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General relativity in the Lagrangian and Hamiltonian formalism

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Abstract

This report presents a comprehensive overview of the Hamiltonian description of general relativity using the variables originally introduced by Arnowitt, Deser and Misner, a foundational framework in the study of the quantisation of Einstein's theory of general relativity. After the introduction of all relevant (canonical) variables, including their physical meaning, the Lagrangian and Hamiltonian are derived, which lie at the core of this theory. By applying a modified variational principle on these quantities, the Einstein field equations as well as field equations for the metric and its corresponding canonical momentum are derived, which are subsequently verified for an FLRW metric. On top of this, from the same quantities, definitions for the mass and momentum within a certain space-time are derived and subsequently validated for a Schwarzschild and Kerr metric, respectively. After establishing these core results, the Lagrangian and Hamiltonian formalisms are compared based on their symmetries, where arguments are provided for either being more fundamental. Finally, to close, this report explores recent developments in quantum gravity research and looks ahead to the near future, anticipating exciting potential breakthroughs.

Contents

1 Introduction

Since the discovery of quantum physics in the previous century [1–3] and, subsequently, quantum electrodynamics [4], a major goal within physics has been to describe all fundamental forces in a theory consistent with quantum mechanics. Though for almost all of these forces, this daunting task has now been completed [4–10], gravity as described by Einstein's theory of general relativity [11] still poses a challenge too large to be conquered [12].

The first to realise the necessity of such a quantum mechanical description of gravity was actually Einstein himself in 1918 (before the advent of modern quantum mechanics!) [13]. Following this prediction and a decade of significant developments within quantum research, the first meaningful attempts to quantise gravity were made by Rosenfeld in the early 1930s [14], in a similar fashion to the quantisation of electromagnetism, for which the methods were already well-known. Whereas renowned physicists of the time such as Pauli and Heisenberg [15] expected the quantisation of gravity to be not much more than a formality using these methods, Rosenfeld encountered several major issues, such as a diverging gravitational self-energy of a light quantum, later known as photon. Despite these obstacles, Bronstein made several important steps forwards in the years after by applying a method similar to Rosenfeld's, [16–18], which are summarized wonderfully by Stachel [19]. Unfortunately, Bronstein's story ends with the untimely death of the protagonist under the regime of Stalin, a fate which befell many other important contributors to research of the time throughout the Second World War. For this reason, little progress was made for several years.

After the war, though, in a time span of a decade, three pivotal research projects to develop a theory of quantum gravity were set up in quick succession, all of which still exist to this date. The first was created in a large-scale research programme set up by Bergmann [20], based on the covariance of the theory of general relativity. Now commonly referred to as the canonical approach to quantum gravity, this research focuses on the non-commutative algebra of the operators within general relativity, especially the Hamiltonian. The covariant approach, on the other hand, attempts to derive a quantum theory of general relativity by linearising the metric around a flat space and quantising the deviations from the flat metric, after which the non-linear terms are reinstated. This method was systematically developed by Gupta [21], continuing on previous work by Rosenfeld, Fierz and Pauli [14, 22]. Finally, Feynman quantisation attempts to reconcile general relativity and quantum mechanics by finding a propagator of a particle by applying Huygens' principle, summing over all possible histories. This idea was already brought up by Feynman in 1948 [23] and was later fully worked out by Misner [24], with the help of Wheeler.

Shortly after the creation of these research directions, Dirac [25] and Arnowitt, Deser and Misner [26] published their papers on the Hamiltonian description of general relativity, overcoming several of the previous issues with Bergmann's research programme. Especially the Arnowitt Deser Misner (ADM) formalism had major impact, introducing new variables to describe the Hamiltonian in a fashion which is still applied to this day. Unfortunately, after several more major developments in the following years by DeWitt, Wheeler, Feynmann [27–31] and several others, research died down around 1970 due to the numerous major issues faced. After 15 years, though, research burst to life again with further developed theories such as string theory and loop quantum gravity.

This report, however, will focus on the theory that originated before these dark middle ages of quantum gravity research. More specifically, this report provides a comprehensive overview of the Hamiltonian formulation of general relativity using the variables introduced by Arnowitt, Deser and Misner, which still lies at the basis of several promising theories such as canonical loop quantum gravity [12] and provides a solid foundation to explore the universe of quantum gravity. For the reader interested in a historical summary of the later developments, as well as a more in-depth view of all previous developments, I highly recommend the paper by Rovelli [32] for a clear overview of developments until the turnover of the century.

Before entering the wondrous world of quantum gravity, please note that the reader is expected to be familiar with the classical Lagrangian and Hamiltonian formalism [33], alongside possessing basic knowledge regarding tensor calculus and general relativity. Those somewhat unfamiliar with the latter two concepts are referred to section 2, in which the basics required for understanding this report are described. The remainder of this report consecutively covers the Lagrangian and Hamiltonian descriptions of general gravity, to end with a comparison of both through the analysis of several symmetries.

2 Theory

2.1 Tensor calculus

Many concepts in relativity are described by tensorial quantities over vector spaces, multilinear maps of vectors and covectors (to be defined later). The key property of a tensor is its invariance under basis transformations, i.e. the value of a tensor for a given point in space is independent of the chosen coordinate basis. As many quantities within physics, such as stresses and curvature of space, generally should not depend on the chosen basis to describe space-time, it is believed that most physical quantities should be described by tensors [34]. Therefore, a basic understanding of tensor calculus is a prerequisite for understanding general relativity, which will be provided in this section. On top of this, the most important types of spaces which will be utilised in the description of general relativity will be defined.

Tensors and dual spaces

Let V be an n-dimensional vector space with the orthonormal set of basis vectors $\{e_i\}$ and inner product $(.|.)_V : V \times V \to \mathbb{R}$. Note that, in the remainder of this report, the subscript of the inner product will be suppressed if the vector space in which the inner product is taken is clear. The dual space of V, with as elements covectors instead of vectors, is defined as $V^* \equiv L(V, \mathbb{R}) = \{x | x : V \to \mathbb{R}, x \text{ linear}\}$, the (vector) space of all linear maps from V to $\mathbb{R}$ [35]. The basis of a dual space is denoted as $\hat{e}^i$, defined uniquely by the relation

$$\hat{e}^i(e_j) = \delta^i_j, \tag{1}$$

where δ^i_j is the Kronecker delta. Similar to elements of the dual space being functions of vectors, vectors can be seen as functions of covectors, by defining that for all $v \in V, \omega \in V^*$, $v(\omega) = \omega(v)$. Therefore, equivalently to equation 1, $e_j(\hat{e}^i) = \delta^i_j$.

As noted before, tensors are multilinear maps of vectors and covectors which are independent of the coordinate basis. More specifically, a k-th order covariant and l-th order contravariant tensor U over a vector space V, $U \in T^l_k(V)$, takes k contravariant vector and l covariant covector arguments and may be decomposed as

$$U = U^{i_1 \dots i_l}_{j_1 \dots j_k} e_{i_1} \otimes \dots \otimes e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}, \tag{2}$$

where $U^{i_1 \dots i_l}_{j_1 \dots j_k}$ is called the holor of the tensor and where

$$(e_{i_1} \otimes \dots \otimes e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k})(x^{m_1}, \dots, x^{m_l}, x_{n_1}, \dots x_{n_k}) \equiv e_{i_1}(x^{m_1}) \cdot \dots \cdot e_{i_l}(x^{m_l}) \cdot \hat{e}^{j_1}(x_{n_1}) \cdot \dots \cdot \hat{e}^{j_k}(x_{n_k}), \tag{3}$$

with the holor adhering to the transformation rule

$$\bar{U}^{i_1 \dots i_l}_{j_1 \dots j_k} = A^{i_1}_{m_1} \dots A^{i_k}_{m_k} A^{n_1}_{j_1} \dots A^{n_k}_{j_k} U^{m_1 \dots m_l}_{n_1 \dots n_k}. \tag{4}$$

Here A^a_b is the Jacobian of an arbitrary coordinate transformation, $U \in T^l_k(V)$ the original tensor and $\bar{U} \in T^l_k(V)$ the tensor after transformation. Note that Einstein's summation convention is applied within equations 2 and 4, stating that a sum over an index can be implicitly written as a distinct combination of an upper and lower index. Conventionally, a Latin index indicates a sum over three dimensions, while a Greek index indicates summation over four dimensions.

An important characteristic of a tensor is symmetry or antisymmetry, i.e. any two indices may be exchanged, freely or at the cost of a minus sign, respectively. Clearly, a mixed covariant and contravariant tensor may never have either of these properties, therefore we consider a general covariant tensor $T \in T^0_k(V)$, though the following equations are fully analogous for a general contravariant tensor. If T is a symmetric tensor, it may be alternatively decomposed as $T = T_{(i_1 \dots i_k)} \hat{e}^{i_1} \vee \dots \vee \hat{e}^{i_k}$, where $\vee$ denotes a symmetric product and the brackets around the indices of the holor denote a symmetrisation as

$$T_{(i_1 \dots i_k)} = \frac{1}{k!} \sum_{\pi} T_{\pi(i_1) \dots \pi(i_k)}, \tag{5}$$

where π is an arbitrary permutation. Analogously, an antisymmetric tensor $U \in T_k^0(V)$ may alternatively be decomposed as $U = U_{[i_1 \dots i_k]} \hat{e}^{i_1} \wedge \dots \wedge \hat{e}^{i_k}$, where $\wedge$ denotes an antisymmetric product and the square brackets around the indices of the holor denote an antisymmetrisation as

$$U_{[i_1 \dots i_k]} = \frac{1}{k!} \sum_{\pi} sgn(\pi) T_{\pi(i_1) \dots \pi(i_k)}. \tag{6}$$

An example of a symmetric tensor vital within general relativity is the second order covariant metric tensor $g \in T_2^0(V)$, defined as $g(v, w) = g_{ij} \hat{e}^i(v) \hat{e}^j(w) \equiv (v|w)_V$ with $v, w \in V$ and $g_{ij} = g(e_i, e_j) = (e_i|e_j)_V$. Alongside the metric tensor itself, the dual metric tensor plays a vital role within physics as well, defined as a second-order contravariant tensor with holor $g^{ij} = (\hat{e}^i|\hat{e}^j)_{V^*}$. It may be swiftly verified that these two metric tensors are related as $g^{ij} g_{jk} = \delta^i_k$ [34], revealing that they are each other's inverse. Note that this is inherent to the (dual) metric tensor and may not hold for an arbitrary tensor.

One important purpose of the metric tensor, due to its connection to the inner product, is defining a reciprocal basis. When the metric tensor is applied to a single vector, the result will be a covector. This operation is called the sharp operation $\# : V \to V^*$ and it transforms basis vectors as $\# e_i \equiv g_{jk} \hat{e}^j(e_i) \hat{e}^k = g_{ik} \hat{e}^k \equiv \hat{e}_i$, with the property $(\hat{e}_i|\hat{e}^j)_{V^*} = g^{jk} g_{ki} = \delta^j_i$, forming a reciprocal basis of V^*. Alternatively, by applying the inverse operation, a reciprocal basis for the vector space V can be found using the 'flat' operator $\flat : V^* \to V$ as $\flat \hat{e}^i \equiv g^{kj} e_k(\hat{e}^i) e_j = g^{ij} e_j \equiv e^i$, with property $(e^i|e_j)_V = g^{ik} g_{kj} = \delta^i_j$. As per these definitions, the metric can be used to raise and lower indices of (basis) vectors, covectors and other tensors.

Manifolds

The space of 4-dimensional space-time, as is the subject of general relativity, is an example of a differentiable manifold [36]. A differentiable manifold M is a locally Euclidean Hausdorff topological space [37], with a set of diffeomorphisms (isomorphisms between manifolds [36]) $\phi_\alpha : \Omega_\alpha \subseteq M \to \phi_\alpha(\Omega_\alpha) \subseteq \mathbb{R}^n$, such that

- $\{\Omega_\alpha\}$ is an open covering of M.
- If $\Omega_\alpha \cap \Omega_\beta \neq \emptyset$, then $\phi_\alpha(\Omega_\alpha \cap \Omega_\beta), \phi_\beta(\Omega_\alpha \cap \Omega_\beta) \subset \mathbb{R}^n$ are open sets, and $\phi_\alpha \circ \phi_\beta^{-1}|_{\phi_\beta(\Omega_\alpha \cap \Omega_\beta)}$ and $\phi_\beta \circ \phi_\alpha^{-1}|_{\phi_\alpha(\Omega_\alpha \cap \Omega_\beta)}$ are diffeomorphisms.
- The atlas $\{(\Omega_\alpha, \phi_\alpha)\}$ is maximal w.r.t. the previous two axioms [35].

The above-defined atlas consists of subsets of M and maps between these subsets and $\mathbb{R}^n$ and can therefore be seen as a way of assigning coordinates $(x_1, \dots, x_n) \in \mathbb{R}^n$ to each point within the space M. In the remainder of this report, the use of an atlas will be implicit and maps over V may equivalently be taken to have the domain $\mathbb{R}^n$, unless a special treatment is required.

Tangent spaces

In many situations in general relativity, the manifold M describing space-time is curved and cannot be described by a global vector space. In these cases, it is useful to define a new Euclidean inner product space $T_x M$ locally tangent to the original space at a point $x \in M$. This is always possible when the space is locally Euclidean everywhere, as is the case for the differentiable manifold representing 4-dimensional space-time. This new tangent space is a vector space and can be described using basis vectors $e_i \equiv \partial_i$, the partial derivative at point $x \in M$, such that $v(f) = v^i \partial_i f|_x$, where $v \in T_x M$ and $f \in C^\infty(M)$. As the tangent space is a vector space, a dual tangent space T^*M can be defined as well, with basis vectors $\hat{e}^i \equiv dx^i$ [35].

The union of all tangent spaces on a manifold M is called a tangent bundle TM, with as elements vectors. Let $\pi : TM \to M$ be the projection map, which maps a vector $v \in T_x M$ to $\pi(v) = x$ for all $x \in M$. A vector field is then defined as a continuous map $X : M \to TM$ such that $\pi \circ X = \mathrm{Id}_M$, i.e. the map X assigns a vector $v \in T_x M$ to each point $x \in M$. The set of all smooth vector fields on M is denoted as $\mathfrak{X}(M)$. Analogously, covector fields can be defined using a map $X : M \to T^*M$, which are grouped into the set containing all smooth covector fields, $\mathfrak{X}^*(M)$.

Similar to vector fields, tensor fields $T^l_k(\mathfrak{X}(M)) : M \to T^l_k(TM)$ are a central part of the Lagrangian formulation of gravity. These assign a tensor to each point in space by providing a value for the holor, keeping the order of the tensor constant at all points. One specific assignment of tensor holors to each point in space is a field configuration, which will be of vital use when describing the variational principle for the Lagrangian formalism of gravity.

