PAPER

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Vacuum initial data on $\mathbb{S}^3$ from Killing vectors

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Abstract

We construct compact initial data of constant mean curvature $\widetilde{K}$ for Einstein's 4d vacuum equations with $\widehat{\Lambda} = \Lambda - (\widetilde{K}^2/3)$ positive, where Λ is the cosmological constant, via the conformal method. To construct a transverse, trace-free (TT) momentum tensor explicitly we first observe that, if the seed manifold has two orthogonal Killing vectors, their symmetrized tensor product is a natural TT candidate. Without the orthogonality requirement, but on locally conformally flat seed manifolds there is a generalized construction for the momentum which also involves the derivatives of the Killing fields found in work by Beig and Krammer (2004 *Class. Quantum Grav.* **21** 73). We consider in particular the round three sphere and classify the TT tensors resulting from all possible pairs of its six Killing vectors, focusing on the commuting case where the seed data are $\mathbb{U}(1) \times \mathbb{U}(1)$—symmetric. As to solving the Lichnerowicz equation, we discuss in particular potential 'symmetry breaking' by which we mean that solutions have less symmetries than the equation itself; we compare with the case of the 'round donut' of topology $\mathbb{S}^2 \times \mathbb{S}$. In the absence of symmetry breaking, the Lichnerowicz equation for a $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric momentum on $\mathbb{S}^3$ reduces to an ODE. We analyze distinguished families of solutions and the resulting data via a combination of analytical and numerical techniques. Finally we investigate marginally trapped surfaces of toroidal topology in our data.

Keywords: conformal method, Lichnerowicz equation, cosmology

(Some figures may appear in colour only in the online journal)

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1. Introduction

We construct certain solutions of the initial value constraints in the compact case for the 4d Einstein equations with cosmological constant Λ. Our tool is the conformal method (see [7, 15] for recent reviews). Simplifying the general procedure, we set out from a 'seed manifold' defined as follows.

Definition 1. A seed manifold $(\mathcal{M}, g_{ij}, L_{ij})$ consists of a compact 3-dim. manifold $(\mathcal{M}, g_{ij})$ with smooth metric in the positive Yamabe class [18] and of a smooth tensor L_{ij} on $\mathcal{M}$ which is transverse and traceless (TT; meaning $g^{ij}L_{ij} = 0 = \nabla^i L_{ij}$ where ∇ is the covariant derivative).

We wish to turn this into an initial data set of the following form:

Definition 2. As CMC initial data $(\widetilde{\mathcal{M}}, \widetilde{g}_{ij}, \widetilde{K}_{ij})$ $(i,j, = 1, 2, 3)$ for vacuum with cosmological constant Λ we take a compact three-dim. Riemannian manifold $\widetilde{\mathcal{M}}$ with smooth metric $\widetilde{g}_{ij}$ and smooth symmetric $(0, 2)$—tensor field $\widetilde{K}_{ij}$ which has constant trace $\widetilde{g}^{ij}\widetilde{K}_{ij} = \widetilde{K} = \mathrm{const}$ and satisfies the constraints

$$\widetilde{R} = \widetilde{K}_{ij}\widetilde{K}^{ij} - \widetilde{K}^2 + 2\Lambda, \qquad \widetilde{\nabla}_i\widetilde{K}^{ij} = 0. \tag{1}$$

Here $\widetilde{\nabla}$ and $\widetilde{R}$ are the covariant derivative and the scalar curvature of $\widetilde{g}_{ij}$.

To do so we need a smooth positive solution ϕ of the Lichnerowicz equation

$$\left(\Delta - \frac{1}{8}R\right)\phi = -\frac{1}{4}\widehat{\Lambda}\phi^5 - \frac{V^2}{8\phi^7} \tag{2}$$

where $\Delta = \nabla^i\nabla_i$ and R are the Laplacian and the scalar curvature of g_{ij}, and we have defined $\widehat{\Lambda} = \Lambda - (\widetilde{K}^2/3)$ and $V^2 = L^{ij}L_{ij}$. For every such ϕ the 'physical' quantities

$$\widetilde{g}_{ij} = \phi^4 g_{ij}, \qquad \widetilde{K}_{ij} - \frac{1}{3}\widetilde{g}_{ij}\widetilde{K} = \phi^{-2}L_{ij} \tag{3}$$

indeed satisfy the constraints (1). The quantities $\widetilde{g}_{ij}$ and $\widetilde{K}_{ij}$ become the induced metric and second fundamental form (with constant mean curvature $\widetilde{K}$) of a spacelike slice in the spacetime resulting from evolution under the $\Lambda-$ vacuum Einstein equations. For zero momentum $V \equiv 0$ equation (2) is equivalent to the Yamabe problem [18]. We restrict ourselves to constructing data for which $\widehat{\Lambda} > 0$; see [7] for the case $\widehat{\Lambda} \leqslant 0$.

Remark on notation. In what follows we abbreviate 'CMC initial data' by 'data' and the 'seed manifold' by 'seed'. Moreover, 'solutions' ϕ of (2) are always understood to be smooth and positive.

Needless to say, the non-linearities of (2) are unpleasant. On the other hand, it is precisely due to this structure that the conformal method is capable in principle of generating 'interesting' data from trivial seeds. In order to commemorate the centenary of the work of our compatriot Friedrich Kottler [17] (The Cracow region was with Austro–Hungary at that time) we recall here the generation of time-symmetric $(\widetilde{K}_{ij} \equiv 0)$ data for the Kottler ('Schwarzschild–de Sitter') solution from a trivial seed. Namely, we consider the 'round unit donut' $\mathbb{S}^2 \times \mathbb{S}^1$ with a unit $\mathbb{S}^2$ and an $\mathbb{S}^1$- circumference B i.e.

$$\mathrm{d}s^2 = \left(\mathrm{d}\xi^2 + \mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\varphi^2\right) \quad \text{where} \quad \xi \in [0, B] \tag{4}$$

and solve (2) for $V \equiv 0$. Since $R = 2$ there is the trivial solution $\phi \equiv \Lambda^{-1/4}$, but in addition we have k solutions of (2) if $B \in (2\pi k, 2\pi(k + 1)]$, $(k \in \mathbb{N}_0)$ which break the $\mathbb{U}(1)$ symmetry of

the seed metric and of the equation. The concept of symmetry breaking used here is the obvious one, but see definition 7 below for the formal statement. Accordingly, there are k non-trivial physical data $(\widetilde{\mathcal{M}}, \widetilde{g}_{ij})$ which contain j pairs $(1 \leqslant j \leqslant k)$ of maximal and minimal surfaces (see [25]). The resulting spacetime (which Kottler of course obtained like Schwarzschild, namely via a spherically symmetric ansatz to Einstein's equations) then contains j pairs of static 'black hole' and 'cosmological' horizons.

In this paper we focus on $\mathbb{S}^3$, which is another well-known example for the Yamabe problem. In this case there is even a 4-(continuous-) parameter family of non-trivial (i.e. symmetry breaking) solutions of (2) with $V \equiv 0$. Curiously, however, none of these solutions leads to new geometry, i.e. conformal rescaling just rescales the round sphere in a non-trivial way. We recall this in section 4.2.

The key issue in the present work is a natural way of constructing TT tensors on seed manifolds with continuous isometries (Killing vectors, KVs). The simplest case consists of any seed which enjoys a pair of orthogonal KVs Π and Υ, since their symmetrized tensor product

$$L_{ij}^{\perp} = \Pi_{(i} \Upsilon_{j)} \tag{5}$$

is TT. Such orthogonal KVs are e.g. $\Pi = \partial/\partial\xi$ and $\Upsilon = \partial/\partial\varphi$ on the donut (4). For a pair of general (but possibly parallel) KVs there is a generalisation of (5), which still yields a TT tensor provided $(\mathcal{M}, g_{ij})$ is of constant curvature, i.e. $3 R_{ij} = R g_{ij}$. On the unit sphere (where $R = 6$) in particular, it reads

$$L_{ij}^{(\Pi,\Upsilon)} = \Pi_{(i}\Upsilon_{j)} + (\operatorname{curl}\Pi)_{(i}(\operatorname{curl}\Upsilon)_{j)} - \frac{1}{3} g_{ij} \left(\Pi^k \Upsilon_k + (\operatorname{curl}\Pi)^k (\operatorname{curl}\Upsilon)_k \right). \tag{6}$$

In this paper we define 'curl' via

$$(\operatorname{curl}\Pi)_i := \frac{1}{2} \epsilon_i{}^{jk} \nabla_j \Pi_k \tag{7}$$

which is 1/2 of the standard definition but saves factors of 2 elsewhere. We call (6) 'Beig–Krammer-tensor' in view of a more general construction [2] requiring just a conformal KV and a divergence-free vector, on any locally conformally flat manifold.

Restricting ourselves now to the round three sphere as a seed, our aim is to classify the momenta (6) which arise from all possible pairs of KVs. We first note that for two generic KVs on $\mathbb{S}^3$ the momentum term (6) (and hence the evolving spacetimes) will not have any symmetries whatsoever. As to classifying the special cases, the key is the unique decomposition of any KV Υ on $\mathbb{S}^3$ (see lemma 1) in terms of its self-dual (sd) and antiself-dual (asd) parts

$$\Upsilon = \Omega + \Sigma \tag{8}$$

defined via $\operatorname{curl}\Omega = \Omega$ and $\operatorname{curl}\Sigma = -\Sigma$. Our result reads as follows. (We omit obvious statements which result from applying the (anti-)symmetry between sd and asd items):

Theorem 1. (Simplified version; for full statement see section 3.) *Let Π and Υ be two Killing vectors on $\mathbb{S}^3$ (possibly parallel). Then the following holds:*

  I. The Λ–Taub-NUT case. If Π is self-dual, and if the anti-self dual parts of Π and Υ are proportional, $L_{ij}^{(\Pi,\Upsilon)}$ is $\mathbb{SO}(3) \times \mathbb{U}(1)$ invariant.

  II. The homogeneous case. If Π is self-dual, $L_{ij}^{(\Pi,\Upsilon)}$ is $\mathbb{SO}(3)$ invariant.

  III. The $\mathbf{U}(1) \times \mathbf{U}(1)$ case. If Π and Υ commute, $L_{ij}^{(\Pi,\Upsilon)}$ is $\mathbb{U}(1) \times \mathbb{U}(1)$ invariant.

  IV. The $\mathbf{U}(1)$ case. If the antiself-dual parts of Π and Υ are proportional, $L_{ij}^{(\Pi,\Omega)}$ is $\mathbb{U}(1)$ invariant.

As to solving the Lichnerowicz equation (2) with momentum term, the key result is due to Premoselli [24]. In essence (we recall the full statement in section 4.1) it reads as follows, in terms of a constant $b \in \mathbb{R}^+$ extracted arbitrarily from $V = b\,\overline{V}$: there exists a $b_\star \in (0, \infty)$ such that (2) has at least two solutions for $0 < b < b_\star$, precisely one solution for $b = b_\star$, and no solution for $b > b_\star$. While this result applies to seeds without any symmetry restrictions, it settles in particular existence and non-existence in the cases of present interest, namely $\mathbb{S}^3$ and $\mathbb{S}^2 \times \mathbb{S}$.

