!(d-2)!k} \frac{1}{\varepsilon^k} + \oint_\Sigma (-L)^{d-1} \log \tau \frac{1}{(d-1)!(d-2)!} \log \varepsilon + \mathcal{O}(\varepsilon^0). \tag{A.1}
\]

Here \(\Sigma\) is some bounded region in the \(t = 1\) coordinate slice. Thus, in this example the hypersurface \(\Sigma\) is not closed, and \textit{a priori} the anomaly and divergences can acquire contributions integrated along \(\partial \Sigma\), arising from the divergence term in the integration by parts result of Theorem 4.1. In fact, by choosing a bulk integration region intersecting \(\Sigma\) orthogonally, these terms vanish for this example. Again we defer a detailed study of
these terms to a sequel article. We work in Euclidean signature but it is not difficult to extend our results to the physical Lorentzian signature in which $t$ becomes a time coordinate and $\Sigma$ is a spatial region.

The mean curvature and the traced-square of the second fundamental form for the hypersurface $\Sigma$ have simple expressions in terms of the parameters $(\alpha, \beta, \gamma)$:

$$H = \frac{\alpha + \beta + \gamma}{3} \quad \Pi^2 := \Pi_{ab} \Pi^{ab} = \alpha^2 + \beta^2 + \gamma^2.$$

Also, the rigidity density of $\Sigma$ is given by

$$K := \Pi_{ab} \Pi^{ab} = \Pi^2 - 3H^2.$$

Note that along $\Sigma$, the scalar curvature obeys

$$J_{\Sigma} = -\frac{K + 6H(2H - 1)}{6}.$$

Imposing the Kasner conditions

$$H = 0 = \Pi^2$$

on the parameters $(\alpha, \beta, \gamma)$, the metric $g := ds^2$ becomes the Ricci-flat Kasner metric, but for added generality, we relax these conditions in the following computation.

Denoting $\sigma = t - 1$, we introduce the defining density $\sigma = [g, \sigma]$ which can, according to Theorem 4.1, be improved to a conformal unit defining density $\bar{\sigma}$. An explicit recursion for finding $\sigma = [g; \bar{\sigma}]$ is given in [GW14, Proposition 4.9] (see also the examples in [GGHW15, Appendix A]). Applying this recursion we find

$$(A.3) \quad \bar{\sigma} = \sigma \left(1 + \frac{H}{2} \sigma + \left[\frac{J_{\Sigma}}{6} + \frac{H(H - 1)}{2}\right] \sigma^2 - \left[\frac{(5H - 6)K}{72} - \frac{H(H - 2)(H - 3)}{24}\right] \sigma^3\right).$$

The corresponding $S$-curvature obeys

$$S = 1 + \sigma^4 [g; B + O(\sigma)],$$

with obstruction density given by $B = [g; B]$ where

$$B = \frac{K(H - 1)^2}{4}.$$ 

Choosing the true scale $\tau = [g; 1]$ and using Equations (2.4) and (2.5) it is not difficult to compute

$$L \frac{1}{\tau^2} \bigg|_{\Sigma} = -4H, \quad L^2 \frac{1}{\tau} \bigg|_{\Sigma} = -2J_{\Sigma}, \quad L^3 \log \tau \bigg|_{\Sigma} = 4K(H - 1).$$

Hence, using Equation (A.1), we have

$$(A.4) \quad \text{Vol}_\varepsilon = A_{\Sigma}^g \left(\frac{1}{3\varepsilon^3} + \frac{H}{\varepsilon^2} - \frac{J_{\Sigma}}{2\varepsilon} - \log \varepsilon \frac{K(H - 1)}{3}\right) + O(1),$$

where $A_{\Sigma}^g$ is the area of the hypersurface $\Sigma$. This equation should be compared with our general result for spaces embedded in four-manifolds in (4.15).