Transitions between manifolds

At times, it may be necessary to transition a tensor field from one manifold N to another manifold M, which may not have the same dimensions as the original. For a general mixed tensor field, the below procedure requires a considerable extension, which is only possible in the special case of a diffeomorphism existing between M and N [37]. Therefore, we will focus on the transition of a purely covariant tensor, as many important tensors in this report and physics in general, such as the metric tensor, are covariant. Define a smooth map $\phi : M \to N$ and define a push-forward operator $d\phi : \mathfrak{X}(M) \to \mathfrak{X}(N)$ for vector fields as

$$(d\phi(V))_{\phi(p)}(f) = V_p(d\phi_0(f)) \equiv V_p(f \circ \phi), \tag{7}$$

where $f \in C^\infty(N)$, $V \in \mathfrak{X}(M)$ and $V_p \equiv V(p) \in TM$ is the vector assigned to point $p \in M$. Then the pull-back of a tensor field $g \in T^0_k(\mathfrak{X}(N))$ can be defined as $\phi^*_k : T^0_k(\mathfrak{X}(N)) \to T^0_k(\mathfrak{X}(M))$ such that

$$(\phi^*_k g)_p(v_1, \ldots, v_k) = g_{\phi(p)}(d\phi(v_1), \ldots d\phi(v_k)), \tag{8}$$

for $v_1, \ldots, v_k \in T_p M$. This pull-back operation thus maps the tensor field g over N to an equivalent tensor field $\phi^*_k g$ over M, effectively transitioning g from N to M. A similar procedure can be applied to covector fields and contravariant tensors, using a smooth mapping $\phi : N \to M$ and the pull-back operator for covector fields $d\phi^* : \mathfrak{X}^* N \to \mathfrak{X}^* M$ defined as

$$(d\phi^* V)_p(w) = V_{\phi(p)}(d\phi(w)) \tag{9}$$

for $V \in \mathfrak{X}^* N, w \in T_p M$ [37].

2.2 Derivatives

Alongside the well-known partial derivatives, two other types of derivatives are often used within the theory of general relativity. The covariant derivative, or affine connection, allows derivatives to be taken on a curved manifold and therefore relates tangent spaces to each other, while the Lie derivative contains information on change along a vector flow field. These derivatives will be formally defined in this section and several important properties and relations will be derived.

Affine connection

An affine connection over the tangent bundle $\nabla : \mathfrak{X}(M) \times \mathfrak{X}(M) \to \mathfrak{X}(M) : \nabla(v, w) \to \nabla_w(v)$ on a manifold M is a multilinear map with the properties

- $\nabla_w(\lambda_1 v_1 + \lambda_2 v_2) = \lambda_1 \nabla_w(v_1) + \lambda_2 \nabla_w(v_2)$ for all $\lambda_1, \lambda_2 \in \mathbb{R}$,
- $\nabla_{(f_1 w_1 + f_2 w_2)}(v) = f_1 \nabla_{w_1}(v) + f_2 \nabla_{w_2}(v)$ for all $f_1, f_2 \in C^\infty(M)$,
- $\nabla_w(fv) = f\nabla_w(v) + v\nabla_w(f)$ for all $f \in C^\infty(M)$,
- $\nabla_w(f) = wf = w^i \partial_i f$ for all $f \in C^\infty(M)$.

A more general definition of the affine connection exists [38], which is valid over any vector bundle, though this definition will not be required for any derivations in this report. The previous definition can be extended to allow for taking covariant derivatives of tensor fields, which can be done by requiring a tensor product rule as

$$\nabla_V(T \otimes S) = \nabla_V T \otimes S + T \otimes \nabla_V S, \tag{10}$$

for any $T, S \in T^l_k(\mathfrak{X}(M))$ and $V \in \mathfrak{X}(M)$, where the affine connection for first order covariant tensor fields is equivalent to the affine connection for vector fields. Additionally, to allow the covariant derivative to be defined for first-order contravariant tensors, a final condition should be added, stating that

$$\nabla_V(tr(T)) = tr(\nabla_V(T)) \tag{11}$$

where $V \in \mathfrak{X}(M)$, $T \in T^l_k(\mathfrak{X}(M))$ and the trace operator $tr : T^l_k(\mathfrak{X}(M)) \to T^{l-1}_{k-1}(\mathfrak{X}(M))$ contracts an arbitrary pair of covariant and contravariant indices of the holor of the tensor it operates on, i.e. $(\text{trace}(T))^{i_1 \cdots i_{l-1}}_{j_1 \cdots j_{m-1}} = T^{i_1 \cdots i_{l-1} m}_{j_1 \cdots j_{k-1} m}$, where m can replace any of the covariant and contravariant indices.

From an extrinsic geometrical point of view, the covariant derivative $\nabla_w v$ describes the rate of change of a vector field $v \in \mathfrak{X}(M)$ when moving in the direction of the vector field $w \in \mathfrak{X}(M)$, along the direction of the vector field w, therefore neglecting the normal component. When the covariant derivative vanishes, the vector field v is said to be parallel transported along the vector field w, i.e. seen intrinsically from the manifold M, the vector field seems constant, such as in figure 1. The concept of parallel transport allows vectors in different tangent spaces $T_x M$ to be compared and is therefore vital for the description of general relativity. On top of this, parallel transport may be used to define an intrinsic curvature to a manifold, as shown in section 2.4. This can already be seen from figure 1, as in a curved space, a vector parallel transported over a loop may not return to its initial state, whereas this will always be the case on a flat manifold.

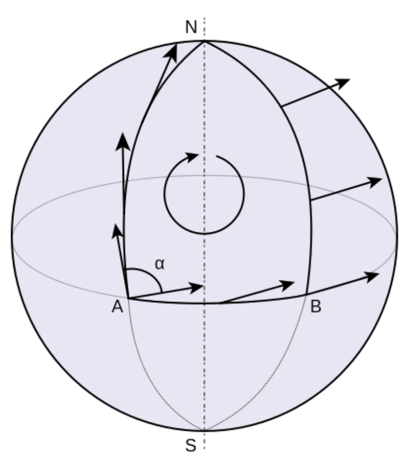

Figure 1: Parallel transport of a vector on a spherical manifold [39]

Due to the previously stated linear and multiplicative properties of the affine connection, it may alternatively be defined by operating on all combinations of basis vectors, for contravariant basis vectors given by

$$\nabla_{e_j} e_i = \Gamma^k_{ij} e_k, \tag{12}$$

where $\Gamma^k_{ij} \in \mathbb{R}$ is a connection coefficient. Then, using the chain rule $\nabla_{e_j}(\hat{e}^i(e_k)) = (\nabla_{e_j}\hat{e}^i)(e_k) + \hat{e}^i(\nabla_{e_j}(e_k))$, the covariant derivative of the covariant basis vectors is found to be

$$\begin{aligned}(\nabla_{e_j}\hat{e}^i)_k &= (\nabla_{e_j}\hat{e}^i)(e_k) \\ &= \nabla_{e_j}(\hat{e}^i(e_k)) - \hat{e}^i(\nabla_{e_j}(e_k)) \\ &= \nabla_{e_j}(\delta^i_k) - \hat{e}^i(\Gamma^l_{kj} e_l) \\ &= 0 - \delta^i_l \Gamma^l_{kj} \\ &= -\Gamma^i_{kj}.\end{aligned} \tag{13}$$

Using these connection coefficients, the covariant derivative of a general tensor can be reduced to an expression containing only partial derivatives. Let $v \in \mathfrak{X}(M)$ and $A \in T^l_k(\mathfrak{X}(M))$ be an arbitrary vector and tensor field, respectively. Then the covariant derivative of A towards v can be found to be

$$\begin{aligned}\nabla_v A &= \nabla_{v^i\partial_i}(A^{i_1\dots i_l}_{j_1\dots j_k} e_{i_1} \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}) \\ &= v^i(\nabla_{\partial_i} A^{i_1\dots i_l}_{j_1\dots j_k})(e_{i_1} \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}) + A^{i_1\dots i_l}_{j_1\dots j_k}(\nabla_{\partial_i}(e_{i_1}) \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}) + \dots \\ &= v^i(\partial_i A^{i_1\dots i_l}_{j_1\dots j_k})(e_{i_1} \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}) + A^{i_1\dots i_l}_{j_1\dots j_k}((\Gamma^{m_1}_{i_1 i} e_{m_1}) \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}) + \dots \\ &= v^i(\partial_i A^{i_1\dots i_l}_{j_1\dots j_k} + A^{m_1 i_2\dots i_l}_{j_1\dots j_k}\Gamma^{i_1}_{m_1 i} + \dots - A^{i_1\dots i_l}_{m_1 j_2\dots j_k}\Gamma^{m_1}_{j_1 i} - \dots)(e_{i_1} \otimes \dots e_{i_l} \otimes \hat{e}^{j_1} \otimes \dots \otimes \hat{e}^{j_k}),\end{aligned} \tag{14}$$

making use of the previously mentioned properties of the affine connection. The components of the covariant derivative of A, $\nabla_{e_j} A \equiv \nabla_j A$, constitute a new tensor of covariant order $k+1$ and contravariant order l, i.e. $\nabla_j A \in T^l_{k+1}(\mathfrak{X}(M))$ [35]. Therefore, the covariant derivative preserves the tensorial properties of a tensor A.

Although the covariant derivative transforms as a tensor, the individual connection coefficients do not. By antisymmetrising the lower indices, though, the torsion tensor $T^k_{ij} = \Gamma^k_{ij} - \Gamma^k_{ji}$ is found, which does transform a tensor [40]. Geometrically, the torsion tensor describes the rotation of a vector or plane under parallel transport. For example, within a flat space-time with non-zero torsion, a plane parallel transported along a straight line will rotate, as shown in figure 2.

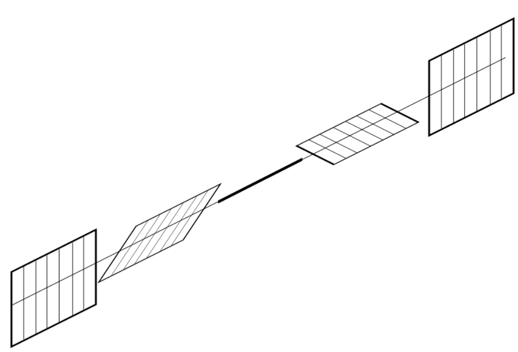

Figure 2: Parallel transport of a plane in a space with non-zero torsion [41]

Within Einstein's theory of general relativity, the torsion tensor is assumed to vanish. This assumption arises from practical experiments, which do not provide any reason to include the possibility of non-zero torsion within theory. The research field which considers space-time with non-zero torsion is Einstein-Cartan theory [42], of which the usefulness has been disputed over the previous century [43].

Finally, using the previously derived relations, an important quantity within general relativity can be determined, being the covariant derivative of the metric tensor. Within Euclidean space, the covariant derivative of an inner product is distributive, i.e. $\nabla_X(V|W) = (\nabla_X V|W) + (V|\nabla_X W)$ [38], where $V, W, X \in \mathfrak{X}(M)$ are arbitrary, implying that $\nabla_X g = 0$ for all $X \in \mathfrak{X}(M)$ through the definition of the metric tensor. On the other hand, on curved (pseudo-)Riemannian manifolds [38], which are used to describe space-time within general relativity, this need not hold. Therefore, Einstein made the assumption that distributivity of the covariant derivative over the inner product and therefore the vanishing of the covariant derivative of the metric tensor holds for any curved pseudo-Riemannian manifold. This assumption, called metric compatibility, holds if and only if the Einstein equivalence principle holds [44, 45], which lies at the basis of general relativity, alongside the assumption on vanishing torsion. Again, removing this assumption from general relativity would bring one to Einstein-Cartan theory.

Intrinsic covariant derivative

The intrinsic covariant derivative over the tangent bundle $D : \mathfrak{X}(M) \times \mathfrak{X}(M) \to \mathfrak{X}(M) : D(v, w) \to D_w(v)$ is defined as the regular covariant derivative, projected down onto a manifold M of lower dimension than the space-time N into which it is embedded, i.e.

$$D_w(v) = w^a D_a(v^b \partial_b) = w^a D_a(v^b)\partial_b + w^a v^b D_a(\partial_b) \equiv w^a \nabla_\alpha(v^\beta) e^\alpha_a e^b_\beta \partial_b + w^a v^b \Gamma^c_{ab} \partial_c, \tag{15}$$

where Γ^c_{ab} is the 3-dimensional connection coefficient and e^a_α is the Jacobian of the projection from space-time onto M. It may be swiftly proven that the intrinsic covariant derivative on N is equivalent to the covariant derivative on manifold M. Therefore, the intrinsic covariant derivative has all properties of a regular covariant derivative, such as compatibility with the metric on M [46].

Lie derivative

The Lie derivative describes the deformation of tensors along a flow generated by a vector field on a manifold M. Similar to the pull-back and push-forward operators defined in section 2.1, we will focus on purely covariant tensors of order k, though the theory can be extended to tensors of any type [38]. Let V be a vector field, generating a smooth flow diffeomorphism $\phi_t : M \to M$, such that a point $p \in M$ is transported along a trajectory $\gamma : \mathbb{R} \to M$ with $\dot{\gamma}(t) = V_{\gamma(t)}$ to $\phi_t(p)$. The transport along the flow of a tensor can then be described using a pull-back map, as defined before, where $\phi_t^* : T^0_k(\mathfrak{X}(M)) \to T^0_k(\mathfrak{X}(M))$ is defined as

$$(\phi_t^* A)_p(v_1, \ldots, v_k) = A_{\phi_t(p)}(d\phi_t(v_1), \ldots, d\phi_t(v_k)), \tag{16}$$

where $v_1, \ldots, v_k \in T_pM$, $A \in T^0_k(\mathfrak{X}(M))$ is a tensor field and $(d\phi_t(v_l))(f) = v_l(f \circ \phi_t)$ for $v_l \in T_pM$ and $f \in C^\infty(M)$. Then the Lie derivative of a covariant tensor $\pounds : \mathfrak{X}(M) \times T^0_k(\mathfrak{X}(M)) \to T^0_k(\mathfrak{X}(M))$ is defined as

$$\pounds_V(A) = \frac{d}{dt}\phi_t^* A|_{t=0}. \tag{17}$$

Intuitively, using the limit definition of the derivative, the Lie derivative can be seen as the difference between the tensor field A at a point p and the tensor field which would be found if the tensor field A at point $\phi_t(p)$ would be transported back along the flow to p, where $t \to 0$. Therefore, the Lie derivative shows how a tensor varies when transported along a vector flow field.

Alongside the flow definition of the Lie derivative using pull-back maps, it can be defined equivalently using algebraic Lie brackets, through the relation $\pounds_V(W) = [V, W]f \equiv (VW - WV)f$, where $V, W \in \mathfrak{X}(M)$ are smooth vector fields and $f \in C^\infty(M)$ [38]. This definition for vector fields can be extended to allow for Lie derivatives of tensor fields in a similar way to the affine connection over tangent bundles, adapting equations 10 and 11 by replacing the covariant derivatives by Lie derivatives. From this description, several properties of the Lie derivative can be deduced, most importantly

- $(\pounds_V W)(V_1, \ldots, V_n) = V(W(V_1, \ldots, V_n)) - W([V, V_1], \ldots, V_n) - \ldots - W(V_1, \ldots, [V, V_n])$ for a smooth vector field $V \in \mathfrak{X}(M)$, an nth-order covariant tensor field $W \in T^0_n(\mathfrak{X}(M))$ and vector fields $V_1, \ldots, V_n \in \mathfrak{X}(M)$. Similar equations can be derived for mixed and contravariant tensors [37].

- $\pounds_t A = \partial_t A$ when $\partial_j t^i = 0$ for all i, j, where $t = t^i \partial_i$ is a smooth vector field and A a smooth tensor field. An example of this is when $t = e_i$, i.e. the flow is along a coordinate vector.

- The Lie derivative is linear.