We are now particularly interested if the 'symmetry breaking' mechanism discussed above for the Yamabe problem ($b = 0$) persists for $b \neq 0$. This is indeed the case in the above-mentioned $\mathbb{S}^2 \times \mathbb{S}$-example—in particular 'rotating Kottler data' arise in a natural way by solving (2) on the donut (4), with a momentum given by (5) (see [4] and section 4.3 below). On the other hand, on $\mathbb{S}^3$ it seems that the symmetry breaking Yamabe solutions mentioned before, and discussed at length in section 4.2, do not survive the addition of any momentum term. More precisely, our findings in the cases listed in theorem 1 are as follows: in the homogeneous case (which clearly includes Λ-Taub-NUT) we have $V^2 = \text{const}$. From a theorem by Brezis and Li [6], this implies $\phi = \text{const}$ for solutions of (2), which yields an algebraic equation for ϕ. On the other hand, for the $\mathbb{U}(1) \times \mathbb{U}(1)$- invariant momenta of point III above, the commuting Killing fields span a torus, and V depends only on one variable x labelling a toroidal foliation of $\mathbb{S}^3$. Combining numerical techniques with analysis we claim that there are no symmetry breaking solutions for $b \neq 0$. More precisely, we conjecture (see conjecture 2 for which we give a partial proof) that ϕ only depends on x as well, whence (2) reduces to an ODE whose observed solutions are just a 'Premoselli pair' for every $b < b_\star$ (see conjecture 1). We display numerical results in the cases that Π and Υ are orthogonal and parallel.

The final section 5 deals with marginally (outer) trapped surfaces (MTSs, MOTSs) and marginally trapped regions (MTRs). The former are two-surfaces $\mathcal{S}$ defined by $\widetilde{\Theta}^\pm = 0$ for at least one of the null expansions $\widetilde{\Theta}^\pm$ on $\mathcal{S}$, while the latter are regions bounded by MTSs. Our motivation comes from a recent criterion for the 'visibility' of such MOTSs and MTSs from timelike infinity in asymptotically de Sitter spacetimes, theorem 2.5. of [8]. We first review this result and discuss it in detail for toroidal MOTSs and MTRs in de Sitter spacetime. We next note that an extension of this discussion to perturbations of de Sitter seems feasible by virtue of Friedrich's general stability results [12]; we formulate a corresponding conjecture. Finally we consider the $\mathbb{U}(1) \times \mathbb{U}(1)$- symmetric data constructed in section 4.2 in the three special cases of Λ− Taub-NUT, and for Π and Υ orthogonal and parallel. These data form one-parameter families in which we can locate toroidal MOTSs analytically (Λ− Taub NUT) or numerically in the other cases. While the orthogonal case only yields the same (Clifford-) torus as de Sitter itself, the MOTSs are quite non-trivial in the parallel case. We leave a discussion of the 'visibility results' for such MOTSs and MTRs in the near-de Sitter setting to future work.

2. The three sphere and its symmetries

The subsequent discussion of $\mathbb{S}^3$ is adapted to our construction (6) of TT momenta discussed in detail the next section, and focuses accordingly on pairs of KVs. While our presentation is largely coordinate independent (in this section, we require coordinates in the proof of lemma 3 only) coordinate expressions are included occasionally to increase clarity. The most useful ones for our purposes are the following.

We restrict ourselves to the unit sphere embedded in flat $\mathbb{R}^4$, viz.

$$\mathrm{d}s^2 = \mathrm{d}z_1^2 + \mathrm{d}z_2^3 + \mathrm{d}z_3^2 + \mathrm{d}z_4^2 \qquad z_1^2 + z_2^3 + z_3^2 + z_4^2 = 1. \tag{9}$$

We define 'toroidal coordinates' (τ, γ, ξ) $\tau \in (0, \pi/2)$, $\gamma, \xi \in (0, 2\pi)$ by

$$z_1 = \sin\tau\sin\gamma, \; z_2 = \sin\tau\cos\gamma, \; z_3 = \cos\tau\sin\xi, \; z_4 = \cos\tau\cos\xi \tag{10}$$

which yields

$$\mathrm{d}s^2 = \mathrm{d}\tau^2 + \sin^2\tau\mathrm{d}\gamma^2 + \cos^2\tau\mathrm{d}\xi^2. \tag{11}$$

The name originates in the toroidal foliation $\tau = \mathrm{const}$.

The Riemann and Ricci tensors and the scalar curvature are given by

$$R_{ijkl} = 2g_{k[i}g_{j]l}, \qquad\qquad R_{ij} = 2g_{ij}, \qquad\qquad R = 6. \tag{12}$$

We write scalar products as $\langle\Pi, \Upsilon\rangle = \Pi_i\Upsilon^i$, the vector product as $(\Pi \times \Upsilon)_i = \epsilon_i{}^{jk}\Pi_j\Upsilon_k$ and the commutator (Lie bracket) $[\Pi, \Upsilon]^j = \Pi^i\nabla_i\Upsilon^j - \Upsilon^i\nabla_i\Pi^j$ is also standard. There are six independent KVs which satisfy

$$\nabla_i\nabla_j\Pi_k = -2g_{i[j}\Pi_{k]}. \tag{13}$$

Next observe that curl defined by (7) maps KVs into KVs and satisfies curl curl $= 1$ on KVs. This leads to the following key definition

Definition 3. We call Killing vectors Ω, Σ selfdual (sd) or antiself-dual (asd) when they obey curl $\Omega = \Omega$ resp. curl $\Sigma = -\Sigma$.

The Lie bracket of KVs can be written as

$$[\Pi, \Upsilon] = (\mathrm{curl}\,\Upsilon) \times \Pi - (\mathrm{curl}\,\Pi) \times \Upsilon. \tag{14}$$

Thus KVs which are curls of each other commute. Furthermore it follows that

$$[\mathrm{curl}\,\Pi, \Upsilon] = [\Pi, \mathrm{curl}\,\Upsilon], \tag{15}$$

so that sd and asd KVs also commute. We next note the identity

$$\mathrm{curl}\,(\Pi \times \Upsilon) = \frac{1}{2}(\Pi\,\mathrm{div}\Upsilon - \Upsilon\,\mathrm{div}\Pi - [\Pi, \Upsilon]) \tag{16}$$

valid for arbitrary vector fields Π, Υ, which obviously reduces to

$$\mathrm{curl}\,(\Pi \times \Upsilon) = -\frac{1}{2}[\Pi, \Upsilon] \tag{17}$$

for KVs. Still for KVs, (14), (15) and (17) now imply

$$\mathrm{curl}\,[\Pi, \Upsilon] = [\Pi, \mathrm{curl}\,\Upsilon] = [\mathrm{curl}\,\Pi, \Upsilon]. \tag{18}$$

The Cartan–Killing metric is proportional to

$$\mathcal{G}(\Pi, \Upsilon) = \frac{1}{2}\left(\langle\Pi, \Upsilon\rangle + \langle\mathrm{curl}\,\Pi, \mathrm{curl}\,\Upsilon\rangle\right). \tag{19}$$

Given Killing vectors Π, Υ, the expression (19) is constant on $\mathcal{M}$. It is positive definite and curl is self-adjoint w.r. to $\mathcal{G}$, i.e.

$$\mathcal{G}(\mathrm{curl}\,\Pi, \Upsilon) = \mathcal{G}(\Pi, \mathrm{curl}\,\Upsilon). \tag{20}$$

It has thus real eigenvalues, namely ± 1 (which we knew already) and we obtain the following result.

Lemma 1. *The Lie algebra of Killing vectors in $\mathbb{S}^3$ decomposes into a direct sum of self-dual and antiself-dual Killing vectors satisfying respectively* $\mathrm{curl}\,\Pi = \pm\Pi$. *In other words we can write every Killing vector* Π *uniquely as*

$$\Pi = \Omega + \Sigma \tag{21}$$

where Ω *is self-dual and* Σ *is antiself-dual. Moreover, we have*

$$\|\Omega\|^2 = \mathcal{G}(\Omega,\Omega) = \langle\Omega,\Omega\rangle = \mathrm{const} \qquad \|\Sigma\|^2 = \mathcal{G}(\Sigma,\Sigma) = \langle\Sigma,\Sigma\rangle = \mathrm{const}. \tag{22}$$

We note that the decomposition (21) is orthogonal w.r. to the Cartan–Killing metric, while there is no orthogonality w.r.t. to g_{ij}: $\langle\Omega,\Sigma\rangle \neq 0$.

We continue with another straightforward result.

Lemma 2. *Killing vectors* Π *and* Υ *on* $\mathbb{S}^3$ *commute iff the self-dual as well as the antiself-dual parts (21) of* Π *and* Υ *are linearly dependent. In terms of the decomposition (21) this means that (possibly after interchanging* Π *and* Υ*) there exist constants* $u \in \mathbb{R}$, $v \in \mathbb{R}$ *with*

$$\Pi = u\,\Omega + \Sigma, \qquad \Upsilon = \Omega + v\,\Sigma. \tag{23}$$

Remark. The statement above includes in particular all pairs involving sd and asd KVs (one has to put either $u = v = 0$, or $\Sigma = 0$, or $\Omega = 0$).

Proof. Inserting the sd-asd decomposition

$$\Pi = \Omega^\Pi + \Sigma^\Pi \qquad \Upsilon = \Omega^\Upsilon + \Sigma^\Upsilon \tag{24}$$

into (14) and using $[\Pi,\Upsilon] = 0$, yields

$$\Omega^\Pi \times \Omega^\Upsilon = \Sigma^\Pi \times \Sigma^\Upsilon. \tag{25}$$

But (14) and (17) imply that the vector product of KVs preserves the sd and asd subspaces. This implies that both sides of (25) vanish which yields the result. $\qquad\square$

We next choose bases Ω^A and Σ^A (capital latin indices take values 1, 2, 3; upper and lower indices mean the same) which are orthonormal w.r. to the Killing–Cartan metric. For the standard scalar product this implies

$$\langle\Omega^A,\Omega^B\rangle = \delta^{AB}, \qquad \langle\Sigma^A,\Sigma^B\rangle = \delta^{AB} \tag{26}$$

$$[\Omega^A,\Omega^B] = -2\epsilon^{AB}_{\ \ C}\,\Omega^C, \qquad [\Sigma^A,\Sigma^B] = 2\epsilon^{AB}_{\ \ C}\,\Sigma^C, \qquad [\Omega^A,\Sigma^B] = 0, \tag{27}$$

where $\epsilon_{ABC} = \epsilon_{[ABC]}$, $\epsilon_{123} = 1$ and, of course, $\mathrm{curl}\,\Omega^A = \Omega^A$ and $\mathrm{curl}\,\Sigma^A = -\Sigma^A$. Equation (27) means that the sd and asd subspaces form $\mathbb{SO}(3)$ Lie algebras, while all pairs with opposite duality commute. The different signs in the commutators are the natural convention in view of (14) which implies $[\Omega^A,\Omega^B] = -\Omega^A \times \Omega^B$ but $[\Sigma^A,\Sigma^B] = \Sigma^A \times \Sigma^B$. Then the remaining freedom in $\{\Omega^A,\Sigma^B\}$ are $\mathbb{SO}(3)$ - transformations $\mathcal{O}^A_{\ B}$, $\widehat{\mathcal{O}}^A_{\ B}$ of the form

$$\Omega^{A\prime} = \mathcal{O}^A_{\ B}\,\Omega^B, \qquad \Sigma^{A\prime} = \widehat{\mathcal{O}}^A_{\ B}\,\Sigma^B, \qquad \mathcal{O}^A_{\ B}\mathcal{O}^B_{\ C} = \delta^A_{\ C}, \qquad \widehat{\mathcal{O}}^A_{\ B}\widehat{\mathcal{O}}^B_{\ C} = \delta^A_{\ C}. \tag{28}$$

The vectors $\{\Omega^A,\Sigma^A\}$ act transitively on the $\mathbb{S}^3$.