As a final check on this result, given the simplicity of the Kasner-type metric in Equation (A.2), we can compute the integral defining the regulated volume in Equation (3.2) by brute force. In particular, we wish to compute

$$(A.5) \quad \text{Vol}_\varepsilon = \int_{D_\varepsilon} \sqrt{\det g} \frac{\varepsilon^4}{\bar{\sigma}^4}.$$
For simplicity, we take $D_\varepsilon$ to be the volume determined by the solid coordinate cylinder
\[(t, x, y, z) \mid (x, y, z) \in \Sigma, \varepsilon \leq \bar{\sigma}(t) \text{ and } t < R\].
This corresponds to the volume of the dark gray trumpet-shaped space-time region depicted below:

To compute the Laurent series expansion in $\varepsilon$ of the integral in Equation (A.5), we expand the integrand in powers of $\sigma = t - 1$ and find
\[
\frac{\sqrt{\det g}}{\bar{\sigma}^4} = \frac{1}{(t-1)^2} + \frac{H}{(t-1)^3} + \frac{K + 3H(H - 3/2)}{9(t-1)^2} + \frac{K(H - 1)}{3(t-1)} + O(1).
\]
We must also solve
\[
\bar{\sigma}(t_0) = \varepsilon,
\]
with $\bar{\sigma}$ given by Equation (A.3), for the starting point of the $t$-integral as a power series in $\varepsilon$. For that we find
\[
t_0 = 1 + \varepsilon + \frac{H}{2} \varepsilon^2 + \frac{K + 12H(H + 1)}{36} \varepsilon^3 + O(\varepsilon^4).
\]
Assembling the above data, the integration over $t$ in Equation (A.5) is easy to perform and gives
\[
\int_{t_0}^R dt \frac{\sqrt{\det g}}{\bar{\sigma}^4} = \frac{1}{3\varepsilon^3} + \frac{H}{\varepsilon^2} - \frac{J|\Sigma|}{2\varepsilon} - \frac{K(H - 1)}{3} \log \varepsilon + O(1).
\]
This matches perfectly the regulated volume expression (A.4).

A.2. Generalized Hawking energies. The Hawking energy associated to a compact spatial region with boundary $\Sigma$ depends on the integral of mean curvature squared $\int_\Sigma H^2$. For conformally flat structures, this quantity recovers the Willmore energy of $\Sigma$. Therefore it is interesting to wonder whether the higher dimensional generalizations of the Willmore functional provided by the anomaly $\mathcal{A}$ are relevant to the problem of constructing quasi-local conserved quantities for general relativity in dimensions greater than four. We will not consider this problem any further except as motivation to compute the regulated volume for spatial regions of a six dimensional Schwarzschild black hole.

The six dimensional Schwarzschild metric is given by
\[
-\left(1 - \frac{r_0^3}{r^3}\right) dt^2 + ds^2,
\]
where the Euclidean signature spatial metric
\[
ds^2 = \frac{dt^2}{1 - \frac{r_0^3}{r^3}} + r^2 d\Omega^2,
\]
and $dQ^2$ is the metric for a round 4-sphere. We take as data for our regulated volume the pair

$$g = ds^2, \quad \Sigma = Z(r - r_0).$$

Here $\Sigma$ is the closed hypersurface given by a 4-sphere of radius $r_0 > r_s$. We then consider the regulated volume of a bounded region $D$ with inner boundary $\Sigma$.

The hypersurface $\Sigma$ is umbilic (vanishing trace-free second fundamental form) with mean curvature

$$H = \sqrt{1 - \frac{r^3}{r_0^3}} \cdot \frac{r^3}{r_0}.$$

The metric $ds^2$ has vanishing (and therefore constant) scalar curvature $J = 0$. However, the hypersurface $\Sigma$ is not a conformal infinity of $ds^2$ so this metric does not solve the our singular Yamabe problem. Indeed

$$\bar{\sigma} = H r_0^2 s \left(1 - \frac{5\mu - 2}{4} s + \frac{\mu(5\mu^2 - 154\mu - 256)}{24} s^2 + \frac{\mu(3\mu^3 + 50\mu^2 + 944\mu + 704)}{384} s^3\right),$$

where

$$s := \frac{r - r_0}{H^2 r_0^3} \quad \text{and} \quad \mu := \frac{r^3}{r_0^3}.$$

determines a conformal unit defining density $\sigma = [g; \bar{\sigma}]$. Moreover, we find that the corresponding $\mathcal{S}$-curvature obeys

$$\mathcal{S} = 1 + \mathcal{O}(\sigma^6),$$

so that the obstruction density vanishes. This implies that the surface $\Sigma$ is a critical point of the generalized Willmore functional $\mathcal{A}$.