Using these properties, the Lie derivative of the metric tensor along a general vector field $V = V^i \partial_i \in \mathfrak{X}(M)$ can be derived. Using the first and second property described above, it is found that

$$\begin{aligned}
\pounds_V g_{ij} &= (\pounds_V g)(e_i, e_j) \\
&= V(g(e_i, e_j)) - g([V, e_i], e_j) - g(e_i, [V, e_j]) \\
&= V^k \partial_k (g(e_i, e_j)) + g(e_i(V^k) e_k, e_j) + g(e_i, e_j(V^k) e_k) \\
&\overset{*}{=} V^k \partial_k (g_{ij}) + \partial_i(V^k) g_{kj} + \partial_j(V^k) g_{ik} \\
&= V^k (\nabla_k(g_{ij}) + \Gamma^l_{ik} g_{lj} + \Gamma^l_{kj} g_{il}) + (\partial_i(V^k) - \Gamma^k_{li} V^l) g_{kj} + (\partial_j(V^k) - \Gamma^k_{lj} V^l) g_{ik} \\
&= V^k \nabla_k(g_{ij}) + \nabla_i(V^k) g_{kj} + \nabla_j(V^k) g_{ik} \\
&= \nabla_i(V_j) + \nabla_j(V_i),
\end{aligned} \tag{18}$$

where in step $(*)$ the linearity of the metric tensor and in the final step metric compatibility was used. Note that $\pounds_V g_{ij}$ denotes the $\{i, j\}$ components of the tensor $\pounds_V g$, not the Lie derivative of an element of the holor of g. The penultimate equation will be valid for any second-order covariant tensor, revealing a relation between the Lie and covariant derivative. In general, analogous relations can be derived between Lie, partial and covariant derivatives for mixed tensors of any order.

2.3 Integrals and volume forms

Many quantities within the Lagrangian and Hamiltonian formalism are described using integrals, not in the least the action functional. In this section, integral conventions are discussed, as well as a common method to solve such integrals, Gauss' theorem.

Volume forms

To allow the formulation of an integral, though, first a volume form should be defined. A volume form describes an infinitesimally small element of space, serving as the basis for defining an integral as a summation over these infinitesimally small volume forms. For an n-dimensional orientable manifold M [37], the volume form is given by an n-th order differential form, i.e. an n-th order antisymmetric tensor $\mathbf{e}_n \in \bigwedge_n(\mathfrak{X}(M))$, describing an infinitesimal n-dimensional oriented volume as shown in [44]. The most basic example of a volume form is the unit volume form

$$\mathbf{e}_n \equiv \mathbf{e} = [i_1 \ldots i_n] \hat{e}^{i_1} \otimes \ldots \otimes \hat{e}^{i_n} = \mathbf{e}_{[i_1 \ldots i_n]} \hat{e}^{i_1} \wedge \ldots \wedge \hat{e}^{i_n}, \tag{19}$$

which is defined such that $\mathbf{e}(e_1,\ldots,e_n)=1$, implying that $\mathbf{e}_{[i_1,\ldots,i_n]}=n!$. It may be proven that the unit volume form transforms as a relative tensor under coordinate transformation, i.e.

$$\bar{\mathbf{e}}_{i_1\ldots i_n}=\det(A)^{-1}A^{j_1}_{i_1}A^{j_2}_{i_2}\ldots A^{j_n}_{i_n}\mathbf{e}_{j_1\ldots j_n}, \tag{20}$$

where $\mathbf{e}$ is the original volume form, $\bar{\mathbf{e}}$ is the transformed volume form and A^j_i is the Jacobian of the coordinate transformation.

More common than the unit volume form is the natural volume form ε, which is designed to transform as a (pseudo-)tensor, cancelling the factor $\det(A)^{-1}$ in equation 20. To this end, consider the term $\sqrt{|g|}$, which transforms as $\bar{g}=\det(A)^2g$, as the metric tensor transforms as a tensor, i.e. $\bar{g}_{ij}=A^k_iA^l_jg_{kl}$. With this relation in mind, the natural volume form may be defined as $\varepsilon=\sqrt{|g|}\mathbf{e}$, which transforms as a pseudo-tensor, i.e.

$$\bar{\varepsilon}_{i_1\ldots i_n}=\mathrm{sgn}(\det(A))A^{j_1}_{i_1}A^{j_2}_{i_2}\ldots A^{j_n}_{i_n}\varepsilon_{j_1\ldots j_n}. \tag{21}$$

Action integral

Using the previously described volume forms, integrals can now be formally introduced. Classically, the most important integral in Lagrangian theory is the action functional, defined as the bounded time integral over the Lagrangian and denoted as

$$S[L]=\int_{t_1}^{t_2}Ldt, \tag{22}$$

where L is the Lagrangian and $dt\equiv\mathbf{e}_1$ is the unit volume form. When using Lagrangian theory to describe general relativity, though, the Lagrangian will not only be integrated over time but the entirety of space-time, as will be explained further in section 3.1. The action functional will in this case be denoted as

$$S[L]=\int_M L\varepsilon, \tag{23}$$

where L is the Lagrangian, M the area of space-time over which is integrated and ε the natural volume form.

Gauss' theorem

Gauss' theorem, also known as the divergence theorem, is a highly useful tool when deriving the equations of motion from the action functional, being applicable in many situations when employing the variational principle. Based on the argument of the integral, the theorem changes slightly. The most common version of Gauss' theorem is

$$\int_M\nabla_\mu\phi^\mu\varepsilon=\oint_{\partial M}\epsilon\phi^\mu n_\mu\varepsilon_3, \tag{24}$$

where M can be a spacelike or timelike hypersurface (will be defined in section 2.4) embedded within space-time, n^μ are the components of the outward pointing unit (normalised) normal vector field to ∂M, $\epsilon=n^\mu n_\mu=\pm1$, $\phi\in\mathfrak{X}(M)$ is a vector field and ε_3 is the natural volume form on the boundary ∂M [47]. Alternatively, in case the argument to the covariant derivative is a scalar field or any other continuous function, i.e. $\phi\in C^\infty(M)$, Gauss' theorem reads

$$\int_M\partial_\nu\phi\varepsilon=\oint_{\partial M}\epsilon\phi n_\nu\varepsilon_3, \tag{25}$$

where the second formulation follows easily from the first by choosing $\phi^\mu=\phi\delta^\mu_\nu$. More extensive equations can be derived for lightlike hypersurfaces [46], though these will not be required for this report.

2.4 Theory of general relativity

The theory of general relativity describes a relation between the structure of space-time and the matter present, attributing the 'force' of gravity to the curvature of space-time instead of using the classical notion of a force. Information on the structure is encapsulated by the relativistic metric tensor, while matter is described by the stress-energy-momentum tensor. In this section, after introducing these and additional relevant derived quantities, the Einstein field equations will be derived, which govern the relation between the metric and stress-energy-momentum tensor. Finally, this section will close with a discussion on different definitions of curvature, a vital concept within the theory of general relativity.

Relativistic metric tensor

The relativistic metric tensor $g \in T_2^0(\mathfrak{X}(M))$, a 4-dimensional second order covariant tensor with holor $g_{\alpha\beta}$, stores most information on the structure of a space-time M and is used to describe the length element as

$$ds^2 \equiv |\delta s|^2 = (\delta s|\delta s) = g_{\alpha\beta}\delta x^\alpha \delta x^\beta \equiv g_{\alpha\beta} dx^\alpha dx^\beta, \tag{26}$$

where $\delta s \equiv \delta x^\alpha e_\alpha$ is an infinitesimal vector and x^α is the 4-dimensional coordinate vector describing the manifold M. From equation 26, it can be deduced that the holor of the relativistic metric tensor can be found by taking the inner product of the unit basis vectors, i.e. $g_{\alpha\beta} = (e_\alpha|e_\beta)$, such that the relativistic metric tensor is equivalent to the metric tensor discussed before in section 2.1. Therefore, the relativistic metric tensor has all properties of the metric tensor, such as the ability to lower and raise indices. Note that, in the remainder of this report, we will use the terms 'metric tensor' and 'metric' interchangeably to refer to this tensor.

Alongside the metric tensor, the connection coefficients $\Gamma^\alpha_{\beta\gamma}$ defined in equation 12 play a central role within the description of space-time as well, as they describe a relation between basis vectors of neighbouring tangent spaces through the notion of parallel transport. Applying the two basic assumptions of Einstein's theory of general relativity, the vanishing of the torsion tensor and metric compatibility, to the definition of these connection coefficients, it may be derived that

$$\Gamma^\alpha_{\beta\gamma} = \frac{1}{2} g^{\alpha\sigma}(\partial_\beta g_{\gamma\sigma} + \partial_\gamma g_{\beta\sigma} - \partial_\sigma g_{\beta\gamma}), \tag{27}$$

by decomposing the vanishing covariant derivative of the metric and cyclically permuting the indices. In this case, the connection coefficients are called the Christoffel symbols of the second kind, which will play a major role in the derivation of the Einstein field equations.

Einstein field equations

The Einstein field equations describe a relation between the matter in and curvature of a given space-time. Within general relativity, the matter within a space is assumed to be described by the symmetric second-order covariant stress-energy-momentum tensor $T = T_{\mu\nu}\hat{e}^\mu \otimes \hat{e}^\nu$, describing the flux of the energy-momentum 4-vector in all directions [48]. Therefore, the tensors describing the curvature of space-time in the Einstein field equations should be symmetric second-order covariant tensors as well. On top of this, these tensors are postulated to depend solely on the metric, due to the previously described relations between the metric tensor, Christoffel symbols and geometry of space-time. Finally, by applying the classical limit and comparing to the Newtonian theory of gravity, it is found that the tensors in the Einstein field equations should not depend on higher-order derivatives of the metric tensor beyond the second and should be linear in such terms.

The Riemann curvature tensor, a tensor which can be formed using only Christoffel symbols, is especially interesting in this case, as it describes the intrinsic curvature of space-time, depends on at most second derivatives of the metric and can be reduced to the second order covariant Ricci tensor as

$$\text{Riemann tensor}: R^{\alpha}_{\beta\gamma\delta} = \partial_\gamma \Gamma^{\alpha}_{\beta\delta} - \partial_\delta \Gamma^{\alpha}_{\beta\gamma} + \Gamma^{\alpha}_{\sigma\gamma}\Gamma^{\sigma}_{\beta\delta} - \Gamma^{\alpha}_{\sigma\delta}\Gamma^{\sigma}_{\beta\gamma}, \tag{28}$$

$$\text{Ricci tensor}: R_{\alpha\beta} = R^{\gamma}_{\alpha\gamma\beta}. \tag{29}$$

The relation between the Riemann curvature tensor and the intrinsic curvature becomes clear when analysing the expression $R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z$, the Riemann tensor applied to vector fields $X, Y, Z \in \mathfrak{X}(M)$ [49]. Using the geometrical meaning of the affine connection and the Lie bracket, it can be deduced that $R(X,Y)Z$ is the vector difference between Z and the vector which is found when Z is parallel transported along an infinitesimally small parallelogram spanned by X and Y [50]. Therefore, any vector Z is parallel transported to itself over any loop if and only if $R(X,Y) = 0$ for all $X, Y \in \mathfrak{X}(M)$. Conversely, it may be proven that $R(X,Y) = 0$ implies that a coordinate transformation exists under which the metric transforms to the Minkowski metric $g_{\alpha\beta} = \text{diag}(-1,1,1,1)$ [38]. Therefore, a vanishing Riemann tensor implies flat space and a non-zero Riemann tensor implies curved space.

Given this relation between the Riemann and Ricci tensor and the curvature of space-time, it may be expected that the Ricci tensor will appear in the Einstein field equations. It may actually be proven that, assuming that quantities in the Einstein field equations are second-order symmetric covariant tensors which depend solely on the metric and are at most linear in the second derivatives of the metric, the most general formulation of the Einstein field equations is

$$\kappa T_{\mu\nu} = \lambda_1 R_{\mu\nu} + \lambda_2 R_{\alpha\beta} g^{\alpha\beta} g_{\mu\nu} + \lambda_3 g_{\mu\nu}, \tag{30}$$

where the Ricci scalar is defined as $R \equiv R_{\alpha\beta} g^{\alpha\beta} \in C^\infty(M)$, $\kappa = \frac{8\pi G}{c^4} \in \mathbb{R}$ and $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$ [51]. It may even be proven that the restriction on the order of derivatives of the metric is superfluous for a 4-dimensional space-time [52], reducing the number of required assumptions.

Alongside the previous assumptions, Einstein assumed that local conservation of energy and momentum, $\nabla_\mu T^{\mu\nu} = 0$, should follow from the field equations, as has been verified by years of physical experiments [11]. Therefore, the covariant derivative of the right-hand side of equation 30 should vanish locally as well. Given that $\nabla_\alpha R_{\mu\nu} = \nabla_\alpha(\frac{1}{2} g_{\mu\nu} R)$ [34], the constants in equation 30 are restricted by the condition $\frac{1}{2}\lambda_1 + \lambda_2 = 0$. Additionally, by taking the classical limit, it can be found that $\lambda_1 = -1$ [34], such that

$$-\kappa T_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} + \Lambda g_{\mu\nu}. \tag{31}$$

Here, $\Lambda \in \mathbb{R}$ is the cosmological constant, which is still undetermined. For physical space-time, the value of the cosmological constant has not yet been found, as several methods provide significantly different results [53]. Therefore, the cosmological constant will be kept arbitrary in the proceedings of this report.

Hypersurfaces and curvature

Hypersurfaces, manifolds of dimension $n-1$ smoothly embedded within a space of dimension n [37], are vital to describe gravity in the Hamiltonian formalism. Specifically, spacelike hypersurfaces will play a major role, where a hypersurface is spacelike if it has a timelike normal vector everywhere and vice versa. A vector $n^\alpha \partial_\alpha \in TM$, in turn, is spacelike if $n^\alpha n_\alpha = g^{\alpha\beta} n_\beta n_\alpha > 0$ and timelike if the same quantity is negative. The value of ϵ in Gauss' theorem thus follows directly from the fact whether the surface is timelike or spacelike.

An important property of these hypersurfaces is their curvature. Previously, the Riemann curvature tensor has been defined, which describes the intrinsic curvature of a surface. Alternatively, an extrinsic curvature K_{ab} can be defined, which contains information on the curvature of the manifold, as embedded in the surrounding space, which can strongly differ from the intrinsic curvature. It is defined as

$$K_{ab} = \nabla_\alpha n_\beta e^\alpha_a e^\beta_b, \tag{32}$$

where $n_\beta \in \mathfrak{X}(M)$ is the normal vector (field) to the manifold and $e^\alpha_a \equiv \frac{\partial x^\alpha}{\partial y^a}$ is the Jacobian of the coordinate basis projection from the space to the hypersurface, where the space is described by coordinates $x^\alpha \in \mathbb{R}^4$ and the hypersurface by coordinates $y^a \in \mathbb{R}^3$. It can be shown that K_{ab} is symmetric [46], such that

$$K_{ab} = \nabla_{(\alpha} n_{\beta)} e^\alpha_a e^\beta_b = \frac{1}{2} \pounds_n (g_{\alpha\beta}) e^\alpha_a e^\beta_b. \tag{33}$$

This shows the relation between the extrinsic curvature, the metric tensor and the normal to a hypersurface. Using the previous description of the Lie derivative, it may be concluded that the extrinsic curvature describes the change in the metric tensor when transported in a flow normal to the hypersurface and therefore depends on the structure of space-time directly surrounding the hypersurface, in contrast to the intrinsic curvature.