In terms of the coordinates introduced in (10) and in terms of 'contravariant' components $\Omega^A = \Omega^{A\,i}(\partial/\partial x^i)$, $\Sigma^A = \Sigma^{A\,i}(\partial/\partial x^i)$, ordered as (τ,γ,ξ), they read

$$\Omega^1 = \begin{pmatrix} \cos(\gamma + \xi) \\ -\cot\tau\,\sin(\gamma + \xi) \\ \tan\tau\,\sin(\gamma + \xi) \end{pmatrix} \quad \Omega^2 = \begin{pmatrix} \sin(\gamma + \xi) \\ \cot\tau\,\cos(\gamma + \xi) \\ -\tan\tau\,\cos(\gamma + \xi) \end{pmatrix} \quad \Omega^3 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \tag{29}$$

$$\Sigma^1 = \begin{pmatrix} -\cos(\gamma - \xi) \\ \cot\tau\,\sin(\gamma - \xi) \\ \tan\tau\,\sin(\gamma - \xi) \end{pmatrix} \quad \Sigma^2 = \begin{pmatrix} -\sin(\gamma - \xi) \\ -\cot\tau\,\cos(\gamma - \xi) \\ -\tan\tau\,\cos(\gamma - \xi) \end{pmatrix} \quad \Sigma^3 = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix} . \tag{30}$$

We now proceed with a more subtle result.

Lemma 3. *Suppose the Killing vectors Π and Υ on $\mathbb{S}^3$ are orthogonal. Then either*

1. *both are either self- or antiself-dual, or*
2. *there are self and antiself-dual KVs Ω and Σ with $\|\Omega\| = \|\Sigma\|$ and a constant $c \in \mathbb{R} \setminus \{0\}$ such that*

$$\Pi = \Omega + \Sigma, \qquad \Upsilon = c(\Omega - \Sigma). \tag{31}$$

Proof. In terms of the decomposition

$$\Pi = c_A\Omega^A + d_B\Sigma^B, \qquad \Upsilon = \bar{c}_A\Omega^A + \bar{d}_B\Sigma^B \tag{32}$$

with constants $c_A, d_B, \bar{c}_A, \bar{d}_B, h_{AB} = (c_A\bar{d}_B + \bar{c}_A d_B)$ the requirement reads

$$0 = \langle \Pi, \Sigma \rangle = c^A\bar{c}_A + d^A\bar{d}_A + h_{AB}\langle \Omega^A, \Sigma^B \rangle. \tag{33}$$

Using the explicit forms (29) and (30) we obtain from (33)

$$\begin{aligned}
0 = {}& c^A\bar{c}_A + d^A\bar{d}_A - [h_{11}\cos(\gamma + \xi)\cos(\gamma - \xi) + h_{21}\sin(\gamma + \xi)\cos(\gamma - \xi) \\
& + h_{12}\sin(\gamma - \xi)\cos(\gamma + \xi) + h_{22}\sin(\gamma + \xi)\sin(\gamma - \xi)] \\
& + \sin(2\tau)[h_{13}\sin(\gamma + \xi) + h_{31}\sin(\gamma - \xi) - h_{32}\cos(\gamma - \xi) - h_{23}\cos(\gamma + \xi)] \\
& + \cos(2\tau)[-h_{11}\sin(\gamma + \xi)\sin(\gamma - \xi) + h_{21}\sin(\gamma - \xi)\cos(\gamma + \xi) \\
& + h_{12}\sin(\gamma + \xi)\cos(\gamma - \xi) - h_{22}\cos(\gamma + \xi)\cos(\gamma - \xi) + h_{33}]
\end{aligned} \tag{34}$$

for all (τ, γ, ξ). From this we first conclude that each bracket vanishes. The next step shows that $h_{AB} \equiv 0$ which also implies $c^A\bar{c}_A + d^A\bar{d}_A = 0$. Contracting now $h_{AB} \equiv 0$ with c^A and d^A we find the following: either all c_A and all $\bar{c}_A$, or all d_B and all $\bar{d}_B$ vanish, which yields the first alternative of the lemma. On the other hand, in the generic case we have non-vanishing constants e, f such that $\bar{c}_A = e.c_A$ and $\bar{d}_A = f.d_A$, and inserting this into $h_{AB} \equiv 0$ gives $f = -e$. Finally, inserting this into $0 = c^A\bar{c}_A + d^A\bar{d}_A = e(c_A c^A - d_A d^A)$ yields $\|\Omega\| = \|\Sigma\|$. This gives the stated result. $\square$

We note an obvious corollary to the above lemmas.

Corollary 1. *Suppose the Killing vectors Π and Υ are orthogonal and commute. Then only the second alternative of lemma 3 applies.*

Remark. The preceding discussion suggests the following definition. Let Ω and Σ be self- and antiself- dual KVs on $\mathbb{S}^3$, respectively. We define the 'toroidal pair' of Killing vectors Γ and Ξ via

$$\Gamma = \left(\frac{\Omega}{\|\Omega\|} + \frac{\Sigma}{\|\Sigma\|} \right), \qquad \Xi = \left(\frac{\Omega}{\|\Omega\|} - \frac{\Sigma}{\|\Sigma\|} \right). \tag{35}$$

The terminology originates in the fact that in toroidal coordinates (10), the tangents $\Gamma^A = \partial/\partial\gamma$ and $\Xi^A = \partial/\partial\xi$) to the torus $\tau = $ const indeed form a toroidal pair. In general, Γ and Ξ are orthogonal, curls of each other, commute, and each one is hypersurface orthogonal as it satisfies $\langle \Gamma, \mathrm{curl}\,\Gamma \rangle = 0 = \langle \Xi, \mathrm{curl}\,\Xi \rangle$. Furthermore, Γ and Ξ have zeros ('axes') aligned along mutually linked great circles of $\mathbb{S}^3$. In contrast, the Ω's and Σ's are neither hypersurface orthogonal nor do they have an axis, since they do not even have zeros.

Clearly, every KV Π enjoys a 'toroidal decomposition' via

$$\Pi = \Omega + \Sigma = p \left(\frac{\Omega}{\|\Omega\|} + \frac{\Sigma}{\|\Sigma\|} \right) + q \left(\frac{\Omega}{\|\Omega\|} - \frac{\Sigma}{\|\Sigma\|} \right) = p\,\Gamma + q\,\Xi \tag{36}$$

in terms of its self- and antiself- dual parts Ω and Σ, and with numbers p and q given by

$$2p = \|\Omega\| + \|\Sigma\|, \qquad 2q = \|\Omega\| - \|\Sigma\|. \tag{37}$$

Note, however, that there is some asymmetry in the decomposition (36) since the first term is always present (as $p > 0$), while the second term is absent if $\|\Omega\| = \|\Sigma\|$. Precisely such a special toroidal pair occurs as point 2 of lemma 3.

3. The Beig–Krammer tensor

Throughout the section, Π, Υ are KVs on $\mathbb{S}^3$, with self- and antiself-dual parts denoted by

$$\Pi = \Omega^\Pi + \Sigma^\Pi, \qquad \Upsilon = \Omega^\Upsilon + \Sigma^\Upsilon, \tag{38}$$

and $\{\Omega^A,\ \Sigma^B\}$ are the bases in the respective subspaces as introduced in (26) and (27).

The task is now to discuss the symmetries of the Beig–Krammer-tensor defined in the Introduction (6). We formulate its key property as follows.

Proposition 1. *On any space of constant curvature, i.e. $3R_{ij} = Rg_{ij}$, the following tensor is TT:*

$$L_{ij}^{(\Pi,\Upsilon)} = \Pi_{(i}\Upsilon_{j)} + (\mathrm{curl}\,\Pi)_{(i}(\mathrm{curl}\,\Upsilon)_{j)} - \frac{1}{3}g_{ij}\left(\Pi^k\Upsilon_k + (\mathrm{curl}\,\Pi)^k(\mathrm{curl}\,\Upsilon)_k \right). \tag{39}$$

Proof. This is a special case of the theorem in [2]; alternatively the result can be obtained by direct calculation. $\qquad\square$

The following lemma the proof of which is obvious from lemma 1 is key for our discussion of this tensor.

Lemma 4. *In terms of the decomposition (38) the tensor (39) reads*

$$L_{ij}^{(\Pi,\Upsilon)} = L_{ij}^{(\Omega)} + L_{ij}^{(\Sigma)} = 2\,\Omega_{(i}^\Pi\,\Omega_{j)}^\Upsilon - \frac{2}{3}\langle \Omega^\Pi, \Omega^\Upsilon \rangle g_{ij} + 2\,\Sigma_{(i}^\Pi\,\Sigma_{j)}^\Upsilon - \frac{2}{3}\langle \Sigma^\Pi, \Sigma^\Upsilon \rangle g_{ij}, \tag{40}$$

which reduces to

$$L_{ij}^{(\Pi,\Upsilon)} = 2u\,\Omega_i\,\Omega_j - \frac{2u}{3}\|\Omega\|^2 g_{ij} + 2v\,\Sigma_i\,\Sigma_j - \frac{2v}{3}\|\Sigma\|^2 g_{ij} \tag{41}$$

in the commuting case (see lemma 2).

The point of this lemma is that the differential expression (39) in terms of (Π, Υ) is replaced by the purely algebraic ones (40) and (41). We note that in these expressions there is no mixing between the sd and asd components. This leads to our key classification relating properties of the KVs Π and Υ to the symmetries of $L_{ij}^{(\Pi, \Upsilon)}$.

Theorem 1. *Let* Π *and* Υ *be two Killing vectors on* $\mathbb{S}^3$ *(possibly parallel). Then in terms of the decomposition (38) and the basis (26) and (27) we find*

I. The $\Lambda-$**Taub-NUT case.** *If* Υ *is self-dual, (i.e.* $\Sigma^\Upsilon = 0$*), and if* $\Omega^\Pi = u\,\Omega^\Upsilon$ *for some constant* $u \in \mathbb{R}$*, then* $L_{ij}^{(\Pi, \Upsilon)}$ *is invariant under the* $\mathbb{SO}(3) \times \mathbb{U}(1)$ *action generated by* $\{\Sigma^A, \Omega^\Pi\}$.

II. The homogeneous case. *If* Υ *is self-dual, (i.e.* $\Sigma^\Upsilon = 0$*), then* $L_{ij}^{(\Pi, \Upsilon)}$ *is invariant under the* $\mathbb{SO}(3)$ *action generated by* $\{\Sigma^A\}$.