Once again, choosing the true scale $\tau = [g; 1]$ and using Equations (2.4) and (2.5), we can compute the local terms appearing in divergences and the anomaly:

$$L^1 \mid_{\Sigma} = -9H, \quad L^2 \mid_{\Sigma} = 6 \left(H^2 + \frac{2}{r_0^3}\right), \quad L^3 \mid_{\Sigma} = 6H \left(H^2 - \frac{4}{r_0^3}\right), \quad L^4 \mid_{\Sigma} = \log \tau.$$

Equation (A.1) then gives the regulated volume

$$\text{Vol}_\epsilon = \frac{8\pi^3}{3} \left(\frac{r_0^3}{4\epsilon^4} + \frac{H r_0^3}{\epsilon^3} + \frac{\epsilon^2 (H^2 r_0^2 + 2)}{4\epsilon^2} + \frac{H r_0^3 (H^2 r_0^2 - 4)}{6\epsilon}\right) - \pi^3 \log \epsilon + \mathcal{O}(1).$$

The coefficients of the four divergences above match our general results given in Equations (A.1), (4.8) and Appendix B.

**Appendix B. NNLO divergence**

The nnlo divergence for the case of a conformal unit defining density is given, according to Equation (1.5), in dimension $d \geq 5$ by

$$-\frac{\int_{\Sigma} L^3 \tau^{4-d}}{3!(d-2)(d-3)(d-4)^2 \epsilon^{d-4}}.$$

The main ingredients required to compute $L^3 \tau^{4-d} \mid_{\Sigma}$ were given in [GW14].

We work in the scale $\tau = [g; 1]$ and first use Equation (2.4) to compute one power of the Laplace–Robin operator

$$L \mid_{\Sigma} = [g; (d-4)((d-6)\rho + \bar{\sigma} J)].$$
Thus
\[
L^2 \tau^{4-d} = -(d-4) \left[ g; (d-4) \left( (d-6)(\nabla_n \rho - (d-3)\rho^2) + J \right) + \bar{\sigma}((d-2)(\nabla_n - (d-2)\rho)J + (d-6)\Delta \rho) + O(\bar{\sigma}^2) \right].
\]

In the above we used that for a conformal unit defining density \(n^2 = 1 - 2\rho\bar{\sigma} + O(\rho^d)\) and that \(\nabla_n u = -d\rho - \bar{\sigma} J\). In turn
\[
L^3 \tau^{4-d} \equiv (d-2)(d-4) \left[ g; (d-4)(d-6)(\nabla_n^2 \rho + (3d-8)H \nabla_n \rho - (d-2)(d-3)H^3) + 2(d-3)(\nabla_n J + (d-2)H J) + (d-6)\Delta \rho \right].
\]

Here we have again used the aforementioned conformal unit defining density properties as well as Lemma 2.3. By virtue of the second identity in Equation (4.11) we have
\[
L^3 \tau^{4-d} \equiv (d-2)(d-4) \left[ g; (d-3)(d-6)(\nabla_n^2 \rho + (3d-10)H \nabla_n \rho - (d-2)(d-4)H^3) + 2(d-3)(\nabla_n J + (d-2)H J) - (d-6)\Delta H \right].
\]

Now we employ Equations (4.12), (4.13) and (4.14) to obtain the required result:
\[
L^3 \tau^{4-d} \equiv (d-4) \left[ g; -2(d-6) \left( \nabla^a \nabla^b H_{ab} - (d-3)(d-4)H \left( (d-2)P_{ab} \hat{a}^a \hat{b}^b + K \right) \right) 
- (d-2)(d-6) \left( (d-2) \nabla^a \nabla \bar{F}_{ab} + (d-4)(\nabla^a (P_{ab} \hat{b}^b)) \right) 
+ (d-2)(d-3)(\hat{a}^a \nabla_a J + (3d-10)H J - (d-2)(d-4)(d-6)H^3) \right].
\]
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