The difference between these two definitions of curvature becomes increasingly clear in the example of a cylinder. When viewing a cylinder from a higher dimensional space, it is clear that its curvature is non-zero, which is confirmed by evaluating the definition of extrinsic curvature as stated in equation 32. Conversely, the cylinder has no intrinsic curvature, as it can be formed from a (curvature-less) plane without tears or deformations. This shows that the intrinsic and extrinsic curvature can contain very different information on the same object, though describing the same concept.

3 Lagrangian formalism

Within this section, the derivation of the Einstein field equations through the Lagrangian formalism will be detailed. A modified variational principle, with as varying quantity a tensor field, will be applied on an action functional, which will be formally defined in section 3.1. By equating the field to the metric tensor and applying the variational principle to the Hilbert action, the vacuum Einstein field equations for relativity will be derived. Then, matter will be added to the system and a stress-energy-momentum tensor will be defined, of which several vital properties will be derived. Alongside this main highlight, it will be shown that this approach naturally induces metric compatibility through the Palatini action.

The setting for this description will be a pseudo-Riemannian Hilbert space representing 4-dimensional curved space-time S, defined by coordinates $x_\mu \in \mathbb{R}^4$ and a symmetric metric tensor $g_{\alpha\beta} \in T^0_2(\mathfrak{X}(S))$ with signature $(-,+,+,+)$, defined on the whole fabric of space-time. Let M be a manifold embedded within this space-time, with an inner product $(.|.) : M \times M \to \mathbb{R}$ defined as $(x|y) = g_{\alpha\beta}x^\alpha y^\beta$. On this manifold M, a one-parameter family of tensor fields $\psi_\lambda \in \mathbb{R} \times T^l_k(\mathfrak{X}(M))$ is defined, which will be the subject of the variational principle. Note that in the following, the indices of the holor of ψ and the corresponding summations will be implicit.

3.1 Variational principle

The variational principle applied to field theory is conceptually the same as that applied to classical mechanics [54], though the specifics are altered. Instead of determining the trajectory corresponding to the stationary value of the action integral for three classical degrees of freedom for an object, now infinite degrees of freedom exist, due to the different values the tensor field ψ can take at each position in space. Therefore, a new type of derivative, the 'functional derivative', should be defined to allow variation of the action functional over a tensor field.

Action functional

First, though, the action functional itself should be defined. Similarly to the classical equivalent, the action functional S will be defined as an integral of a Lagrangian density function L, which may depend on the tensor field ψ and the metric tensor $g_{\alpha\beta}$, as well as any of their derivatives [34]. Whereas in classical Lagrangian mechanics, the coordinates over which the variation is performed are a function of purely time, ψ varies as both a function of time and space. This implies that, instead of integrating only over time, integration should be performed over the entire manifold M, inducing the name Lagrangian density.

Furthermore, it is believed that physical theories should be generally covariant. This symmetry must be reflected in the action S, which therefore has to behave as scalar under general coordinate transformations [34]. It will be assumed in the following that all coordinate transformations will preserve the orientation of the manifold describing space-time, implying that all pseudotensors will transform as tensors [55]. The Lagrangian density should then behave as a tensor under transformation, as the natural volume form $\varepsilon = \sqrt{-g}[i_1 \dots i_n]\hat{e}^{i_1} \otimes \dots \otimes \hat{e}^{i_n}$ transforms as a tensor as well. To ensure this behaviour, the Lagrangian density will depend only on covariant instead of partial derivatives of ψ, alongside scalar combinations of the metric tensor and its derivatives. Therefore, we find that the action functional in its most general form can be written as

$$S[L] = \int_M L(\psi, \nabla_\alpha \psi, ..., \nabla^k_\alpha \psi, g_{\alpha\beta}, \partial_\mu g_{\alpha\beta}, ...)\varepsilon, \tag{34}$$

where the field ψ and its derivatives are assumed independent. Note that not only the Lagrangian density depends on the metric, but the volume form as well. Therefore, if the action functional is varied towards the metric to determine the equations of motion, the volume form will vary as well. There are two main approaches to account for this variation. The first approach will be to calculate the variation in the volume form by brute force, adding many additional terms to the calculations. The second, more insightful approach will be to adopt a new volume form, being the unit volume form $\mathbf{e} = [i_1 \dots i_n] \hat{e}^{i_1} \otimes \dots \otimes \hat{e}^{i_n}$, which is independent of the metric tensor. When applying this method, the Lagrangian density is commonly redefined to the scalar density $\mathcal{L} = L \cdot \sqrt{-g}$ [56], such that the action functional can be rewritten as

$$S[\mathcal{L}] = \int_M L \varepsilon = \int_M \mathcal{L} \mathbf{e}. \tag{35}$$

Variation operator

Before the functional derivative is defined, first our focus shifts to the variation operator δ. In the classical case, the Euler-Lagrange equations are derived by defining a path $\bar{y}(x) = y(x) + \epsilon \eta(x)$, where $y(x)$ is the path with a minimal value of the action functional. For field theory, equivalently, a one-parameter family of tensor field configurations $\psi_\lambda = \psi_0 + \lambda \eta \in \mathbb{R} \times T^l_k(\mathfrak{X}(M))$ is defined, where $\eta \in T^l_k(\mathfrak{X}(M))$ and $\lambda \in \mathbb{R}$ are arbitrary and where $\psi_0 \in T^l_k(\mathfrak{X}(M))$ is the field which solves the field equations. The variation operator δ is then defined as the derivative of a function towards λ, evaluated at $\lambda = 0$, i.e.

$$\delta L[\psi] \equiv \frac{dL[\psi_\lambda]}{d\lambda}|_{\lambda=0}, \tag{36}$$

where L is an arbitrary continuously differentiable function of ψ. From this definition, it can be deduced that the variation operator contains information on the variation of a function when the field ψ is varied infinitesimally around the field which satisfies the field equations, ψ_0. Therefore, it must be that $\delta S[\psi] = 0$ if ψ is the field which minimizes S, i.e. if ψ satisfies the field equations.

Several important properties of the variation operator can be derived from its definition, equation 36. First, note that all properties of the derivative operator apply to the variation operator as well, such as linearity over sums, the chain rule and the product rule. This implies that the variation operator commutes with integration through Leibniz' integral rule as well.

Next, the commutative relations between the variation operator and other derivatives are investigated. For this, we will need to view δ from a slightly different perspective. Using the definition of $\delta\psi$, the Taylor expansion of ψ_λ around $\lambda = 0$ is determined to be

$$\psi_\lambda = \psi_0 + (\delta\psi)\lambda + \mathcal{O}(\lambda^2), \tag{37}$$

as ψ_0 is independent of λ. By realising that, when applying the variational principle, variations in λ (and thus λ itself) will be infinitesimal, terms of second order in λ are negligible, reducing equation 37 to

$$\delta\psi = \lim_{\lambda \to 0} \frac{\psi_\lambda - \psi_0}{\lambda}. \tag{38}$$

An equivalent relation can be derived for the variation of the action functional [57]. Using equation 38, the commutation relation between the variation and partial derivatives is found to be

$$\partial(\delta\psi) = \partial \left(\lim_{\lambda \to 0} \frac{\psi_\lambda - \psi_0}{\lambda} \right) = \lim_{\lambda \to 0} \frac{\partial(\psi_\lambda) - \partial(\psi_0)}{\lambda} = \delta(\partial\psi). \tag{39}$$

On the other hand, using the relations derived in section 2.2 between the partial, covariant and Lie derivative, it can be determined that the variation operator and covariant or Lie derivative do not commute in general, only when the variation in the connection coefficients and variation in the vector flow field vanish, respectively.

Functional derivative

The variation operator can be used to define the functional derivative of the action functional S towards the field $\psi \in T^l_k(\mathfrak{X}(M))$, $\frac{\delta S}{\delta \psi}$. Analogous to the previous section, define a smooth family of tensor field configurations $\psi_\lambda \in T^l_k(\mathfrak{X}(M))$, where ψ_0 is the solution to the field equations. Now suppose $\delta S = \frac{dS}{d\lambda}|_{\lambda=0}$ exists for all such smooth one parameter families ψ_λ. Then, if there exists a smooth tensor field $\chi \in T^k_l(\mathfrak{X}(M))$ dual to ψ such that

$$\delta S \equiv \frac{dS}{d\lambda}|_{\lambda=0} = \int_M \chi^{j_1 j_2 \dots j_k}_{i_1 i_2 \dots i_l} \frac{d\psi^{i_1 i_2 \dots i_l}_{j_1 j_2 \dots j_k, \lambda}}{d\lambda}|_{\lambda=0}\varepsilon \equiv \int_M \chi^{j_1 j_2 \dots j_k}_{i_1 i_2 \dots i_l} \delta\psi^{i_1 i_2 \dots i_l}_{j_1 j_2 \dots j_k, \lambda}\sqrt{-g}\mathbf{e} \tag{40}$$

for all families ψ_λ, S is functionally differentiable at ψ_0 and the functional derivative is defined as $\frac{\delta S}{\delta \psi}|_{\psi_0} = \chi^{j_1 j_2 \dots j_k}_{i_1 i_2 \dots i_l}$ [58]. In the rest of this report, the indices of the holor of χ will be suppressed, similar to the indices of ψ.

Note that, for a field ψ which is symmetric in at least 2 indices, this definition of S is ambiguous. In that case, the antisymmetric part of χ in those indices will not contribute to the integral in equation 40 and thus any tensor antisymmetric in the given indices can be added to χ. To remove this ambiguity, it is defined that, should the field ψ be symmetric in some indices, χ should be symmetric in those as well.

As the variation in the field $\delta\psi$ is arbitrary, $\delta S = 0$ only holds in general if and only if $\chi = 0$. Therefore, both the functional derivative and variation operator can be used to determine the field which satisfies the field equations. In the remainder of this report, the variation operator is the preferred choice, as the previously derived properties simplify notation considerably.

Boundary conditions

Finally, several boundary conditions need to be enforced to ensure the well-definedness of the variational principle. Firstly, the area of space-time within which the variation will occur should be a bounded, compact manifold $U \subseteq M$, to ensure the existence of a stationary value of the action. We will additionally assume U to be non-null, to reduce complexity, as these surfaces require a slightly different treatment [46]. Secondly, analogously to classical theory, which requires that the variation of the path at its endpoints must be 0, it is required that the variation of the field on the boundary of the manifold, ∂U, is equal to 0.

3.2 Field Euler-Lagrange equations

In a similar fashion to the classical Euler-Lagrange equations [59], equations of motion for fields can be found by applying the techniques of calculus of variations to the previously defined variational principle. One important relation required for this derivation is the variation of the terms alongside the Lagrangian density, $\delta(\sqrt{-g}\mathbf{e})$. To be able to determine this relation, first a relation should be found between the variation in the metric and its inverse. Using the product rule of the variation operator, it is easily found that

$$g_{\alpha\beta}\delta g^{\beta\gamma} + g^{\mu\gamma}\delta g_{\alpha\mu} = \delta(g_{\alpha\beta}g^{\beta\gamma}) = \delta(\delta^\gamma_\alpha) = 0, \tag{41}$$

which can be reorganised to find $\delta g_{\mu\nu} = -g_{\alpha\mu}g_{\beta\nu}\delta g^{\alpha\beta}$. Using this and the Jacobi rule for variation in determinants [46], it can be found that

$$
\begin{aligned}
\delta(\sqrt{-g}\mathbf{e}) &= \delta(\sqrt{-g})\mathbf{e} \\
&= -\frac{1}{2\sqrt{-g}}\delta g\mathbf{e} \\
&= -\frac{1}{2\sqrt{-g}}(g \cdot g^{\mu\nu} \cdot \delta g_{\mu\nu})\mathbf{e} \\
&= -\frac{1}{2}\sqrt{-g}(g^{\mu\nu} \cdot g_{\alpha\mu} \cdot g_{\beta\nu} \cdot \delta g^{\alpha\beta})\mathbf{e} \\
&= -\frac{1}{2}\sqrt{-g}(g_{\alpha\beta}\delta g^{\alpha\beta})\mathbf{e}.
\end{aligned}
\tag{42}
$$

Using equation 42, the field Euler-Lagrange equations can be derived for a scalar field, as found in appendix I. Assuming that only first-order derivatives of the field occur in the Lagrangian, the field Euler-Lagrange equations are given by

$$
\frac{\partial L}{\partial \psi} - \nabla_\mu \left(\frac{\partial L}{\partial(\nabla_\mu \psi)} \right) = 0. \tag{43}
$$

Similar equations can be derived for a Lagrangian which depends on higher order derivatives of the field [34].

Example: Klein-Gordon equations

To illustrate the previously defined variational principle and field Euler-Lagrange equations, the Klein-Gordon equations, which describe the evolution of a field containing spinless particles [60, 61], will be derived using the Lagrangian formalism. Similar to the classical Lagrangian $L = T - V$, the Klein-Gordon Lagrangian is proposed to be

$$
L = -\frac{1}{2}(g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi + M^2\psi^2), \tag{44}
$$

where $\psi \in C^\infty(U)$ is the particle wave function and $M = \frac{mc^2}{\hbar}$.

Before applying the variational principle, it should first be proven that the action functional corresponding to this Lagrangian is functionally differentiable. Using the chain rule and the previously described commutative relations between differentiation and δ, it is found that

$$
\begin{aligned}
\delta S &= \int_U -\frac{1}{2}\delta[g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi + M^2\psi^2]\varepsilon \\
&= -\int_U [g^{\mu\nu}\delta(\nabla_\mu\psi)\nabla_\nu\psi + M^2\psi\delta\psi]\varepsilon \\
&= -\int_U [g^{\mu\nu}\nabla_\mu(\delta\psi)\nabla_\nu\psi + M^2\psi\delta\psi]\varepsilon \\
&= -\int_U [g^{\mu\nu}\nabla_\mu(\delta\psi\nabla_\nu\psi) - g^{\mu\nu}\nabla_\mu(\nabla_\nu\psi)\delta\psi + M^2\psi\delta\psi]\varepsilon \\
&= -\int_U [-g^{\mu\nu}\nabla_\mu(\nabla_\nu\psi) + M^2\psi]\delta\psi\varepsilon + \oint_{\partial U} \epsilon[g^{\mu\nu}\delta\psi n_\mu\nabla_\nu\psi]\varepsilon_3 \\
&= -\int_U [-g^{\mu\nu}\nabla_\mu(\nabla_\nu\psi) + M^2\psi]\delta\psi\varepsilon,
\end{aligned}
\tag{45}
$$

where in the penultimate step Gauss' theorem was used and in the final step the boundary condition $\delta\psi|_{\partial U} = 0$ was used. From this final line, it can be read that $\chi = g^{\mu\nu}\nabla_\mu(\nabla_\nu\psi) - M^2\psi$, which is a smooth function, thus the action is functionally differentiable.