III. The $\mathbb{U}(1) \times \mathbb{U}(1)$ **case.** *If* Π *and* Υ *commute,* $L_{ij}^{(\Pi, \Upsilon)}$ *is* $\mathbb{U}(1) \times \mathbb{U}(1)$ *invariant. From lemmas 2 and 4, the invariance is generated by* $\{\Omega, \Sigma\}$ *unless one of these latter vectors vanishes, in which case the invariance group enlarges to* $(\mathbb{SO}(3) \times \mathbb{U}(1)) \supset (\mathbb{U}(1) \times \mathbb{U}(1))$ *and yields* $\Lambda-$*Taub-NUT data (see I).*

IV. The unitary case. *If* $\Omega^\Pi = c\,\Omega^\Upsilon$ *for some constant* $c \in \mathbb{R}$*, then* $L_{ij}^{(\Pi, \Omega)}$ *is invariant under the* $\mathbb{U}(1)$ *action generated by* Ω^Π.

Proof. The main statements (*If..., then...*) of cases I, II and IV are immediate consequences of lemmas 1, 4, and the commutation relations (27). In addition, the proof that case I indeed produces $\Lambda-$ Taub-NUT data is postponed to the Appendix. As to case III, it is obvious that $L_{ij}^{(\Pi, \Upsilon)}$ in the original form (39) is $\mathbb{U}(1) \times \mathbb{U}(1)$ invariant under the action of its commuting generators Π and Υ, and hence under any linear combination thereof, *unless these vectors are parallel*. In this special case the full invariance still holds and follows from lemmas 2 and 4 as stated in III above. $\qquad\square$

Remarks.

1. We have omitted obvious counterparts to the above statements which result from applying the (anti-)symmetry between sd and asd items.
2. If Π and Υ are orthogonal, then the data are either homogeneous (case II) or $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric (case III), which follows immediately from the two cases of lemma 3.
3. Concerning the $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric data, there are the following interesting special cases (in the notation of lemma 2):

   Λ-**Taub-NUT:** Applies if one of the following holds: $\Sigma \equiv 0$, $\Omega \equiv 0$, $u = 0$, $v = 0$, or $u = v = 0$.

   the 'parallel' case: $u\,v = 1$ (but neither $\Sigma \equiv 0$ nor $\Omega \equiv 0$).

   the 'orthogonal' case: $u\,v = -1$ and $u\|\Omega\| = \|\Sigma\|$ (see point 2 of lemma 3). On these data we will focus our discussion of the Lichnerowicz equation in section 4 below, and determine the marginally trapped surfaces in the data in section 5.

4. From the previous remark it is clear that case I is a special case of any other one, while III is a special case of IV.

5. Some converse of the above theorem holds as well, i.e. invariances of $L_{ij}^{(\Pi, \Upsilon)}$ imply statements on Π and Υ. The proof is non-trivial in case III only; we refrain from giving details.

6. Clearly, the list in the above theorem is not exhaustive, i.e. there is a generic case (no continuous symmetries) as well.

4. The Lichnerowicz equation

4.1. Existence, stability and symmetry

We recall here key results [24] on solving the Lichnerowicz equation (2) and on proving properties of its solutions. Since both our seed manifold as well as the momentum term V^2 enjoy symmetries, it will in particular be important to examine the conditions under which the solutions inherit or break these symmetries. We recall from [4] some definitions and results on this issue. We then compare their application to the $\mathbb{S}^3$ and $\mathbb{S}^2 \times \mathbb{S}^1$ cases [4], respectively. We recall from the Introduction that a 'solution' is always understood to be smooth and positive.

Definition 4. The linearized Lichnerowicz operator L_ϕ and eigenvalue λ:

$$L_\phi \zeta := \left(-\Delta + \frac{R}{8} - \frac{5\widehat{\Lambda}}{4}\phi^4 + \frac{7V^2}{8\phi^8} \right) \zeta = \lambda \zeta. \tag{42}$$

Definition 5. Stability of solutions and initial data sets.

1. A solution ϕ of (2) is strictly stable/stable/marginally stable/unstable/strictly unstable iff the lowest eigenvalue λ is positive/nonnegative/zero/nonpositive/negative respectively.
2. An initial data set $(\widetilde{\mathcal{M}}, \widetilde{g}_{ij}, \widetilde{K}_{ij})$ is stable iff the solution $\phi \equiv 1$ is stable, and analogously for the other stability properties.

We remark that stability of a data set implies that in fact *every solution* (generating that data from an an arbitrary seed) is stable (see lemma 1 of [4]). Again this extends to all stability properties.

Proposition 2. *Uniqueness of stable solutions for convex potentials, see [10]. If stable solutions of (2) exist, they are unique.*

To see this, note that the potential term in equation (2) is strictly convex in the sense of proposition 1.3.1. of [10]. Thus, the latter result just requires adaptation from the autonomous case to the present non-autonomous one, and from Dirichlet boundary conditions to the present compact case. Both generalisations are trivial.

The Yamabe theorem (see [18, 26]). *Let $(\mathcal{M}, g_{ij})$ be compact and of positive Yamabe type. Then (2) with $V \equiv 0$ has at least one solution ϕ.*

Premoselli's theorem [24]. *Let $(\mathcal{M}, g_{ij})$ be compact and of positive Yamabe type. Writing $V = b.\overline{V}$ for a positive constant b and a function $\overline{V} \not\equiv 0$, the following holds:*

There exists $b_\star \in (0, \infty)$ such that equation (2) has, for

$b < b_\star$: more than one solution precisely one of which, ϕ_s, is strictly stable;
$b = b_\star$: a unique marginally stable solution;
$b > b_\star$: no solution.

Moreover, the unique stable solution $b \to \phi_s(b)$ for $b \in (0, b_\star]$ satisfies

1. $\lim_{b \to 0} \phi_s(b) = 0$;
2. the map $b \to \phi_s(b)$ is continuous and increasing in the sense that $\phi_s(b) < \phi_s(b')$ for $b < b'$, everywhere on $\mathcal{M}$;
3. every $\phi_s(b)$ is minimal in the sense that $\phi_s(b) < \phi$ everywhere, for any other solution ϕ.

This formulation combines theorem 1.1, proposition 3.1 (positivity), proposition 6.1 (stability and minimality) and lemma 7.1 (continuity) of [24]. Note that theorem 1.1 applies to a more general setting in which uniqueness of stable solutions need not hold; in the present case it does follow from proposition 2 above.

We turn now to the symmetry properties of solutions.

Definition 6 (Symmetric Lichnerowicz equation). We call equation (2) symmetric iff $(\mathcal{M}, g_{ij})$ and V^2 are invariant under some (discrete or continuous) isometry.

Clearly this definition is *a priori* less restrictive than the invariance of $(\mathcal{M}, g_{ij})$ and K_{ij} used in the remaining part of this paper.

Definition 7 (Symmetry inheritance/breaking). A solution ϕ of a symmetric Lichnerowicz equation (2) inherits a continuous symmetry Π iff the corresponding Lie derivative satisfies $\mathcal{L}_\Pi \phi \equiv 0$ while otherwise it breaks the symmetry. An analogous definition applies to discrete symmetries.

Proposition 3 (Symmetry inheritance/breaking; see proposition 2 and corollary 1 of [4]). *The stable solutions ϕ_s of (2) inherit continuous and discrete symmetries.*

Premoselli's theorem also implies that the solutions form branches parametrized by b. Of particular interest are results which characterize the behaviour of these branches near their end points $b = 0$ and $b = b_\star$. The minimal stable branch indeed enjoys such a 'universal' behaviour on either end; the precise results are as follows

Lemma 5 (Modified part of proposition 4 of [4]). *There is an $\epsilon > 0$ such that for all $b \in (b_\star - \epsilon, b_\star)$ there is precisely one stable and one unstable solution.*

Lemma 6 (Modified proposition 3 of [4]). *For the minimal, stable solutions $\lim_{b \to 0} b^{-1/4} \phi_s$ is finite.*

On the other hand, the number and the properties of the unstable branches largely depend on the seed and on V^2, which is revealed in particular by the examples discussed shortly. Nevertheless, some general information can be obtained via the implicit function theorem, bifurcation theory, and general results on elliptic PDEs. We recall in particular that a necessary condition for a bifurcation to occur at some b is that the linearized operator L defined as (42) has a zero eigenvalue.

In the next section 4.2 we discuss the $\mathbb{S}^3$ case which we compare in section 4.3 with the round unit donut $\mathbb{S}^2 \times \mathbb{S}$ (see (4)) elaborated in [4]. Noting that $R = 6$ in the former and $R = 2$ in the latter case, it proves useful to remove $\widehat{\Lambda}$ from (2) via the rescaling

$$\psi = \left(\frac{2\widehat{\Lambda}}{R}\right)^{1/4} \phi, \qquad W = 2\frac{\widehat{\Lambda} V}{R} \tag{43}$$

which yields

$$\left(\Delta - \frac{R}{8}\right)\psi + \frac{R}{8}\psi^5 + \frac{W^2}{8\psi^7} = 0 \tag{44}$$

for any $R = \text{const} > 0$. Note that $\psi \equiv 1$ now solves (44) for $W \equiv 0$. In terms of these variables, the linearization (42) reads

$$L_\psi \rho := \left(-\Delta + \frac{R}{8} - \frac{5R}{8}\psi^4 + \frac{7W^2}{8\psi^8}\right)\rho = \lambda\rho. \tag{45}$$

4.2. $\mathbb{S}^3$

In this case equation (44) becomes

$$\Delta\psi - \frac{3}{4}\left(\psi - \psi^5\right) + \frac{W^2}{8\psi^7} = 0. \tag{46}$$

When we use the coordinate system (11) with the substitution $x = \cos(2\tau), \quad x \in (-1, 1)$, we obtain

$$ds^2 = \frac{dx^2}{4(1-x^2)} + \frac{1+x}{2}d\gamma^2 + \frac{1-x}{2}d\xi^2 \tag{47}$$

which we will use occasionally in what follows.

We discuss in turn the Yamabe case $W \equiv 0$, the case that W is constant, and the generic $\mathbb{U}(1) \times \mathbb{U}(1)$-symmetric one.

(a) **$W \equiv 0$**: This case is well-known, see e.g. [18] for a review. We recall the Yamabe theorem and its proof which provides the most instructive example of symmetry-breaking and is required for the analysis of the generic case. It is based on the existence of nontrivial conformal isometries of the standard three-sphere.