Now the equations of motion can be derived. It can be seen from equation 44 that this Lagrangian only depends on first-order derivatives of the field ψ, allowing equation 43 to be applied. Note that covariant, partial and Lie derivatives are equivalent when acting on ψ (as ψ is a scalar field). Using this equivalence, the field equations may be found to be

$$\begin{aligned} 0 &= \frac{\partial(-g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi - M^2\psi^2)}{\partial\psi} - \nabla_\alpha\left[\frac{\partial(-g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi - M^2\psi^2)}{\partial(\nabla_\alpha\psi)}\right] \\ &= -2M^2\psi + \nabla_\alpha[g^{\mu\nu}(\delta^\alpha_\mu\nabla_\nu\psi + \delta^\alpha_\nu\nabla_\mu\psi)] \\ &= -2M^2\psi + \nabla_\nu(g^{\mu\nu}\nabla_\mu\psi) + \nabla_\mu(g^{\mu\nu}\nabla_\nu\psi) \\ &= -2(M^2\psi - \nabla^\mu\nabla_\mu\psi), \end{aligned} \tag{46}$$

which is equivalent to the Klein-Gordon equations

$$M^2\psi - \nabla^\mu\nabla_\mu\psi = 0. \tag{47}$$

Note that this equation is equivalent to $\chi = 0$, confirming the validity of the derived field Euler-Lagrange equations.

3.3 Einstein field equations

Einstein field equations in vacuo

In the derivation of the Einstein field equations, the varying field is defined to be the inverse metric $g^{\alpha\beta}$. As the variation in the metric and inverse metric are directly related, the choice for the inverse is made to ease later computations. As $\psi = g^{\alpha\beta}$, the Lagrangian will be a function of purely the (inverse) metric and its derivatives. Given that the Lagrangian should be a scalar and related to the vacuum Einstein field equations as described in equation 31, the most obvious choice for a non-trivial Lagrangian is the Ricci scalar R, as first realised by Hilbert in 1915 [62]. Therefore, the 'Hilbert' action is defined as

$$S_H[\mathcal{L}] = \int_U R\varepsilon = \int_U R\sqrt{-g}\mathbf{e}. \tag{48}$$

The equations of motion follow directly from the variation of this Hilbert action, the derivation of which can be found in appendix II, with as result

$$\delta S_H = \int_U (R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta})\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e} - \oint_{\partial U} \epsilon h^{\alpha\beta}\delta(\partial_\mu g_{\alpha\beta})n^\mu\sqrt{|h|}\mathbf{e}_3, \tag{49}$$

where $n_\mu \in \mathfrak{X}(\partial U)$ is the unit (normalised) normal to ∂U, $\epsilon = n^\mu n_\mu = \pm 1$ and $\mathbf{e}_3$ is the 3-dimensional unit volume form. The term $h_{\alpha\beta}$ denotes the extension of the metric on ∂U, h_{ab}, into the whole of space-time U, defined through the relation $h_{\alpha\beta} = h_{ab}e^a_\alpha e^b_\beta$, where e^a_α is the Jacobian of the coordinate transformation from ∂U to U. This extension is equivalent to a pull-back operation using a function $\phi : U \to \partial U, \phi(v) = v^\alpha e^a_\alpha \partial_a$ with $v \in \mathfrak{X}(U)$.

Without the second boundary integral, equation 49 would produce the vacuum Einstein field equations for a vanishing cosmological constant as the equations of motion for the field. Therefore, adaptations should be made to the initial Lagrangian density to remove the boundary term in the variation of the action. One approach to this focuses on the extrinsic curvature, $K \in C^\infty(M)$, defined in section 2.4 as $K = K_{ab}h^{ab} \equiv \nabla_\beta n_\alpha e^\alpha_a e^\beta_b h^{ab} = \nabla_\beta n_\alpha h^{\alpha\beta}$. Therefore, on the boundary ∂U, the variation of the extrinsic curvature is equal to

$$\begin{aligned}\delta K &= \delta(\nabla_\beta n_\alpha h^{\alpha\beta}) \\ &\overset{*}{=} h^{\alpha\beta}\delta(\partial_\beta n_\alpha - \Gamma^\gamma_{\alpha\beta} n_\gamma) \\ &\overset{**}{=} -h^{\alpha\beta}\delta\Gamma^\gamma_{\alpha\beta} n_\gamma \\ &= -h^{\alpha\beta}\delta[\frac{1}{2}g^{\gamma\mu}(\partial_\alpha g_{\mu\beta} + \partial_\beta g_{\alpha\mu} - \partial_\mu g_{\alpha\beta})]n_\gamma \\ &= -\frac{1}{2}h^{\alpha\beta}\delta(\partial_\alpha g_{\mu\beta} + \partial_\beta g_{\alpha\mu} - \partial_\mu g_{\alpha\beta})n^\mu \\ &= \frac{1}{2}h^{\alpha\beta}\delta(\partial_\mu g_{\alpha\beta})n^\mu,\end{aligned} \tag{50}$$

where in the last step the fact was used that derivatives of the variation of the metric tangential to the boundary should vanish, as the variation on the boundary itself vanishes everywhere. Additionally, in step $(*)$, the boundary condition $\delta g^{\alpha\beta} = \delta h^{\alpha\beta} = 0$ is directly applied, whereas in step $(**)$, a consequence of these boundary conditions is used, namely that the variation in the normal vector vanishes everywhere.

The found equation for the variation in the extrinsic curvature closely resembles the integrand of the boundary term of the variation of the Hilbert action. Therefore, define a new boundary action as

$$S_B = \oint_{\partial U} 2\epsilon K\sqrt{|h|}\mathbf{e}_3. \tag{51}$$

Once this boundary action is varied and added to the varied Hilbert action, where it should be noted that $\delta\sqrt{|h|}|_{\partial U} = 0$ due to boundary conditions, the boundary terms will cancel each other, providing the equation

$$\delta S = \delta(S_H + S_B) = \int_U (R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta})\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e}. \tag{52}$$

Comparing the previous result with the Einstein field equations 52, we realise that the cosmological constant should still be accounted for. To this end, define an additional action functional

$$S_\Lambda = -2\int_U \Lambda\sqrt{-g}\mathbf{e}, \tag{53}$$

where Λ is the cosmological constant. Using equation 42, the variation in this action is found to be

$$\delta S_\Lambda = -2\int_U \Lambda\delta\sqrt{-g}\mathbf{e} = \int_U \Lambda g_{\alpha\beta}\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e}, \tag{54}$$

which may be added to the total varied action 52 to find

$$\delta S = \delta(S_H + S_B + S_\Lambda) = \int_U (R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta})\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e}. \tag{55}$$

As the action $S = S_H + S_B + S_\Lambda$ is clearly functionally differentiable, with $\chi = R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta}$, the field equations which follow from $\chi = 0$ are exactly the Einstein field equations in vacuo,

$$R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta} = 0. \tag{56}$$

Value of the action

Though the correct equations of motion follow from the proposed action $S = S_H + S_B + S_\Lambda$, there is still one major issue. Assume space-time is flat, i.e. $S = M = \mathbb{R}^4$, meaning that the Ricci scalar vanishes and assume zero cosmological constant, such that the action reduces to $S = S_B$. Now define U as the volume bounded by two hypersurfaces of constant time, connected by a cylinder of radius R, as depicted in figure 3. Note that the figure is 3-dimensional, while the actual space is 4-dimensional.

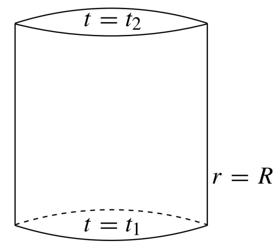

Figure 3: Two surfaces of constant time connected by a cylinder of radius R [46]

On the hypersurfaces of constant time, the extrinsic curvature clearly vanishes. On the cylinder, however, this is not the case. There, the metric is given by $ds^2 = -c^2dt^2 + R^2 d\Omega^2$, where $d\Omega^2 = d\theta^2 + \sin(\theta)^2 d\phi^2$, such that $\sqrt{|h|} = cR^2\sin(\theta)$. As the normal to the cylinder is given by $n_\alpha = \partial_\alpha r$, the extrinsic curvature may be computed to be

$$K = K_{ab}h^{ab} = (\nabla_\alpha n_\beta)e^\alpha_a e^\beta_b h^{ab} = \Gamma^\gamma_{\alpha\beta}(\partial_\gamma r)e^\alpha_a e^\beta_b h^{ab} = \Gamma^r_{ab}h^{ab} = \frac{2}{R}, \tag{57}$$

using the values of the Christoffel symbols for spherical coordinates [63]. The value of the action is thus given by

$$S_B = \oint_{\partial U} 2\epsilon K\sqrt{|h|}\mathbf{e}_3 = \int_0^{2\pi}\int_0^\pi\int_{t_1}^{t_2}\frac{4}{R}cR^2\sin(\theta)dtd\theta d\phi = 8\pi R(t_2 - t_1)c\int_0^\pi \sin(\theta)d\theta = 16\pi R(t_2 - t_1)c, \tag{58}$$

where $\epsilon = 1$ as $n_\alpha = \partial_\alpha r$, such that $n^\alpha n_\alpha = h^{rr}n_r n_r = 1$. Therefore, when the radius of the cylinder is extended towards infinity, the value of the action diverges. To remedy this, an additional regularisation term is added to the action, defined as

$$S_0 = -\oint_{\partial U} 2\epsilon K_0\sqrt{|h|}\mathbf{e}_3, \tag{59}$$

where $K_0 \in C^\infty(M)$ is the extrinsic curvature of ∂U in flat space-time. As K_0 is independent of the metric, the functional derivative of S_0 towards the metric vanishes, such that the variation of the total action still provides the Einstein field equations.

Adding a matter term

When matter is present in the system, an additional action S_M describing matter should be defined:

$$S_M[L_M] \equiv \int_U L_M(\phi, \nabla_\alpha\phi, g_{\alpha\beta})\varepsilon = \int_U L_M(\phi, \nabla_\alpha\phi, g_{\alpha\beta})\sqrt{-g}\mathbf{e}, \tag{60}$$

where L_M is the matter Lagrangian and $\phi \in T^i_j(\mathfrak{X}(M))$ is a tensor field of arbitrary order describing the matter in the system. Note that the Lagrangian has been restricted to be a function of at most first-order derivatives of the matter field and no derivatives of the metric tensor to simplify the following derivations [64]. The variation of this matter action can be found to be

$$\begin{aligned}
\delta S_M &= \delta \int_U L_M(\phi, \nabla_\alpha \phi, g_{\alpha\beta})\sqrt{-g}\mathbf{e} \\
&= \int_U \left[\delta L_M \sqrt{-g} + L_M \delta\sqrt{-g}\right]\mathbf{e} \\
&= \int_U \left[\delta g^{\alpha\beta}\frac{\partial L_M}{\partial g^{\alpha\beta}}\sqrt{-g} + \delta\phi\frac{\partial L_M}{\partial \phi}\sqrt{-g} + \delta(\nabla_\alpha\phi)\frac{\partial L_M}{\partial(\nabla_\alpha\phi)}\sqrt{-g} - L_M\frac{1}{2}\sqrt{-g}g_{\alpha\beta}\delta g^{\alpha\beta}\right]\mathbf{e} \\
&= \int_U \left[\frac{\partial L_M}{\partial g^{\alpha\beta}}\sqrt{-g} - L_M\frac{1}{2}\sqrt{-g}g_{\alpha\beta}\right]\delta g^{\alpha\beta}\mathbf{e} \\
&\equiv \int_U \frac{\delta S_M}{\delta g^{\alpha\beta}}\delta g^{\alpha\beta}\mathbf{e},
\end{aligned} \tag{61}$$

where $\delta\phi = \delta\nabla_\alpha\phi = 0$, as the matter field and the metric tensor are independent. With the addition of this term, the variation of the total action $S_H + S_B + S_\Lambda + S_0 + S_M$ reads

$$\delta S = \delta(S_H + S_B + S_\Lambda + S_0 + S_M) = \int_U \left[(R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta}) + \frac{\partial L_M}{\partial g^{\alpha\beta}} - L_M\frac{1}{2}g_{\alpha\beta}\right]\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e}, \tag{62}$$

yielding the field equations

$$R_{\alpha\beta} - \frac{1}{2}Rg_{\alpha\beta} + \Lambda g_{\alpha\beta} = -\frac{\partial L_M}{\partial g^{\alpha\beta}} + L_M\frac{1}{2}g_{\alpha\beta}. \tag{63}$$

Defining the 'dynamical' stress-energy-momentum tensor as $\kappa T_{\alpha\beta} \equiv -\frac{\partial L_M}{\partial g^{\alpha\beta}} + L_M\frac{1}{2}g_{\alpha\beta}$, where $\kappa = \frac{8\pi G}{c^4}$ is the Einstein gravitational constant, equation 63 is equivalent to the Einstein field equations including matter. In the remainder of this report, through the use of arbitrary units, κ is set to 1.

Dynamical stress-energy-momentum tensor

Previously, two important properties of the relativistic stress-energy-momentum tensor, conservation under covariant differentiation and symmetry, have been postulated to derive the Einstein field equations, as described in section 2.4. Alternatively, instead of these assumptions, equation 63 may be used to define the stress-energy-momentum tensor, from which conservation under covariant differentiation and symmetry naturally follow. Whereas the latter is easily confirmed by equation 63, as $g_{\alpha\beta}$ is symmetric, the former requires more effort and a shift of focus.

An important property of the Lagrangian (and Hamiltonian) formalism is invariance under diffeomorphisms, due to their tensorial nature. More specifically, each of the previously described action terms should be diffeomorphism invariant, including the matter action. By applying Noether's theorem [65], a conservation law can be derived from this invariance, as follows.

Suppose $\phi_\lambda : \mathbb{R} \times U \to U$ is a smooth one-parameter family of diffeomorphisms, generated by a vector field V^α, which vanishes on the boundary ∂U (to ensure smoothness). Assume that the matter field ϕ and its derivatives satisfy the matter equations, such that the functional derivatives of the action towards these values vanishes. Then diffeomorphism invariance implies that

$$\frac{dS_M}{d\lambda}|_{\lambda=0} \equiv \delta S_M = \int_U \frac{\delta S_M}{\delta g^{\alpha\beta}}\delta g^{\alpha\beta}\varepsilon + \int_U \frac{\delta S_M}{\delta\phi}\delta\phi\varepsilon + \int_U \frac{\delta S_M}{\delta\nabla_\alpha\phi}\delta\nabla_\alpha\phi\varepsilon = \int_U \frac{\delta S_M}{\delta g^{\alpha\beta}}\delta g^{\alpha\beta}\varepsilon = 0. \tag{64}$$

The functional derivative of the matter action functional towards the inverse metric has already been determined in equation 61 to be $\frac{\delta S_M}{\delta g^{\alpha\beta}} = \frac{\partial L_M}{\partial g^{\alpha\beta}} - L_M\frac{1}{2}g_{\alpha\beta} = -T_{\alpha\beta}$. Additionally, it may be proven that

$\delta g^{\alpha\beta} = \pounds_V g^{\alpha\beta} = 2\nabla^{(\alpha} v^{\beta)}$ [58]. Note that $\pounds_V g^{\alpha\beta}$ is the α, β-component of $\pounds_V g$, not the Lie derivative of an element of the holor of g. Combining the previous equations, it is found that

$$\begin{aligned}
\int_U \frac{\delta S_M}{\delta g^{\alpha\beta}} \delta g^{\alpha\beta} \varepsilon &= \int_U -T_{\alpha\beta} 2\nabla^{(\alpha} V^{\beta)} \varepsilon \\
&= -2 \int_U T_{\alpha\beta} \nabla^\alpha V^\beta \varepsilon \\
&= -2 \left(\int_U \nabla^\alpha (T_{\alpha\beta} V^\beta) \varepsilon - \int_U \nabla^\alpha (T_{\alpha\beta}) V^\beta \varepsilon \right) \\
&= -2 \left(\oint_{\partial U} \epsilon n^\alpha (T_{\alpha\beta} V^\beta) \varepsilon_3 - \int_U \nabla^\alpha (T_{\alpha\beta}) V^\beta \varepsilon \right) \\
&= 2 \int_U \nabla^\alpha (T_{\alpha\beta}) V^\beta \varepsilon \\
&= 0,
\end{aligned} \tag{65}$$

where the boundary term vanishes as the flow field V^β vanishes on the boundary. As the diffeomorphism and thus the flow field is arbitrary, to satisfy the above equations, it must hold that $\nabla^\alpha (T_{\alpha\beta}) = 0$ locally, thus $T_{\alpha\beta}$ is locally conserved under covariant differentiation. It has thereby been proven that both symmetry and conservation under covariant differentiation follow directly from the definition of the dynamical stress-energy-momentum tensor and therefore do not need to be postulated.

3.4 Palatini action

This section introduces the Palatini action, which, rather than requiring metric compatibility as a postulate, lets it follow naturally from the variational principle instead. Without this starting assumption, the Levi-Civita connection no longer applies, such that the metric and connection coefficients $\Gamma^\alpha_{\beta\gamma}$ may be assumed to be independent. Note that this assumption only holds when the matter term is independent of the connection coefficients [66]. The Palatini action, which is otherwise equivalent to the Hilbert action, is therefore a function of the metric, the connection coefficients and first-order derivatives of the connection coefficients. Varying the vacuum Palatini action towards the metric, we find

$$\begin{aligned}
\delta(S_H + S_B + S_\Lambda + S_0) &= \int_U [\delta(g^{\alpha\beta} R_{\alpha\beta}) \sqrt{-g} + (g^{\alpha\beta} R_{\alpha\beta} - 2\Lambda) \delta \sqrt{-g}] \mathbf{e} + \oint_{\partial U} 2\epsilon \delta K \sqrt{|h|} \mathbf{e}_3 \\
&= \int_U [R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} g^{\mu\nu} R_{\mu\nu} + g_{\alpha\beta} \Lambda] \delta g^{\alpha\beta} \sqrt{-g} \mathbf{e} \\
&= \int_U [R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} R + g_{\alpha\beta} \Lambda] \delta g^{\alpha\beta} \sqrt{-g} \mathbf{e},
\end{aligned} \tag{66}$$

which yields the Einstein field equations in vacuo, as expected. The discussion of the matter action S_M, which has been assumed independent of the connection coefficients, is unaltered from the previous section.

Alternatively, the Palatini action may now be varied towards the connection coefficients. Only the variation in the vacuum action $S_H + S_B + S_\Lambda + S_0$ needs to be considered, as the matter term is independent of the connection coefficients. Applying the variation operator yields

$$
\begin{aligned}
\delta(S_H + S_B + S_\Lambda + S_0) &= \int_U g^{\alpha\beta}\delta R_{\alpha\beta}\sqrt{-g}\mathbf{e} + \oint_{\partial U} 2\epsilon\delta K\sqrt{|h|}\mathbf{e}_3 \\
&\overset{*}{=} \int_U g^{\alpha\beta}[\nabla_\sigma(\delta\Gamma^\sigma_{\alpha\beta}) - \nabla_\beta(\delta\Gamma^\sigma_{\alpha\sigma})]\sqrt{-g}\mathbf{e} - \oint_{\partial U} 2\epsilon h^{\alpha\beta}\delta\Gamma^\gamma_{\alpha\beta}n_\gamma\sqrt{|h|}\mathbf{e}_3 \\
&= \int_U [\nabla_\sigma(g^{\alpha\beta}\delta\Gamma^\sigma_{\alpha\beta}) - \nabla_\sigma(g^{\alpha\beta})\delta\Gamma^\sigma_{\alpha\beta} - \nabla_\beta(g^{\alpha\beta}\delta\Gamma^\sigma_{\alpha\sigma}) + \nabla_\beta(g^{\alpha\beta})\delta\Gamma^\sigma_{\alpha\sigma}]\sqrt{-g}\mathbf{e} \\
&= \int_U [-\nabla_\sigma(g^{\alpha\beta})\delta\Gamma^\sigma_{\alpha\beta} + \nabla_\beta(g^{\alpha\beta})\delta\Gamma^\sigma_{\alpha\sigma}]\sqrt{-g}\mathbf{e} + \int_U \nabla_\beta[g^{\alpha\sigma}\delta\Gamma^\beta_{\alpha\sigma} - g^{\alpha\beta}\delta\Gamma^\sigma_{\alpha\sigma}]\sqrt{-g}\mathbf{e} \\
&= \int_U [-\nabla_\sigma(g^{\alpha\beta}) + \nabla_\nu(g^{\alpha\nu})\delta^\beta_\sigma]\delta\Gamma^\sigma_{\alpha\beta}\sqrt{-g}\mathbf{e} + \oint_{\partial U} \epsilon n_\beta[g^{\alpha\sigma}\delta\Gamma^\beta_{\alpha\sigma} - g^{\alpha\beta}\delta\Gamma^\sigma_{\alpha\sigma}]\sqrt{|h|}\mathbf{e}_3 \\
&= \int_U [-\nabla_\sigma(g^{\alpha\beta}) + \nabla_\nu(g^{\alpha\nu})\delta^\beta_\sigma]\delta\Gamma^\sigma_{\alpha\beta}\sqrt{-g}\mathbf{e},
\end{aligned}
\tag{67}
$$

where at several points the boundary conditions $\delta\Gamma^\beta_{\alpha\sigma} = 0$ are used and where in step $(*)$ equations II.2 and 50 are used. Given that the connection coefficients are symmetric in their two lower indices, the functional derivative of the total action $\frac{\delta S_H + S_B + S_0 + S_M}{\delta\Gamma^\sigma_{\alpha\beta}} \equiv \chi$ should be symmetric in the indices α and β as well. Therefore $\chi = -\nabla_\sigma(g^{\alpha\beta}) + \nabla_\nu(g^{\nu(\alpha}\delta^{\beta)}_\sigma$, which yields the equations of motion

$$
-\nabla_\sigma(g^{\alpha\beta}) + \frac{1}{2}\nabla_\nu(g^{\alpha\nu})\delta^\beta_\sigma + \frac{1}{2}\nabla_\nu(g^{\nu\beta})\delta^\alpha_\sigma = 0. \tag{68}
$$

This set of 40 equations of 40 variables only has $\nabla_\sigma(g^{\alpha\beta}) = 0$ as solution [49], which immediately implies $\nabla_\sigma(g_{\alpha\beta}) = 0$ as well. Therefore, in contrast to the Hilbert action, metric compatibility and thereby the Levi-Civita connection are a direct result of the variation of the Palatini action, instead of a postulate.

4 Hamiltonian formalism

Within classical mechanics, a Legendre transform is applied to the Lagrangian to obtain a Hamiltonian, which defines a system through the equations of motion

$$\begin{cases} \frac{\partial H}{\partial q} = -\dot{p}, \\ \frac{\partial H}{\partial p} = \dot{q}, \end{cases} \tag{69}$$

where q is the generalised coordinate and p the canonical momentum. A similar approach will be taken for field theory, though now some preliminary steps are required to be taken, as, due to the Lorentz covariance of the Lagrangian, no explicit time-direction has been defined, leaving an inability to define a canonical momentum as in the classical sense. Therefore, first a 3+1 decomposition of space-time into space and time should be made, to allow the definition of time derivatives.

After performing the decomposition, the Hamiltonian density and corresponding equations of motion can be derived. Alongside the equations of motion, the Hamiltonian density contains additional information on the system, which will be derived in section 4.4. Finally, some important symmetries of the Hamiltonian formalism will be discussed and compared to the Lagrangian formalism.

Similar to the Lagrangian formalism, the setting for the Hamiltonian description of relativity will be a Hilbert space representing 4-dimensional curved space-time S, defined by coordinates $x_\mu \in \mathbb{R}^4$ and a symmetric metric tensor $g_{\alpha\beta} \in T^0_2(\mathfrak{X}(S))$ with signature $(-,+,+,+)$, within which the manifold M is embedded, with inner product $(.|.) : M \times M \to \mathbb{R}$, defined as $(x|y) = g_{\alpha\beta}x^\alpha y^\beta$.

4.1 3+1 decomposition of space-time

To perform the 3+1 decomposition, a foliation of 4-dimensional space-time is made using an infinite set of spacelike 3-dimensional hypersurfaces which partition space-time, as shown in figure 4. These surfaces are defined through an arbitrary scalar field $t(x^\mu) : S \to \mathbb{R}$, where each hypersurface Σ_t corresponds to a different constant value of $t(x^\mu)$.

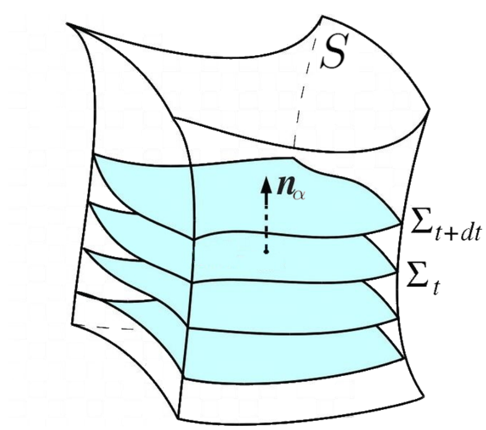

Figure 4: Conceptual visualisation of a foliation of space-time S [67]

Additionally, each hypersurface Σ_t has their own coordinates $y^a \in \mathbb{R}^3$, metric $h_{ab} \in T^0_2(\mathfrak{X}(\Sigma_t))$ and future-directed timelike normal vector $n^\alpha \in \mathfrak{X}(\Sigma_t)$. Per the definition of the foliation, the coordinates on different surfaces need not be related in any way, though this would be convenient. Therefore, a congruence of curves $\gamma_m : \mathbb{R} \times M \to M$ is defined with $m \in M$, such that $\gamma_m(t)$ returns the intersection of the curve through point m and hypersurface Σ_t, as shown in figure 5. The congruence of curves relates the coordinates of all hypersurfaces by requiring that the point $\gamma_m(0)$ is assigned the same coordinates y^a on Σ_0 as $\gamma_m(t)$ on Σ_t, for any $t \in \mathbb{R}$.

Note that these curves need not intersect the surfaces orthogonally. Rather, if t^α is the tangent to the curve and $t \equiv t(x^\mu)$ is the curve parameter, the tangent can be decomposed in the directions perpendicular and tangential to the surfaces Σ_t as

$$t^\alpha = N \cdot n^\alpha + N^a \cdot e^\alpha_a \equiv N \cdot n^\alpha + N^a \cdot \frac{\partial x^\alpha}{\partial y^a}, \tag{70}$$

where $N \in C^\infty(M)$ is the lapse and $N^a \in T^0_1(\mathfrak{X}(M))$ is the shift vector.

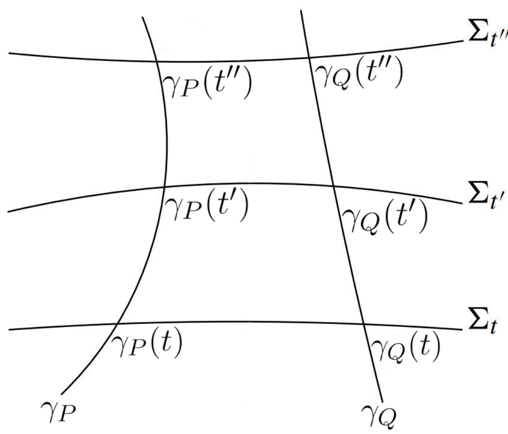

Figure 5: Conceptual visualisation of a congruence of curves through a foliation of space-time S [46]

The lapse may alternatively be defined through the relation $n_\alpha = -N\nabla_\alpha t$. The equivalence of this relation and the previous can be found by realising that $n_\alpha \propto \nabla_\alpha t$, as both are perpendicular to the surface Σ_t, and determining the proportionality constant using equation 70, $t^\alpha \nabla_\alpha t = 1$ (which holds by construction) and contractions.

As a 3+1 decomposition of space-time is made, general Lorentz covariance is lost within the Hamiltonian formalism. Though this is the case, arguments can still be made that the Hamiltonian is a more fundamental approach than the Lagrangian [68]. More on this will be discussed in section 4.5.

Relations between coordinate systems

The definition of the congruence of curves allows for an alternate coordinate system describing 4-dimensional space-time, being (t, y^α). This coordinate system can be related to the original x^μ through the relations

$$\begin{cases} t^\alpha = (\frac{\partial x^\alpha}{\partial t})_{y^a}, \\ e^\alpha_a = (\frac{\partial x^\alpha}{\partial y^a})_t, \end{cases} \tag{71}$$

where the subscript denotes a coordinate which is held constant. This implies that an infinitesimal displacement can be decomposed as

$$dx^\alpha = t^\alpha dt + dy^a e^\alpha_a = (Ndt)n^\alpha + (N^a dt + dy^a)e^\alpha_a, \tag{72}$$

yielding the length element

$$ds^2 = g_{\alpha\beta} dx^\alpha dx^\beta = \epsilon N^2 dt^2 + h_{ab}(dy^a + N^a dt)(dy^b + N^b dt), \tag{73}$$

where $\epsilon = -1$ as Σ_t are spacelike. This shows that the 3- and 4-dimensional metric are related through the projection $h_{ab} = g_{\alpha\beta} e^\alpha_a e^\beta_b$, equivalent to the application of a pull-back operation using the map $\phi : \Sigma_t \to M, \phi(v) = v^a e^\alpha_a \partial_\alpha$ for $v \in \mathfrak{X}(\Sigma_t)$.

Now, given that $g_{\alpha\beta}$ is an invertible, symmetric matrix, it holds that $g^{tt} = \text{adjugate}(g_{tt})/g \equiv \frac{\partial g}{\partial g_{tt}}/g = h/g$, where the final step can be deduced from equation 73 [69]. Alternatively, it is known that $g^{tt} = g^{\alpha\beta}\partial_\alpha t \partial_\beta t = g^{\alpha\beta} N^{-2} n_\alpha n_\beta = \epsilon N^{-2}$, where $\epsilon = -1$ as the surfaces are spacelike. Combining these two statements shows that $\sqrt{-g} = N\sqrt{h}$, which will often be used to transition between 3- and 4-dimensional volume forms.

Summarising all previously stated relationships between space-time and Σ_t, it has been found that

$$\begin{cases} t(x^\alpha)|_{\Sigma_t} = \text{constant}, \\ e^\alpha_a = (\frac{\partial x^\alpha}{\partial y^a})_t, \\ t^\alpha = (\frac{\partial x^\alpha}{\partial t})_{y^a}, \\ h_{ab} = g_{\alpha\beta} e^\alpha_a e^\beta_b, \\ \sqrt{-g} = N\sqrt{h}. \end{cases} \tag{74}$$

Finally, the completeness relation $g^{\alpha\beta} = \epsilon n^\alpha n^\beta + h^{ab} e^\alpha_a e^\beta_b$ will be of importance later, which can be verified element-wise by utilising equations 72 and 73 for the length element.