By means of preparation let us start with the following observations: there is a four-parameter family of solutions of the equation

$$\nabla_i\nabla_j\sigma + g_{ij}\sigma = 0. \tag{48}$$

Namely, these can be taken to be constant linear combinations of the Euclidean coordinates (z_1, z_2, z_3, z_4) (see (9)), restricted to $\mathbb{S}^3$. As a corollary they satisfy

$$(\Delta + 3)\sigma = 0, \tag{49}$$

whence are the $n = 1$ spherical harmonics on $\mathbb{S}^3$. Next observe that by virtue of (48) the vector fields $\sigma^i = \nabla^i\sigma$ are conformal Killing vectors. They form a 4-dimensional linear space, but not a Lie algebra. Note that the quantity $(\nabla\sigma)^2 + \sigma^2$ is constant; we find it convenient to rescale σ such that

$$(\nabla\sigma)^2 + \sigma^2 = 1. \tag{50}$$

Each of the functions (z_1, z_2, z_3, z_4) has this property. Note finally that each solution of (48,50) can be characterized as follows: pick a ('reference' or 'north pole') point P on $\mathbb{S}^3$ and require $\sigma|_P = -1$, whence P is a critical point due to (50). The function σ will then monotonically increase along the flow of $\nabla^i \sigma$ while being constant on two-spheres. It goes to zero on the equatorial sphere and then to $+1$ on the point antipodal to P, which is also a critical point.

Proposition 4 (The Yamabe theorem on $\mathbb{S}^3$). *The solutions of (46) with $W \equiv 0$ form a four-parameter family given by*

$$\psi_a = \sqrt{\frac{2\,a}{(1+\sigma)a^2 + 1 - \sigma}} \tag{51}$$

where $a \in \mathbb{R}^+$.

Proof. Checking that ψ_a solves (46) with $W = 0$ is a straightforward exercise based on (48) and (49). As the reference point (north pole) can be chosen arbitrarily on $\mathbb{S}^3$, the full family of solutions is in fact four-parametric. For uniqueness recall a theorem by Obata (see [18, 22]), which states that all rescalings of the standard metric having the same constant curvature come, apart from a constant rescaling, from conformal isometries of $(\mathbb{S}^3, g_{ij})$. We state without proof that the functions ψ_a, up to a constant rescaling by $a^{1/2}$, do come from the conformal flow Ψ_t generated by $\nabla^i \sigma$ with $a = e^t$. $\qquad\square$

Suppose we choose the north pole for σ on the limiting great circle $x = -1$ on which the toroidal foliation given by $x = \text{const}$ is based. Then

$$\sigma = \cos \tau \cos \xi, \tag{52}$$

and we observe the following: while the Yamabe equation (46) with $W \equiv 0$ is invariant under the six-parameter family of isometries of $\mathbb{S}^3$, its solutions (51) are of the form $\psi(r) = \psi(\tau, \xi)$ - hence in particular the invariance under the KV $\Xi = \partial/\partial\xi$ is broken.

In view of proposition 2, this symmetry breaking signals an instability under conformal rescalings. In the present context, in particular for $R = 6$, $W = 0$ and $\psi = 1$, equation (45) becomes

$$-\Delta\rho = (3 + \lambda)\rho. \tag{53}$$

As is well known, the spectrum of $-\Delta$ on $\mathbb{S}^3$ is $n(n + 2)$, where $n \in \mathbb{N}_0$. Thus, the lowest eigenvalue is $\lambda = -3$. In terms of the coordinates (47), the higher eigenmodes either depend on x only, or they result from excitation of the γ and ξ- modes on a fixed torus $x = \text{const}$. Explicitly, with the separation ansatz $\rho(x, \gamma, \xi) = \exp(ik\gamma + im\xi)\,\chi(x)$, where $i = \sqrt{-1}$ and $k, m \in \mathbb{Z}$, equation (53) takes the form

$$\left(-4\frac{\mathrm{d}}{\mathrm{d}x}(1 - x^2)\frac{\mathrm{d}}{\mathrm{d}x} + \frac{2k^2}{1 - x} + \frac{2m^2}{1 + x}\right)\chi = (3 + \lambda)\chi. \tag{54}$$

In particular, the second eigenvalue $\lambda = 0$ has multiplicity four with the associated eigenfunctions

$$\chi_1 = \sqrt{1 - x}\cos\xi, \quad \chi_2 = \sqrt{1 - x}\sin\xi, \quad \chi_3 = \sqrt{1 + x}\cos\gamma, \quad \chi_4 = \sqrt{1 + x}\sin\gamma. \tag{55}$$

Of course, these eigenfunctions correspond to the four directions of the general four-parameter solution of the Yamabe problem described above.

(b) $\mathbf{W} = \mathbf{const} \neq \mathbf{0}$. In terms of the classification theorem for $L_{ij}^{(\Pi,\Upsilon)}$ of section 3, this case arises precisely for the homogeneous case II in theorem 1, as follows from (40) and $\langle \Omega, \Sigma \rangle \neq 0$. (Recall, however, that this homogeneous case overlaps with the other cases of the theorem).

In this case, equation (46) has obviously constant solutions determined by the positive roots of the polynomial

$$\psi^{12} - \psi^8 + \frac{1}{6} W^2 = 0. \tag{56}$$

These solutions come in pairs for all $0 < W^2 < W_{\max}^2 = 8/9$, in accordance with Premoselli's theorem quoted in the previous subsection. There now arises the question of uniqueness of these solutions, particularly in view of the symmetry breaking exposed above for the case $W \equiv 0$. However, it turns out that this ambiguity disappears as soon as W is turned on, due to the following result.

Theorem (Corollary 1 of theorem 1 of Brezis and Li [6]) *On* $\mathbb{S}^3$, *the Lichnerowicz equation (46) with* $W = \text{const}$ *has only constant solutions.*

(c) $\mathbf{W} = \mathbf{W}(\mathbf{x})$. We finally turn to the case of $\mathbb{U}(1) \times \mathbb{U}(1)$ symmetric data. From (41) we obtain, in terms of the notation of lemma 2,

$$W_{(\Pi,\Upsilon)}^2 = \frac{1}{9}\widehat{\Lambda}^2 V_{(\Pi,\Upsilon)}^2 = \frac{8\widehat{\Lambda}^2}{27} \left[\left(u^2 \|\Omega\|^4 - u\,v\,\|\Omega\|^2\,\|\Sigma\|^2 + v^2\,\|\Sigma\|^4 \right) + 3\,u\,v\,\langle \Omega,\,\Sigma \rangle^2 \right]. \tag{57}$$

We now choose Ω and Σ as follows

$$\Omega = \sqrt{\frac{3}{\widehat{\Lambda}}}\,\Omega^3 \quad \text{and} \quad \Sigma = u\sqrt{\frac{3}{\widehat{\Lambda}}}\,\Sigma^3, \tag{58}$$

where Ω^3, and Σ^3 are elements of a basis defined via (26) and (27). This choice is compatible with (23) and no loss of generality in view of the remaining scaling ambiguity and the rotation freedom (28). In terms of adapted coordinates (29) and (30) with $x = \cos(2\tau)$ this entails $\langle \Omega, \Sigma \rangle = 3\widehat{\Lambda}^{-1}u\,x$, and simplifies (57) as follows

$$W_{(\Pi,\Upsilon)}^2 = \frac{8}{3}u^2\left(1 - u\,v + u^2\,v^2\right) + 8\,u^3\,v\,x^2. \tag{59}$$

As to solving the Lichnerowicz equation (46) we conjecture that, as for $W = \text{const} \neq 0$ and in accordance with Premoselli's theorem quoted above, there is exactly one pair of solutions for $0 < b < b_\star$. Below we split this conjecture into an ODE and a PDE part, and formulate it for arbitrary $W^2(x) = b^2\overline{W}^2(x)$ rather than for the special form (59). We call a solution even if $\psi(x) = \psi(-x)$.

Conjecture 1. The Lichnerowicz-ODE, which results from (46) by assuming that $\psi = \psi(x)$, viz.

$$4(1-x^2)\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - 8x\frac{\mathrm{d}\psi}{\mathrm{d}x} - \frac{3}{4}(\psi - \psi^5) + \frac{b^2\overline{W}^2(x)}{8\psi^7} = 0 \tag{60}$$

has for every $0 < b \leqslant b_\star$ a unique stable, even solution and a unique unstable, even solution which coincide at $b = b_\star$. For $b \to 0$ the solutions on the stable branch tend to zero like $b^{1/4}$, while the unstable ones converge to $\psi \equiv 1$.

Partial proof and numerical evidence. For the stable branch, the result follows from Premoselli's theorem and proposition 2 and lemma 6 above. For the unstable branch an adaption of Premoselli's theorem (in terms of suitably restricted function spaces) might still apply. Alternatively, the implicit function applied to the linearized ODE operator (the ODE restriction of (45)) would guarantee existence and uniqueness directly as long as this operator had a trivial kernel. This is easily verified for $b = 0$ because the linearized Yamabe operator around $\psi = 1$, given by $L = -\Delta - 3$, has a trivial kernel when restricted to functions depending only on x, hence it holds for small b. It also holds for b near $b_\star$ by virtue of lemma 5. In the intermediate range we rely on numerical observations. $\square$

As to the full Lichnerowicz equation (46) with $b > 0$, we now discuss non-existence of symmetry breaking bifurcations, first from the Yamabe solutions and then from the unstable ODE branch.

Proposition 5. *Equation (46) has no symmetry breaking solutions bifurcating at $b = 0$ from the zero eigenvalue of the four-parameter family of the Yamabe solutions.*

Proof. We already know that for $W = W(x)$ and small b there exists an ODE solution of equation (46) of the form $\psi = \psi(x) = 1 + b^2\psi_1(x) + \mathcal{O}(b^4)$. To see if there are other solutions bifurcating from $\psi = 1$ at $b = 0$, we seek them in the form

$$\psi = 1 + bv + z, \tag{61}$$

where $v \in N$ (kernel of L) and $z \in N^\perp$ is of the order $\mathcal{O}(b^2)$. We recall that $N = \mathrm{span}\{\chi_1, \chi_2, \chi_3, \chi_4\}$, where χ_k are given in (55). Substituting the expansion $z = b^2z_2 + b^3z_3 + \dots$ into (46), at the order $\mathcal{O}(b^2)$ we get

$$Lz_2 = \frac{15}{2}v^2 + \frac{1}{8}\overline{W}^2. \tag{62}$$

Since v^2 is orthogonal to N, by the Fredholm alternative the solution z_2 exists iff

$$(\overline{W}^2, \chi_k) = 0, \quad k = 0, \dots, 4, \tag{63}$$

where $(,)$ denotes the L^2-inner product on $\mathbb{S}^3$. Assuming that the orthogonality conditions (63) hold, at the order $\mathcal{O}(b^3)$ we get

$$Lz_3 = 15vz_2 + \frac{15}{2}v^3 - \frac{7}{8}v\overline{W}^2. \tag{64}$$

Let $v = \sum_{k=1}^{4} c_k\chi_k$. By the Fredholm alternative, the coefficients c_k are constrained by the orthogonality conditions

$$(15vz_2 + \frac{15}{2}v^3 - \frac{7}{8}v\overline{W}^2, \chi_k) = 0. \tag{65}$$

In general, this will give a system of four cubic polynomial equations for the coefficients c_k, however in our case the cubic terms vanish identically and we are left with the trivial linear equations $c_k = 0$ (the vanishing of the cubic terms is a consequence of existence of the 4-parameter family of solutions for $b = 0$; more precisely, for $W = 0$ the v and particular solutions $z_2, z_3, ...$ correspond to the Taylor series expansion of this 4-parameter family). This excludes symmetry-breaking solutions that bifurcate from $\psi = 1$ at $b = 0$, thereby proving the uniqueness of the x-dependent continuation (unstable branch) in b of the trivial solution $\psi = 1$.

Thanks to the conformal symmetry for $b = 0$, an analogous argument proves the absence of bifurcations from the whole four-parameter family of Yamabe solutions.   □

Conjecture 2. Equation (46) has no symmetry breaking solutions bifurcating from the unstable ODE branch for $b > 0$.

Partial proof and numerical evidence. We were not able exclude bifurcation and corresponding symmetry breaking by general theorems such as those of Brezis and Li [6] used for $W = $ const, or by the results of Jin *et al* [16] employed in [9]. We rather have to resort to numerical evidence. In particular we will consider now the eigenvalue problem for the linearized operator on the unstable branch

$$\left(-4\frac{d}{dx}(1-x^2)\frac{d}{dx} + \frac{3}{4}(1-5\psi^4) + \frac{7W^2(x)}{8\psi^8} + \frac{2k^2}{1-x} + \frac{2m^2}{1+x} \right) \chi = \lambda\chi \tag{66}$$

for special choices of $W(x)$.

We focus on the three cases listed in remark 3 after theorem 1, namely Λ-Taub NUT (where we set $v = 0$), and the parallel ($uv = 1$) and the orthogonal ($uv = -1$) cases. Note that (58) is consistent with this Remark.

For the respective momentum densities $W_{\bowtie}$, $W_{\parallel}$ and $W_{\perp}$ we obtain from (57)

$$W_{\bowtie}^2 = \frac{8}{3}u^2, \qquad W_{\parallel}^2 = 8u^2(\frac{1}{3} + x^2), \qquad W_{\perp}^2 = 8u^2(1-x^2). \tag{67}$$

We can now consider $b = u$ as scaling parameter in Premoselli's theorem, which then in particular implies existence of solutions up to a maximal value $u_\star$. Recall from the previous subsection b) that in the Λ-Taub NUT case where $W_{\bowtie} = $ const we have only constant solutions (see the upper diagrams in figure 1). As to the other cases, numerics and perturbative calculations show that along the unstable branches the lowest eigenvalues grow monotonically from -3 at $u = 0$ to 0 at u_* while all higher eigenvalues remain positive. This absence of zero modes supports the above conjectures. The ODE branches are plotted in figure 1.   □

We finally remark that an elementary perturbative calculation gives the following approximations for the *unstable solutions* for small values of u

$$\psi_{\parallel}(x) = 1 - \frac{5-x^2}{21}u^2 + \mathcal{O}(u^4), \qquad \psi_{\perp}(x) = 1 - \frac{3x^2+13}{63}u^2 + \mathcal{O}(u^4). \tag{68}$$

The corresponding eigenvalues (66) can be obtained perturbatively as well.

Remark. It is known from point 2. in Premoselli's theorem quoted above in section 4.1 that solutions on the stable branch are pointwise strictly monotonically *increasing* with u. We
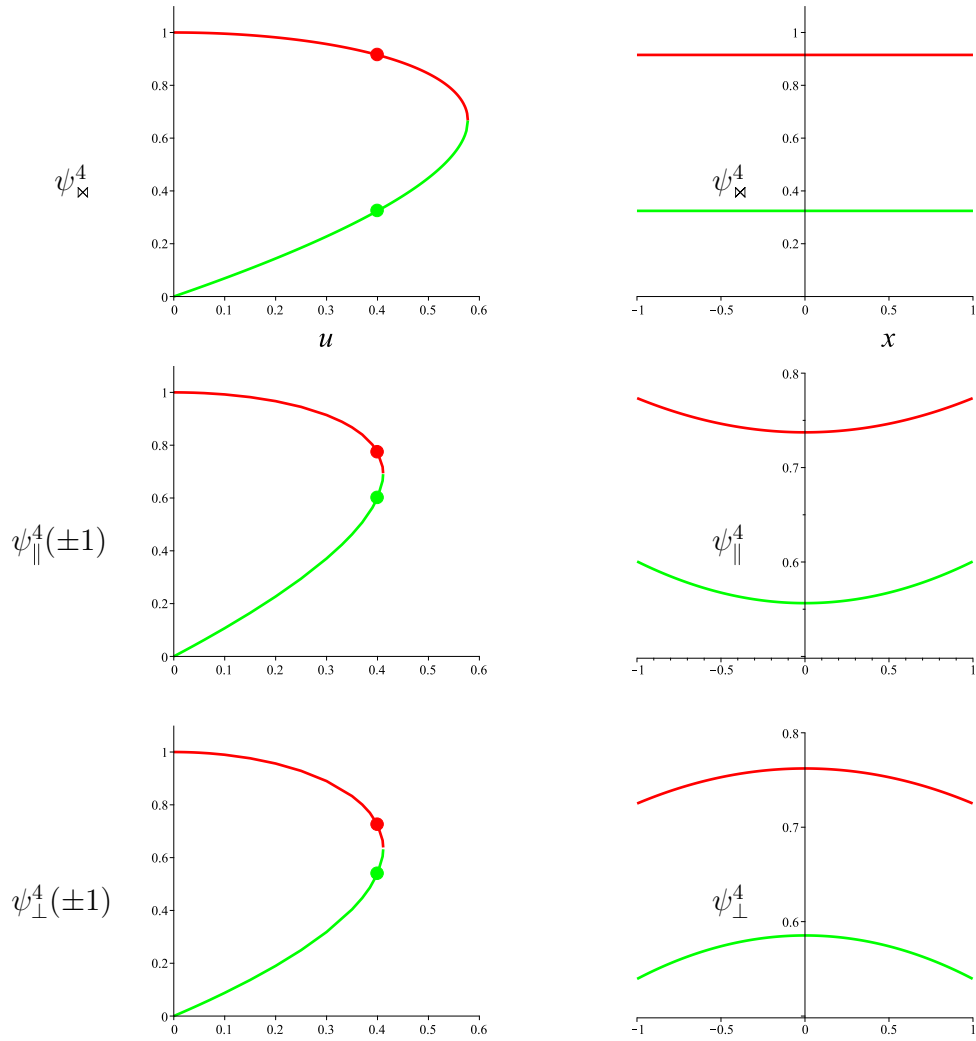
Figure 1. The diagrams on the left show the stable (green) and unstable (red) branches of solutions of the Lichnerowicz-ODE equation (60), for the choices $W = W_{\bowtie} = \text{const}$, $W(x) = W_{\parallel}(x)$ and $W(x) = W_{\perp}(x)$ given by (67); in the latter two cases, there are plotted the values of ψ^4 at the polar circles $x = \pm 1$ against u. For a sample value $u = 0.4$ (indicated by dots) the diagrams on the right show the respective functions $\psi^4(x)$.

observe numerically that the solutions on the unstable branch are pointwise strictly monotonically *decreasing* with u (for small u this follows from the perturbative solutions, see (68)). If proven, this would imply that the potential term in (66) is strictly monotonically increasing with u and consequently the same holds for the eigenvalues. This would prove that all the eigenvalues but the lowest one are positive, thereby excluding symmetry breaking bifurcations.

4.3. $\mathbb{S}^2 \times \mathbb{S}^1$

It is instructive to compare the data constructed above with similar ones of topology $\mathbb{S}^2 \times \mathbb{S}^1$. In this case the seed manifold is the donut (4) whose symmetry group is obviously $\mathbb{SO}(2) \times \mathbb{U}(1)$. We consider here equation (44) for $R = 2$ and distinguish, in analogy with the $\mathbb{S}^3$ case, momenta with $W \equiv 0$, $W = $ const and axially symmetric ones, i.e. $W = W(\theta)$.

(a) **$W \equiv 0$**: As we sketched in the introduction, the Yamabe- case is already non-trivial for such data since 'symmetry breaking generates black holes'—in particular, the family of time-symmetric Kottler data (k solutions if $B \in (2\pi k, 2\pi(k + 1)]$) arises via breaking the $\mathbb{U}(1)$ symmetry of the donut. We refer to [25] for details.

(b) **$W = $ const $\neq 0$**. In this case, the constant solutions are determined by the positive roots of the polynomial

$$\psi^{12} - \psi^8 + \frac{1}{2}W^2 = 0, \tag{69}$$

which exist up to a maximum value $W_{\text{max}}^2 = 8/27$. However, in contrast to the $\mathbb{S}^3$ case, there are also symmetry-breaking solutions; we refer to Chruściel and Gicquaud [9]. On the other hand, these authors show that $\phi = \phi(\xi)$, i.e. the solutions are necessarily still $\mathbb{S}^2$-spherically symmetric.

(c) **$W = W(\theta)$**. In [4] we considered a three-parameter family of 'Bowen-York' data which endows all $\mathbb{S}^2$ sections with an angular momentum of arbitrary magnitude and direction. We recall that the ten-parameter family of Bowen-York-data [5] was originally defined on flat space, but the definition carries over straightforwardly to the present locally conformally flat setting. Analyzing then the Lichnerowicz equation via Premoselli's theorem and numerically reveals a rich structure of rotating data, which exist up to a limiting angular momentum $J_\star$. Among them are both $\mathbb{U}(1)$-symmetry-preserving as well as -breaking ones, corresponding to their stability properties [19]. Although the data with broken symmetry very likely contain 'black holes' in the sense of marginally trapped surfaces (as it is the case without rotation), this is unproven.

We show how the momenta considered in [4] are related to the scheme of section 3. above. To reinterpret this family of data in the present context, we consider, in the coordinates (4), the orthogonal, commuting Killing vectors

$$\Xi = \frac{\partial}{\partial \xi}, \qquad \Phi = \frac{\partial}{\partial \varphi}. \tag{70}$$

We note that, in contrast to $\mathbb{S}^3$, the present $\mathbb{S}^2 \times \mathbb{S}$ space is not of constant curvature, whence the construction of TT tensors described in Sect 3 does not apply. Nevertheless, we recall from equation (5) of the Introduction that the symmetrized tensor product of Φ and Ξ, viz.

$$L_{ij} = 6J\,\Xi_{(i}\,\Phi_{j)} \quad \text{where} \quad J = \frac{1}{8\pi}\int_{\mathcal{S}} L_{ij}\Phi^i \mathrm{d}S^j \tag{71}$$

is a TT tensor on any background. The ('Komar'-) angular momentum J is conformally invariant and the same for all compact two-surfaces $\mathcal{S}$ within a given homology class; here in particular for any spherical surface. As ingredient for the Lichnerowicz equation we find

$$W^2 = \widehat{\Lambda}^2 V^2 = \widehat{\Lambda}^2 K_{ij}K^{ij} = 18\widehat{\Lambda}^2 J^2 \sin^2\theta \tag{72}$$

which agrees with [4] except for the different Λ- scaling (which is already present in the respective seed manifolds) and that [4] is restricted to the maximal case $\widetilde{K} = 0$. We refer to that paper and to [19] for the discussion of the solutions.