Boundary conditions

Similar to the Lagrangian case, a bounded, compact region U should be defined to perform integration and variation over. In this case, it is chosen to let U be bounded by two spacelike surfaces Σ_{t_1} and Σ_{t_2}, connected by an arbitrary timelike boundary B, as shown in figure 6, such that U describes space-time between times t_1 and t_2, in the spatial area bounded by B. This new region will again be foliated by Σ_t, with $t_1 < t < t_2$. Additionally, given that $\partial\Sigma_t = \Sigma_t \cap B \equiv S_t$, the boundary B is foliated by S_t. Similar relations to those provided in equation 74 can be described between B and the surface S_t, which are described in appendix III, as well as direct relations between S_t, B and 4-dimensional space-time.

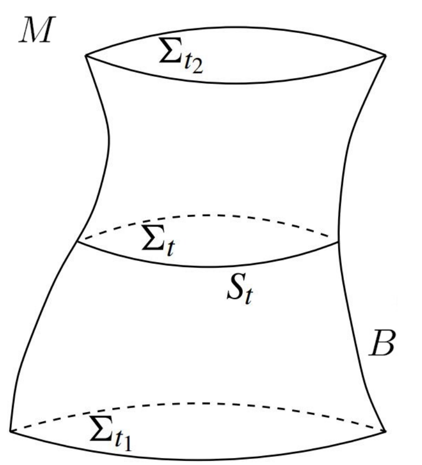

Figure 6: Conceptual visualisation the compact subset U of space-time [46]

Variation operator

Within the Hamiltonian formalism, the definition of the variation operator is modified slightly from the original in section 3.1. Instead of only considering the variation towards the field ψ, now the variation operator is redefined to include the variation towards both the field ψ as well as the canonical momentum π (to be formally defined later), to allow the field equations for both these variables to be derived. This implies that for an arbitrary continuously differentiable function $S[\psi, \pi]$,

$$\delta S[\psi, \pi] \equiv \int_U \left(\frac{\delta S}{\delta \psi} \delta \psi + \frac{\delta S}{\delta \pi} \delta \pi \right) \varepsilon. \tag{75}$$

Similar to the Lagrangian formalism, the variation of the field ψ is required to vanish at the boundary ∂U. The variation of the canonical momentum, on the other hand, need not vanish at the boundary to derive the Hamiltonian equations of motion for gravity, as will be shown in section 4.3.

4.2 Hamiltonian density and field equations

The first step in developing a Hamiltonian description of general relativity is to define the canonical momentum. Analogous to the classical definition $p = \frac{\partial L}{\partial \dot{q}}$, where $\dot{q} = \frac{dq}{dt}$, the canonical momentum will be defined as $\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}}$, where $\dot{\psi} = \pounds_t \psi$. Assuming the Lagrangian is a function of at most first derivatives of the field ψ [64], these canonical momentum can be used to define the Hamiltonian density as

$$\mathcal{H}(\pi, \psi, \nabla_a \psi, g_{\alpha\beta}, \partial_\mu g_{\alpha\beta}) = \pi \dot{\psi} - \sqrt{-g} L. \tag{76}$$

Note that the Hamiltonian density does not depend explicitly on $\dot{\psi}$, only π and spatial derivatives of ψ. Additionally, observe that π and $\mathcal{H}$, due to the factor $\sqrt{-g}$, do not transform as tensorial quantities under coordinate transformations. This has been chosen to slightly ease the difficulty of future calculations, given that a tensorial description of these variables does not provide many advantages [46].

It should still be proven that the above definition for the Hamiltonian density does provide the required equations of motion for π and ψ. We will assume for the following derivations that ψ is a scalar field, though similar equations can be derived for tensorial fields [70]. Inverting and integrating equation 76, while keeping the 3+1 decomposition explicit, provides

$$S = \int_{t_1}^{t_2} \int_{\Sigma_t} (\pi \dot{\psi} - \mathcal{H}) \mathbf{e}. \tag{77}$$

For the solution of the field equations, the variation in S should vanish, such that

$$\delta S = \int_{t_1}^{t_2} \int_{\Sigma_t} \delta(\pi \dot{\psi} - \mathcal{H}) \mathbf{e} = \int_{t_1}^{t_2} \int_{\Sigma_t} \left[\dot{\psi} \delta \pi + \pi \delta \dot{\psi} - \frac{\partial \mathcal{H}}{\partial \psi} \delta \psi - \frac{\partial \mathcal{H}}{\partial \pi} \delta \pi - \frac{\partial \mathcal{H}}{\partial (\nabla_a \psi)} \delta (\nabla_a \psi) \right] \mathbf{e} = 0, \tag{78}$$

where the variation in $g_{\alpha\beta}$ and $\partial_\mu g_{\alpha\beta}$ has been omitted, as ψ is a scalar field and therefore independent of the metric. The second term can be rewritten as

$$\begin{aligned} \int_{t_1}^{t_2} \int_{\Sigma_t} \pi \delta \dot{\psi} \mathbf{e} &= \int_{t_1}^{t_2} \left(\int_{\Sigma_t} \frac{\partial}{\partial t} (\pi \delta \psi) \mathbf{e}_3 - \int_{\Sigma_t} \dot{\pi} \delta \psi \mathbf{e}_3 \right) dt \\ &= \int_{t_1}^{t_2} \left(\int_{S_t} \epsilon \pi \delta \psi r_t \mathbf{e}_2 - \int_{\Sigma_t} \dot{\pi} \delta \psi \mathbf{e}_3 \right) dt \\ &= - \int_{t_1}^{t_2} \int_{\Sigma_t} \dot{\pi} \delta \psi \mathbf{e}, \end{aligned} \tag{79}$$

where $dt \equiv \mathbf{e}_1$, Gauss' rule was applied and the surface integral vanishes due to the boundary conditions.

Similarly for the last term,

$$
\begin{aligned}
\int_{t_1}^{t_2}\int_{\Sigma_t}\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\delta(\nabla_a\psi)\mathbf{e} &= \int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\delta\psi\right)\mathbf{e}-\int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\right)\delta\psi\mathbf{e}\\
&= \int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(\nabla_a\psi)}\sqrt{h}\delta\psi\right)\mathbf{e}-\int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(\nabla_a\psi)}\sqrt{h}\right)\delta\psi\mathbf{e}\\
&\overset{*}{=} \int_{t_1}^{t_2}dt\int_{\Sigma_t}\nabla_a\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(D_a\psi)}\delta\psi\right)\sqrt{h}\mathbf{e}_3-\int_{t_1}^{t_2}\int_{\Sigma_t}D_a\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(\nabla_a\psi)}\right)\delta\psi\sqrt{h}\mathbf{e}\\
&= \int_{t_1}^{t_2}dt\oint_{S_t}\epsilon\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(\nabla_a\psi)}\delta\psi\right)r_a\sqrt{|\sigma|}\mathbf{e}_2-\int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}_{scalar}}{\partial(\nabla_a\psi)}\sqrt{h}\right)\delta\psi\mathbf{e}\\
&= -\int_{t_1}^{t_2}\int_{\Sigma_t}\partial_a\left(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\right)\delta\psi\mathbf{e},
\end{aligned}
\tag{80}
$$

where $\mathcal{H}_{scalar}\equiv\frac{\mathcal{H}}{\sqrt{h}}$ is a scalar, equation ($*$) holds due to the divergence formula for vector fields [46] and the boundary term vanishes due to the boundary conditions. Returning to equation 78, inserting the previous two relations and grouping terms yields

$$
\int_{t_1}^{t_2}\int_{\Sigma_t}\left[\left(\dot{\psi}-\frac{\partial\mathcal{H}}{\partial\pi}\right)\delta\pi+\left(\partial_a\left(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\right)-\frac{\partial\mathcal{H}}{\partial\psi}-\dot{\pi}\right)\delta\psi\right]\mathbf{e}=0. \tag{81}
$$

The previous equation should hold for arbitrary variations of the canonical momentum π and field ψ independently, such that the equations of motions are found to be

$$
\begin{cases}\dot{\psi}=\frac{\partial\mathcal{H}}{\partial\pi},\\ \dot{\pi}=\partial_a\left(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}\right)-\frac{\partial\mathcal{H}}{\partial\psi}.\end{cases} \tag{82}
$$

Example: Klein-Gordon equations

The Hamiltonian field equations will now be verified for the Klein-Gordon equations, similar to section 3.2. Recall the Klein-Gordon Lagrangian, which was defined using the particle wave function $\psi\in C^\infty(U)$ as

$$
L=-\frac{1}{2}(g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi+M^2\psi^2). \tag{83}
$$

For simplicity, choose $N^a=0$. This ensures that $g_{ab}=h_{ab}$ for $a,b\in\{1,2,3\}$ and $g_{t\alpha}=0$ for $\alpha\neq t$, yielding the canonical momentum

$$
\begin{aligned}
\pi &= \frac{\partial\sqrt{-g}L}{\partial\pounds_t\psi}\\
&= \frac{1}{2}\sqrt{-g}\frac{\partial(-g^{\mu\nu}\nabla_\mu\psi\nabla_\nu\psi-M^2\psi^2)}{\partial\pounds_t\psi}\\
&= \frac{1}{2}\sqrt{-g}\frac{\partial(-g^{tt}\pounds_t\psi\pounds_t\psi-h^{ab}\nabla_a\psi\nabla_b\psi-M^2\psi^2)}{\partial\pounds_t\psi}\\
&= -\sqrt{-g}g^{tt}\pounds_t\psi.
\end{aligned}
\tag{84}
$$

Entering this result into the definition of the Hamiltonian density yields

$$\begin{aligned}\mathcal{H} &= \pi\dot{\psi} - \sqrt{-g}L \\ &= -\sqrt{-g}g^{tt}(\pounds_t\psi)^2 - \frac{1}{2}\sqrt{-g}(-g^{tt}\pounds_t\psi\pounds_t\psi - h^{ab}\nabla_a\psi\nabla_b\psi - M^2\psi^2) \\ &= \frac{1}{2}\sqrt{-g}(-g^{tt}(\pounds_t\psi)^2 + h^{ab}\nabla_a\psi\nabla_b\psi + M^2\psi^2) \\ &= \frac{1}{2}\sqrt{-g}(\frac{-\pi^2}{-g\cdot g^{tt}} + h^{ab}\nabla_a\psi\nabla_b\psi + M^2\psi^2).\end{aligned} \tag{85}$$

Finally, using the previous result and equation 82, the equations of motion can be determined to be the coupled system of first-order differential equations

$$\begin{cases}\dot{\pi} = \partial_a(\frac{\partial\mathcal{H}}{\partial(\nabla_a\psi)}) - \frac{\partial\mathcal{H}}{\partial\psi} = \partial_a(\sqrt{-g}h^{ab}\nabla_b\psi) - \sqrt{-g}M^2\psi, \\ \dot{\psi} = \frac{\partial\mathcal{H}}{\partial\pi} = \frac{-\pi}{\sqrt{-g}\cdot g^{tt}}.\end{cases} \tag{86}$$

These equations can easily be solved by realising that, due to the vanishing shift, $\sqrt{-g}$ and g^{tt} are independent of t. Using this, the equations of motion may be combined by taking the Lie derivative of the second and inserting the first, yielding

$$\begin{aligned}\ddot{\psi} &= \frac{-\dot{\pi}}{\sqrt{-g}\cdot g^{tt}} \\ &= \frac{-\partial_a(\sqrt{-g}h^{ab}\nabla_b\psi) + \sqrt{-g}M^2\psi}{\sqrt{-g}\cdot g^{tt}} \\ &\overset{*}{=} g_{tt}M^2\psi - \frac{1}{\sqrt{-g}}g_{tt}\partial_a(\sqrt{-g}h^{ab}\nabla_b\psi) \\ &\overset{**}{=} g_{tt}M^2\psi - \frac{1}{\sqrt{-g}}g_{tt}\partial_\alpha(\sqrt{-g}g^{\alpha\beta}\nabla_\beta\psi) + \frac{1}{\sqrt{-g}}g_{tt}\partial_t(\sqrt{-g}g^{tt}\nabla_t\psi) \\ &= g_{tt}M^2\psi - g_{tt}\nabla_\alpha(g^{\alpha\beta}\nabla_\beta\psi) + \frac{1}{\sqrt{-g}}g_{tt}\partial_t(-\pi) \\ &= g_{tt}M^2\psi - g_{tt}g^{\alpha\beta}\nabla_\alpha(\nabla_\beta\psi) + \ddot{\psi},\end{aligned} \tag{87}$$

where equation $(*)$ and $(**)$ both hold due to the vanishing shift, which implies the relations $g^{tt} = \frac{1}{g_{tt}}$, $g_{ab} = h_{ab}$ for $a, b \in \{1, 2, 3\}$ and $g_{t\alpha} = 0$ for $\alpha \neq t$. By manipulating the last line of this equation, the field equations are found to be

$$M^2\psi - g^{\alpha\beta}\nabla_\alpha(\nabla_\beta\psi) = 0, \tag{88}$$

exactly the Klein-Gordon equations. Though this shows the validity of the found field equations, this derivation has been considerably more laborious than its Lagrangian equivalent. The usefulness of the Hamiltonian formalism therefore does not lie in the computation of the field equations of simple systems, but in its ability to define a Hamiltonian operator, of which the quantisation procedure is well known.

4.3 Einstein field equations

Einstein field equations in vacuo

Recall the vacuum action functional as described in equations 48, 51 and 59. To allow the Hamiltonian technique to be applied, the action should be decomposed into space and time, the procedure for which is described in appendix IV. The final result for the decomposed action is

$$S = \int_{t_1}^{t_2}\left(\int_{\Sigma_t}({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)N\sqrt{h}\mathbf{e}_3 + 2\oint_{S_t}(k - k_0)N\sqrt{|\sigma|}\mathbf{e}_2\right)dt, \tag{89}$$

where ${}^3R \in C^\infty(\Sigma_t)$ is the 3-dimensional Ricci scalar and $K \in C^\infty(\Sigma_t)$ is the extrinsic curvature scalar.