5. Marginally trapped surfaces

We finally locate and discuss toroidal (marginally, outer) trapped surfaces (MTSs, MOTSs) as well as marginally trapped regions (MTRs) in our data. Before doing so in section 5.3, we recall in section 5.1 key definitions, a result on '(non)-visibility' of MTRs due to Chruściel *et al* [8] (reproduced below as theorem 2) which motivates our discussion, and in section 5.2 the situation in de Sitter spacetime and its perturbations. We adopt the notation of [8] except that our tilded quantities refer to the physical spacetime, while compactifications are untilded. In particular, the spacetime is denoted by $(\widetilde{\mathcal{N}}, \widetilde{\gamma}_{\mu\nu})$ $(\mu, \nu = 0, 1, 2, 3)$ and its compactification by $(\mathcal{N}, \gamma_{\mu\nu})$.

5.1. Definitions, results, motivation

Definition 8.

- A marginally trapped surface (MTS) is a compact 2-surface for which least one of the families of orthogonally emanating, future directed null geodesics with tangents $\widetilde{l}^+$ and $\widetilde{l}^-$ has vanishing expansion ($\widetilde{\Theta}^+ = 0$ or $\widetilde{\Theta}^- = 0$).
- A compact, connected spacelike hypersurface is called a marginally trapped region (MTR) if its (only) boundary is a MTS with respect to the outward normal $\widetilde{l}^+$. In this case the bounding MTS is called a marginally outer trapped surface (MOTS).

Remarks.

1. The above definition of a MOTS is in line with [8] (which contains the more general definition of a weakly trapped region). However, it differs in general from others (e.g. definition 2.1. of [1]) as to the 'outer' assignment.
2. A MOTS (and hence the boundary of a MTR) need not be connected.
3. A MOTS itself is *never* a marginally trapped region as the 'outer' direction is ill-defined.
4. A MTR need not contain any *outer trapped surfaces* defined by $\widetilde{\Theta}^\pm < 0$.

The original motivation for studying such surfaces and regions comes from the singularity theorems. We recall in particular Hawking's classical theorem (theorem 4, section 8.2 of [13]) which asserts past geodesic incompleteness in spatially closed spacetimes that are at some stage future expanding and satisfy the strong energy condition. However, as the latter condition is violated in our Λ- vacuum case (while the dominant energy condition still holds for positive Λ), the conclusion need not hold; in fact de Sitter space which is geodesically complete is an example. Nevertheless, as we shall see shortly, de Sitter space itself is awash with MTSs and MTRs. We also recall that Friedrich's stability results for de Sitter space [12] indicate that, under 'weak' energy conditions, a cosmological singularity theorem can only hold under substantial modifications of the other requirements.

On the other hand, Chruściel *et al* [8] recently obtained results concerning the 'visibility' (from infinity) of MTSs and MTRs. The key differences to the singularity theorems are that only the null energy condition is required, and some asymptotics compatible with de Sitter is assumed. In precise terms, the result which concerns us here reads as follows.

Theorem 2 ((In)visibility of trapped regions from $\mathcal{J}$; slightly adapted theorem 2.5 of [8]). *Consider a future asymptotically de Sitter spacetime $(\widetilde{\mathcal{N}}, \widetilde{\gamma}_{\mu\nu})$ which is future causally simple and satisfies the null energy condition. Then either the causal future of some set $\widetilde{\mathcal{A}} \subset \mathcal{N}$ contains all of infinity, i.e. $J^+(\widetilde{\mathcal{A}}, \mathcal{N}) \supset \mathcal{J}^+$, or else there are no marginally trapped regions in $J^+(\widetilde{\mathcal{A}}, \mathcal{N}) \cap \mathcal{I}^-(\mathcal{J}^+, \mathcal{N})$.*

Turning to calculations, we recall the decomposition of the expansion on any two-surface $\widetilde{\mathcal{U}}$ with mean curvature $\widetilde{H}$, outer normal $\widetilde{n}^i$, and induced metric $\widetilde{q}_{ij} = \widetilde{g}_{ij} - \widetilde{n}_i \widetilde{n}_j$ in terms of the data, viz.

$$\widetilde{\Theta}^{\pm} = \pm \widetilde{H} + \widetilde{Q} = \pm \widetilde{\nabla}_i \widetilde{n}^i + \widetilde{q}^{ij} \widetilde{K}_{ij} = \pm \frac{1}{\sqrt{\widetilde{g}}} \partial_i \left(\sqrt{\widetilde{g}} \, \widetilde{n}^i \right) + \widetilde{q}^{ij} \widetilde{K}_{ij} \qquad \text{on } \widetilde{\mathcal{U}}. \tag{73}$$

We now restrict ourselves to MOTSs of toroidal topology. Such MOTSs have been found and studied before, in particular in asymptotically flat $\Lambda = 0$-vacuum data [14] as well as in closed Friedmann–Lemaître–Robertson–Walker spacetimes [11, 20]. We remark that topology results (see lemma 9.2 of [1], or [21]) imply that MOTSs which are *stable* with respect to their outward normals within their defining MTRs, (as defined e.g. in definition 5.1. and proposition 5.1. of [1]) must be spherical. Therefore, toroidal MOTSs must be *strictly unstable* in the sense that the lowest eigenvalue of the stability operator (see definition 3.1 of [1]) must be negative; this will be used in the discussion of conjecture 3 in the next subsection.

5.2. Toroidal MOTSs and MTRs in de Sitter spacetime

We next determine toroidal MOTSs on 'standard' CMC slices of de Sitter space, by which we mean $\sigma = \text{const}$, slices of (A.3). The induced metric and extrinsic curvature of such a slice read

$$\widetilde{g}_{ij} = \frac{3}{\Lambda \cos^2 \sigma} \, \mathrm{d}S_{ij}^2, \qquad \widetilde{K}_{ij} = \sqrt{\frac{3}{\Lambda}} \frac{\sin \sigma}{\cos^2 \sigma} \mathrm{d}S_{ij}^2, \tag{74}$$

where $\mathrm{d}S_{ij}^2$ is the standard metric on the unit three-sphere. Hence the mean curvature is $\widetilde{K} = \widetilde{K}_{ij} \widetilde{g}^{ij} = \sqrt{3\Lambda} \sin \sigma$.

Restricting ourselves now to toroidal surfaces of the form $\tau = \tau_0 = \text{const}$ in the coordinates (11), we obtain

$$\widetilde{\Theta}^{\pm} \Big|_{\tau_0} = \left(\pm \widetilde{H} + \widetilde{q}^{ij} \widetilde{K}_{ij} \right) \Big|_{\tau_0} = \sqrt{\frac{\Lambda}{3}} \left[\pm \frac{\cos \sigma}{\sin(2\tau)} \frac{\partial}{\partial \tau} \left(\sin(2\tau) \right) + 2 \sin \sigma \right]_{\tau_0}$$

$$= 2\sqrt{\frac{\Lambda}{3}} \left(\pm \cos \sigma \cot(2\tau_0) + \sin \sigma \right). \tag{75}$$

This implies that

$$\widetilde{\Theta}^{\pm} = 0 \text{ iff } \tau = \tau_0^{\pm} = \pm \sigma/2 + \pi/4; \tag{76}$$

in particular MOTSs exist for all times, i.e. for all $\sigma \in (-\pi/2, \pi/2)$. The corresponding MTRs are given by $\tau \in [0, \tau_0^+]$ and $\tau \in [\tau_0^-, \pi/2]$, respectively; curiously, neither region contains toroidal outer trapped surfaces.

As to applying theorem 2 in this setup it should be kept in mind that the set $\widetilde{\mathcal{A}}$ can in particular be chosen to be a MTS, but alternatively to be a MTR, while the conclusion refers to MTRs in either case.

We first recall from [8] the example of the time-symmetric case $\sigma_0 = 0$. We take $\widetilde{\mathcal{A}}$ to be the Clifford torus at $\tau = \pi/4$ which satisfies $\widetilde{\Theta}^{\pm} = 0$. We find that $J^+(\widetilde{\mathcal{A}}, \mathcal{N})$ contains $\mathcal{J}^+$ given by $\sigma = \pi/2$ in the compactification $\mathcal{N}$; in fact it contains all slices $\sigma \in [\pi/4, \pi/2]$. These latter slices also contain MTRs, as determined after equation (76), while $J^+(\widetilde{\mathcal{A}}, \mathcal{N}) \cap (\sigma = \mathrm{const})$ does not contain any MTRs for $\sigma \in [0, \pi/4)$. This is obviously consistent with theorem 2. A similar behaviour is found for MOTSs $\widetilde{\mathcal{A}}$ given by (76) on any slice $\sigma_0 \in (0, \pi/6)$: $J^+(\widetilde{\mathcal{A}}, \mathcal{N})$ contains all slices $\sigma \in [3\sigma_0/2 + \pi/4, \pi/2]$, and only for such slices $J^+(\widetilde{\mathcal{A}}, \mathcal{N}) \cap (\sigma = \mathrm{const})$ contains MRTs. On the other hand, for MOTSs on slices $\sigma_0 \in (\pi/6, \pi/2)$, $J^+(\widetilde{\mathcal{A}}, \mathcal{N}) \cap (\sigma = \mathrm{const})$ contains neither $\mathcal{J}^+$ nor any MTRs, again in agreement with theorem 2.

Needless to say, one would like to have a more interesting example for this theorem. A natural candidate would be a perturbation of de Sitter. In fact Friedrich's stability result, theorem 3.3 of [12] together with remark 3.4, asserts that, roughly speaking, the compactification survives small perturbations of the data, which is a prerequisite in order for theorem 2 to apply. This motivates the following

Conjecture 3. Under perturbations of de Sitter data which preserve its global stucture according to Friedrich's stability result theorem 3.3. of [12], the toroidal marginally outer trapped surfaces and marginally outer trapped regions remain close to those of de Sitter as determined above.

The difficulty of proving such a statement is that, as mentioned at the end of the previous subsection, toroidal MOTSs must be *strictly unstable* in the present Λ—vacuum case. On the other hand, *strict stability* guarantees the persistence of MOTSs under small perturbation of the data. This follows, via an implicit function argument, from a slight adaption of theorem 9.1 of [1]. The same could be proven, by the same method, in the present *strictly unstable* case provided the adjoint of the stability operator (definition 3.1 of [1]) had a trivial kernel. The latter, however, is unknown in the general setting as discussed above. Below we will revisit conjecture 3 in the context of the special data constructed in section 4, without giving a proof either.

5.3. Toroidal MOTSs and MTRs in our data

We now track toroidal MOTSs in the $\mathbb{U}(1) \times \mathbb{U}(1)$ -symmetric data constructed in section 4 on $\mathbb{S}^3$. We restrict ourselves to the maximal case $\widetilde{K} = 0$. As before the tori are given by $\tau = \tau_0 = \mathrm{const}$ in the coordinates (11), but now we include the momentum of lemma 4. For the last term in (73), we obtain from (41) and (43)

$$\widetilde{q}^{ij}\widetilde{L}_{ij} = \frac{2}{3\,\phi^6}\left(u\|\Omega\|^2 + v\|\Sigma\|^2\right) = \frac{2}{3\,\psi^6}\left(\frac{\Lambda}{3}\right)^{3/2}\left(u\|\Omega\|^2 + v\|\Sigma\|^2\right) = 2\sqrt{\frac{\Lambda}{3}}\frac{c}{\psi^6} \tag{77}$$

which defines c *as a constant on* $\mathbb{S}^3$, in particular c does not depend on the torus $\tau = \tau_0$.

Hence (73) can be rewritten on $\widetilde{\mathcal{U}}$ in the coordinates (11) as

$$\widetilde{\Theta}^{\pm} = \pm\frac{1}{\phi^6\sin(2\tau)}\frac{\partial}{\partial\tau}\left(\phi^4\sin(2\tau)\right) + \widetilde{q}^{ij}\widetilde{L}_{ij} = \pm\frac{1}{\psi^6\sin(2\tau)}\sqrt{\frac{\Lambda}{3}}\frac{\partial}{\partial\tau}\left(\psi^4\sin(2\tau)\right) + 2\sqrt{\frac{\Lambda}{3}}\frac{c}{\psi^6}, \tag{78}$$

and the condition for $\tau = \tau_0^\pm$ to be a MOTS becomes

$$\left[\frac{1}{\sin(2\tau)}\frac{\partial}{\partial \tau}\left(\psi^4 \sin(2\tau)\right)\right]_{\tau_0^\pm} = \mp 2c. \tag{79}$$

We finally restrict ourselves to the special cases singled out in remark 3 after theorem 1 and further elaborated in the previous section, namely Λ-Taub-NUT ($v = 0$) and the parallel ($uv = 1$) and orthogonal ($uv = -1$) cases. Furthermore we adopt the choice (58), which gives $\|\Omega\| = \sqrt{3/\Lambda}$ and $\|\Sigma\| = u\sqrt{3/\Lambda}$. We find from the definition (77) that the respective constants c take the values

$$c_\bowtie = \frac{u}{3} \qquad c_\| = \frac{2u}{3} \qquad c_\perp = 0. \tag{80}$$

In the following closer analysis of toroidal MOTSs in the above cases we restrict ourselves to the $\widetilde{\Theta}^+ = 0$ ones; the case $\widetilde{\Theta}^- = 0$ involves some sign changes.

Λ-**Taub-NUT:** Recall that here $W_\bowtie$ is constant given by the first of (67) and therefore $\psi_\bowtie$ is the constant determined by (56). From (79) and (80) the condition for a torus $\tau = \tau_\bowtie$ to be a MOTS then reads

$$\psi_\bowtie^4 = -\frac{u}{3}\tan(2\tau_\bowtie). \tag{81}$$

Using (56) and (67) we can eliminate either $\psi_\bowtie$ or u to obtain

$$\frac{u}{3} = \cot(2\tau_\bowtie)[4\cot(2\tau_\bowtie) - 1], \qquad \cot(2\tau_\bowtie) = \pm\frac{\sqrt{1 - \psi_\bowtie^4}}{2}. \tag{82}$$

This calculation is interpreted as follows. Recall from (56) that, for any u with $u^2 \in (0, 1/3)$, there are precisely two values for $\psi_\bowtie \in (0, 1)$ which yield a stable and an unstable 'Premoselli pair' of data. Either data have *precisely one* MOTS at $\tau_\bowtie$ given by the second equation in (82), where the sign has to be chosen such that $u\tan(2\tau_\bowtie) < 0$ by virtue of (81). We now recover a behaviour analogous to the de Sitter case: (78) implies that each torus given by $\tau \in (0, \tau_\bowtie)$ is *outer untrapped* in the sense that $\widetilde{\Theta}^+ > 0$; on the other hand, the region covered by these tori is called a MTR according to definition 8.

The parallel case: In the previous section we determined numerically the stable and the unstable branches of solutions $\psi_\|$ of the Lichnerowicz equation (60) with $W_\|$ from (67). Solving now also the MOTS equation, namely the $\widetilde{\Theta}^+$ part of (75) with the choice (80) numerically reveals a behavior which is qualitatively the same as in the previous Λ-Taub-NUT case: in particular we find *precisely one MOTS $\tau = \tau_\|$ on each branch*. We remark that for the unstable branch, the small-u approximation (68) gives $\cos(2\tau_\|) = 2u/3 + O(u^2)$.

The orthogonal case: The numerical solutions of the Lichnerowicz equation (60) now involve $W_\perp$ from (67). Since $c_\perp$ vanishes from (80), the MOTS equation (75) becomes

$$4\,\psi_\perp^{-1}\left.\frac{\mathrm{d}\psi_\perp}{\mathrm{d}x}\right|_{x_\perp} = \cot 2\tau_\perp. \tag{83}$$

A numerical analysis now shows that the respective sides of (83) have different signs unless both vanish. Hence we are left with the Clifford torus at $\tau_\perp = \pi/4$ as only MOTS, like in the time-symmetric de Sitter case described earlier.

To conclude, we found numerically toroidal MOTSs in all $\mathbb{U}(1) \times \mathbb{U}(1)$-symmetric, maximal Λ-Taub-NUT, 'parallel' and 'orthogonal' data. While in the first two cases there is a unique $\widetilde{\Theta}^+ = 0$ and $\widetilde{\Theta}^- = 0$- pair of different MOTSs, these MOTSs coincide at the Clifford torus in the latter case. Being boundaries of MTRs, all these MOTSs qualify in principle as tests for the (non-)visibility theorem of [8] quoted above as theorem 2. Clearly, the constructed data are in general unlikely to satisfy the 'cosmic-no-hair'-type requirement of this theorem, namely an evolution towards a causally simple asymptotically de Sitter spacetime $(\widetilde{\mathcal{N}}, \widetilde{\gamma}_{\mu\nu})$. We rather return now to the perturbative setting of conjecture 3. For our special families of data this means that we need to restrict ourselves *both to small u as well as to the unstable solutions of the Lichnerowicz equation*, (in the sense of definition 5 above), since the stable ones go to zero for $u \to 0$. Clearly, $\Lambda-$ Taub NUT can for small NUT parameter be interpreted as a perturbation of de Sitter, see [3]. On the other hand, understanding the structure of toroidal MOTSs and MTRs in the other cases could be achieved by generalizing the calculations of this subsection from the maximal to the CMC-case. We leave this to future work.

Acknowledgments

Appendix

Λ-*Taub-NUT data*

The Λ-Taub-NUT metric can be written as (see e.g. [3, 23])

$$\widetilde{\gamma}_{\mu\nu} = \frac{3D}{\Lambda} \left[-\frac{1}{f(t)} t_{,\mu} t_{,\nu} + f(t) \Omega^1_\mu \Omega^1_\nu + (1 + t^2)(\Omega^2_\mu \Omega^2_\nu + \Omega^3_\mu \Omega^3_\nu) \right], \qquad \text{(A.1)}$$

where the one-forms Ω^A_μ are related to the vectors (29) via $\Omega^A_\mu \mathrm{d}x^\mu = g_{ij} \Omega^{Aj} \mathrm{d}x^i$, and

$$f(t) = \frac{Dt^4 + 2(3D - 2)t^2 + Ct + 4 - 3D}{1 - t^2} \qquad \text{(A.2)}$$

with constants C and $D > 0$ so that $f > 0$. We remark that the relation to the one-forms ω^A_i of [23] is $2\,\Omega^A_\mu \mathrm{d}x^\mu = \omega^A_i \mathrm{d}x^i$ where the coordinates are related via $\tau = \theta/2$, $\gamma = (\psi - \phi)/2$ and $\xi = (\psi + \phi)/2$.

Note also that de Sitter spacetime is obtained for $C = 0$, $D = 1$ in the form

$$\widetilde{\gamma}_{\mu\nu} = \frac{3}{\Lambda \cos^2 \sigma} \left(-\sigma_{,\mu} \sigma_{,\nu} + \Omega^1_\mu \Omega^1_\nu + \Omega^2_\mu \Omega^2_\nu + \Omega^3_\mu \Omega^3_\nu \right), \qquad \text{(A.3)}$$

where $t = \tan \sigma$.

The intrinsic metric of $t = t_0$ is given by

$$\widetilde{g}_{ij}(t_0) = \frac{3D}{\Lambda} [f(t_0) \Omega^1_i \Omega^1_j + (1 + t_0^2)(\Omega^2_i \Omega^2_j + \Omega^3_i \Omega^3_j)] \qquad \text{(A.4)}$$

and the extrinsic curvature by

$$\widetilde{K}_{ij}(t_0) = \sqrt{\frac{3Df(t_0)}{\Lambda}} \left[\frac{1}{2}f'(t_0)\Omega_i^1\Omega_j^1 + t_0(\Omega_i^2\Omega_j^2 + \Omega_i^3\Omega_j^3)\right]. \tag{A.5}$$

The slice $t = t_0$ is conformal to the standard $\mathbb{S}^3$ iff $f(t_0) = 1 + t_0^2$. This leads to a relation between t_0 and the parameters C and D which we do not give explicitly. For the mean curvature of the spherical surfaces we obtain

$$\widetilde{K} = \widetilde{K}_{ij}\widetilde{g}^{ij} = \sqrt{\frac{\Lambda}{3D(1+t_0^2)}} \left(\frac{1}{2}f'(t_0) + 2t_0\right). \tag{A.6}$$

For a more detailed discussion we restrict ourselves to maximal slices (still with round metrics), which satisfy $f'(t_0) = -4\,t_0$. A computation shows that

$$C = 2t_0 \frac{t_0^4 + 6t_0^2 - 3}{1 + t_0^2}, \qquad D = \frac{1 - t_0^2}{1 + t_0^2}. \tag{A.7}$$

Assuming without loss that $0 \leqslant t_0 < 1$, the necessary and sufficient condition for the existence of such a t_0 is

$$C = 4\sqrt{\frac{1 - D}{1 + D}} \frac{1 - 2D - 2D^2}{1 + D} \tag{A.8}$$

and we are left with

$$\widetilde{g}_{ij}(t_0) = \frac{6D}{\Lambda(1+D)} g_{ij}, \qquad \widetilde{K}_{ij}(t_0) = 3\sqrt{\frac{3D}{2\Lambda}} \frac{\sqrt{1-D}}{1+D} \left(2\Omega_i^1\Omega_j^1 - \frac{2}{3}g_{ij}\right). \tag{A.9}$$

One easily checks that this family of initial data is a map from $0 < D \leqslant 1$ to solutions of the initial value constraints (1), as it has to be, and this map is injective. To make contact with case I. of theorem 1 in section 3. note that

$$\phi^2 = \sqrt{\frac{6D}{\Lambda(1+D)}}, \qquad u^2 = \frac{9D^2(1-D)}{(1+D)^3} \tag{A.10}$$

where we have used (41) with the choice $v = 0$ and (58). From the second relation in (A.10) we see that each $u^2 \in [0, \frac{1}{3})$ has 2 inverse images $D \in [0, 1]$, and this corresponds precisely to the (at least) 2 solutions of the Lichnerowicz equations predicted by Premoselli's theorem.

In any case we have shown that, with u^2 given as above for $0 < D \leqslant 1$, our case I of theorem 1 evolves into a Λ—Taub—NUT metric with C given by (A.8). We finally notice that, for D close to 1 (which implies C close to 0) they must have regular future and past infinity as a consequence of Friedrich's stability result theorem 3.3 of [12]. As to the global structure of the general case we refer to [3].

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