Due to the 3+1 decomposition, the tensor field $\psi = h_{ab}$ will be used as the subject of the variational principle instead of $g^{\alpha\beta}$ as in the Lagrangian formalism. This implies that the Hamiltonian will only be integrated over a single hypersurface Σ_t and will therefore have a different value for each $t \in \mathbb{R}$. To define the Hamiltonian, though, first the Lie derivative of the metric should be determined. Using the fact that e^α_a is by definition independent of time, we find

$$\begin{aligned}
\pounds_t h_{ab} &= \pounds_t(g_{\alpha\beta}e^\alpha_a e^\beta_b) \\
&\equiv \pounds_t(g_{\alpha\beta})e^\alpha_a e^\beta_b \\
&= (\nabla_\beta t_\alpha + \nabla_\alpha t_\beta)e^\alpha_a e^\beta_b \\
&= (\nabla_\beta(Nn_\alpha + N_\alpha) + \nabla_\alpha(Nn_\beta + N_\beta))e^\alpha_a e^\beta_b \\
&= ((\nabla_\beta N)n_\alpha + \nabla_\beta N_\alpha + N(\nabla_\beta n_\alpha + \nabla_\alpha n_\beta) + (\nabla_\alpha N)n_\beta + \nabla_\alpha N_\beta)e^\alpha_a e^\beta_b \\
&\overset{*}{=} (\nabla_\beta N_\alpha + \nabla_\alpha N_\beta)e^\alpha_a e^\beta_b + N(\nabla_\beta n_\alpha + \nabla_\alpha n_\beta)e^\alpha_a e^\beta_b \\
&= (\nabla_\beta N_\alpha + \nabla_\alpha N_\beta)e^\alpha_a e^\beta_b + 2NK_{ab} \\
&\equiv D_b N_a + D_a N_b + 2NK_{ab},
\end{aligned} \tag{90}$$

where $N_\alpha \equiv N_a e^a_\alpha$, D_a is the intrinsic covariant derivative as defined in section 2.2 and ($*$) holds as a normal vector projected down to the surface it is defined on, $n_\alpha e^\alpha_a$, vanishes. Inverting this relation for K_{ab} yields

$$K_{ab} = \frac{1}{2N}(\pounds_t h_{ab} - D_b N_a - D_a N_b). \tag{91}$$

Given that the current formulation of the Lagrangian does depend on K_{ab}, but neither on $\dot{h}_{ab}$ nor $D_a N_b$, the chain rule can be applied to find $\pi^{ab} = \frac{\partial K_{mn}}{\partial \dot{h}_{ab}} \frac{\partial L\sqrt{-g}}{\partial K_{mn}}$. As the boundary term of the action is independent of the 3-dimensional extrinsic curvature, the canonical momenta depend only on the bulk Lagrangian

$$L_B = {}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda = {}^3R + (h^{ac}h^{bd} - h^{ab}h^{cd})K_{ab}K_{cd} - 2\Lambda, \tag{92}$$

where the last equality can be swiftly verified by distributing the term in brackets. Therefore, the canonical momenta are found to be

$$\begin{aligned}
\pi^{ab} &= \frac{\partial K_{mn}}{\partial \dot{h}_{ab}} \frac{\partial L_B\sqrt{-g}}{\partial K_{mn}} \\
&= \frac{\delta^a_m \delta^b_n}{2N}\sqrt{-g}\frac{\partial({}^3R + (h^{ce}h^{df} - h^{cd}h^{ef})K_{cd}K_{ef} - 2\Lambda)}{\partial K_{mn}} \\
&= \sqrt{h}(h^{ac}h^{bd} - h^{ab}h^{cd})K_{cd} \\
&= \sqrt{h}(K^{ab} - h^{ab}K).
\end{aligned} \tag{93}$$

Using this relation, the bulk Hamiltonian density is determined to be

$$\begin{aligned}
\mathcal{H}_B &= \pi^{ab}\dot{\psi}_{ab} - \sqrt{-g}L_B \\
&= \sqrt{h}(K^{ab} - h^{ab}K)(D_b N_a + D_a N_b + 2NK_{ab}) - \sqrt{-g}({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda) \\
&= 2\sqrt{h}(K^{ab} - h^{ab}K)D_a N_b - N\sqrt{h}(-2K_{ab}(K^{ab} - h^{ab}K) + {}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda) \\
&= 2\sqrt{h}(K^{ab} - h^{ab}K)D_a N_b - N\sqrt{h}({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda) \\
&= 2\sqrt{h}[D_a((K^{ab} - h^{ab}K)N_b) - D_a(K^{ab} - h^{ab}K)N_b - \frac{N}{2}({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)].
\end{aligned} \tag{94}$$

The full Hamiltonian is then found by integrating the previously found bulk density over space and re-adding the boundary terms, yielding

$$
\begin{aligned}
H_G &= \int_{\Sigma_t} \mathcal{H}_B \mathbf{e}_3 - \sqrt{-g}\left(\int_{\Sigma_t} L\mathbf{e}_3 - \int_{\Sigma_t} L_B \mathbf{e}_3\right) \\
&= \int_{\Sigma_t} \mathcal{H}_B \mathbf{e}_3 - \left(\int_{\Sigma_t} ({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)N\sqrt{h}\mathbf{e}_3 + 2\oint_{S_t}(k-k_0)N\sqrt{|\sigma|}\mathbf{e}_2 - \int_{\Sigma_t} L_B N\sqrt{h}\mathbf{e}_3\right) \\
&= \int_{\Sigma_t} \mathcal{H}_B \mathbf{e}_3 - 2\oint_{S_t}(k-k_0)N\sqrt{|\sigma|}\mathbf{e}_2 \\
&= \int_{\Sigma_t} 2[D_a((K^{ab} - h^{ab}K)N_b) - D_a(K^{ab} - h^{ab}K)N_b - \frac{N}{2}({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)]\sqrt{h}\mathbf{e}_3 \\
&\qquad\qquad - 2\oint_{S_t}(k-k_0)N\sqrt{|\sigma|}\mathbf{e}_2 \\
&= \int_{\Sigma_t} [-2D_a(K^{ab} - h^{ab}K)N_b - N({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)]\sqrt{h}\mathbf{e}_3 \\
&\qquad\qquad - 2\oint_{S_t}[(k-k_0)N - r_a(K^{ab} - h^{ab}K)N_b]\sqrt{|\sigma|}\mathbf{e}_2,
\end{aligned}
\tag{95}
$$

where in the final step Gauss' theorem has been applied with $\epsilon = 1$ (as S_t is timelike). Due to the boundary terms present in the action and Hamiltonian, no 'full' Hamiltonian density corresponding to the entire Hamiltonian can be constructed and equations 82 cannot be used. Therefore, another method should be used to derive the equations of motion. In this case, the variation of the action and thereby the equations of motion can be determined directly from the full Hamiltonian, using that

$$
S = \int_{t_1}^{t_2}\int_{\Sigma_t} L\sqrt{-g}\mathbf{e} = \int_{t_1}^{t_2}\int_{\Sigma_t} \pi^{ab}\dot{h}_{ab}\mathbf{e} - \int_{t_1}^{t_2} H_G dt. \tag{96}
$$

The variation in the action can be derived swiftly using equation 79, yielding

$$
\delta S = \int_{t_1}^{t_2}\int_{\Sigma_t} (\delta\pi^{ab}\dot{h}_{ab} + \pi^{ab}\delta\dot{h}_{ab})\mathbf{e} - \int_{t_1}^{t_2}\delta H_G dt = \int_{t_1}^{t_2}\int_{\Sigma_t} (\delta\pi^{ab}\dot{h}_{ab} - \dot{\pi}^{ab}\delta h_{ab})\mathbf{e} - \int_{t_1}^{t_2}\delta H_G dt, \tag{97}
$$

Finally, the variation of the Hamiltonian should still be found, for which the procedure is described in appendix V. The results are given by

$$
\begin{cases}
\delta H_G = \int_{\Sigma_t}(\mathcal{P}^{ab}\delta h_{ab} + \mathbb{H}_{ab}\delta\pi^{ab} - \mathcal{C}\tilde{\delta}N - 2\mathcal{C}_a\tilde{\delta}N^a)\mathbf{e}_3, \\
\mathcal{P}^{ab} = \pi^{cb}D_c(N^a) + \pi^{ca}D_c(N^b) + \sqrt{h}D_d(h^{ab}D^d(N) - D^a(N)h^{bd}) - \sqrt{h}D_d(N^d\frac{\pi^{ab}}{\sqrt{h}}) \\
\qquad + N(\sqrt{h}G^{ab} + \frac{1}{\sqrt{h}}(2\pi^{da}\pi^b_d - \pi\pi^{ab}) - \frac{1}{2\sqrt{h}}h^{ab}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) + \sqrt{h}\Lambda h^{ab}), \\
\mathbb{H}_{ab} = \frac{2N}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + 2D_{(b}N_{a)}, \\
\mathcal{C} = ({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)\sqrt{h}, \\
\mathcal{C}_a = D_b(K^b_a - h^b_a K)\sqrt{h},
\end{cases}
\tag{98}
$$

where $\tilde{\delta}N$ and $\tilde{\delta}N^a$ denote an arbitrary variation in the lapse and shift, respectively. Combining the previous two equations, it is found that the variation of the action is

$$
\delta S = \int_{t_1}^{t_2}\int_{\Sigma_t}[(\dot{h}_{ab} - \mathbb{H}_{ab})\delta\pi^{ab} - (\dot{\pi}^{ab} + \mathcal{P}^{ab})\delta h_{ab} + \mathcal{C}\tilde{\delta}N + 2\mathcal{C}_a\tilde{\delta}N^a]\mathbf{e} = 0. \tag{99}
$$

Using that the variation of the canonical momenta, field, shift and lapse can independently vary arbitrarily, such that the integrand corresponding to each variation should vanish, the equations of motion are found to be

$$\begin{cases} \dot{h_{ab}} = \mathbb{H}_{ab}, \\ \dot{\pi^{ab}} = -\mathcal{P}^{ab}, \\ \mathcal{C} = 0, \\ \mathcal{C}_a = 0, \end{cases} \tag{100}$$

where the final two equations are boundary conditions which pose restrictions on the choice of coordinate basis. These equations arise due to the freedom in choosing arbitrary lapse and shift for the system, as introducing additional freedom induces an equal amount of constraints. Therefore, to solve the above set of equations for a given metric, first a coordinate transformation should be applied to satisfy the boundary conditions, after which the evolution equations for the metric and canonical momenta can be determined.

Adding a matter term

Once matter is added to the system and the corresponding matter term is added to the Lagrangian, the Hamiltonian and therefore the equations of motion change. To allow the analysis of a system in an area with matter present, all previous derivations for the equations of motion should be redone. The starting point for this will be equations 93 and 97, as the stress-energy-matter tensor is inherent to a system and therefore independent of the foliation of space-time and extrinsic curvature of the spacelike surfaces K_{ab}. Therefore, the equations of motion can be derived by solely analysing the effect of the matter Lagrangian on the variation of the Hamiltonian H. The Hamiltonian in a system with matter is given by

$$H = H_G - \int_{\Sigma_t} L_M \sqrt{-g}\mathbf{e}_3 \equiv H_G - H_M, \tag{101}$$

where L_M is the matter Lagrangian as defined in section 3.3. The variation of the matter Lagrangian towards the 4-dimensional metric has been previously defined as

$$\delta L_M \sqrt{-g} = -T_{\alpha\beta}\sqrt{-g}\delta g^{\alpha\beta} = T^{\alpha\beta}\sqrt{-g}\delta g_{\alpha\beta}, \tag{102}$$

where $T_{\alpha\beta}$ is the 4-dimensional stress-energy-matter tensor and where equation 41 was used. Using equation 73, this variation of the matter Lagrangian towards the 4-dimensional metric can be decomposed into variations towards the canonical variables N, N^a and h_{ab}. The functional derivative of the matter Hamiltonian towards the canonical momenta, on the other hand, will vanish, as the stress-energy-matter tensor is independent of K^{ab}, leaving the equations of motion for the canonical momenta unaltered from equation 98.

First, consider the variation towards the lapse, which may be swiftly determined to be

$$\delta \int_{\Sigma_t} L_M \sqrt{-g}\mathbf{e}_3 = \int_{\Sigma_t} T^{00}\delta(g_{00})\sqrt{-g}\mathbf{e}_3 = \int_{\Sigma_t} T^{00}\delta(-N^2)\sqrt{-g}\mathbf{e}_3 = -\int_{\Sigma_t} 2N^2 T^{00}\delta N\sqrt{h}\mathbf{e}_3. \tag{103}$$

Similarly, the variation towards the 3-dimensional metric is found to be

$$\begin{aligned} \delta \int_{\Sigma_t} L_M \sqrt{-g}\mathbf{e}_3 &= \int_{\Sigma_t} (T^{ab}\delta g_{ab} + T^{00}\delta g_{00})\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} (T^{ab}\delta h_{ab} + T^{00}\delta(h_{ab}N^a N^b))\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} (T^{ab}\delta h_{ab} + T^{00}N_a N_b \delta h^{ab})\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} N(T^{ab} - N^a N^b T^{00})\sqrt{h}\delta h_{ab}\mathbf{e}_3, \end{aligned} \tag{104}$$

where in the final step equation 41 was used. Finally, the variation of the matter Lagrangian towards the shift is determined to be

$$\begin{aligned}\delta \int_{\Sigma_t} L_M \sqrt{-g}\mathbf{e}_3 &= \int_{\Sigma_t} (T^{0a}\delta g_{0a} + T^{a0}\delta g_{a0} + T^{00}\delta g_{00})\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} (T^{0a}\delta N_a + T^{a0}\delta N_a + T^{00}\delta h^{ab} N_b N_a)\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} (T^{0a}\delta N_a + T^{a0}\delta N_a + 2T^{00} N^a \delta N_a)\sqrt{-g}\mathbf{e}_3 \\ &= \int_{\Sigma_t} 2N(T^{0a} + T^{00}N^a)\delta N_a \sqrt{h}\mathbf{e}_3.\end{aligned} \tag{105}$$

Adding these terms to the vacuum field equations 100, the matter field equations are found, stating

$$\begin{cases} \dot{h}_{ab} = \mathbb{H}_{ab}, \\ \dot{\pi}^{ab} = -\mathcal{P}^{ab} - N(T^{ab} - N^a N^b T^{00})\sqrt{h}, \\ \mathcal{C} - 2N^2 T^{00}\sqrt{h} = 0, \\ \mathcal{C}_a + N(2T^{0a} + 2T^{00}N^a)\sqrt{h} = 0. \end{cases} \tag{106}$$

Example: Equations of motion for FLRW metric

The above determined equations of motion for space-times with matter will be verified by application on a Friedmann-Lemaître-Robertson-Walker (FLRW) metric defined with respect to the basis (t, r, θ, ϕ), with line element

$$ds^2 = -c^2 dt^2 + a(t)^2 \left(\frac{dr^2}{1 - kr^2} + r^2 d\Omega^2 \right), \tag{107}$$

where $d\Omega^2 = d\theta^2 + \sin(\theta)^2 d\phi^2$, $a(t)$ is the scale factor [44] which is an arbitrary function of time and k is a constant containing information on the curvature of space-time. This metric describes a space-time which is homogeneous and isotropic, equivalent to a space-time filled homogeneously with a perfect fluid, with stress-energy-matter tensor

$$T^{\mu\nu} = \begin{pmatrix} \rho & 0 & 0 & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & 0 & 0 & p \end{pmatrix}, \tag{108}$$

where p is the pressure and ρ the density of the fluid. Due to the size and complexity of the equations involved in determining the equations of motion, the tool Wolfram Mathematica has been utilised. The code used can be found in appendix VI. In the derivation of the equations of motion, it has been chosen to define Σ_t as hypersurfaces of constant time t and S_t as surfaces of constant time t and radius r, as these surfaces generate a lapse and shift which satisfy the boundary conditions. For this choice of surfaces, the canonical momenta are given by

$$\pi^{ab} = -\frac{2r^2 \sin(\theta)\alpha(t)^2\alpha'(t)}{c\sqrt{1 - kr^2}} h^{ab}. \tag{109}$$

Using these canonical momenta, the equations of motion are found to be

$$\begin{cases} \dot{h}_{ab} = 2a(t)a'(t)h_{ab}, \\ \dot{\pi}^{ab} = -\frac{2r^2 \sin(\theta)\alpha(t)^2 a''(t)}{c\sqrt{1-kr^2}} h^{ab}, \\ \mathcal{C} - 2N^2 \rho\sqrt{h} = 0, \\ \mathcal{C}_a = 0, \end{cases} \tag{110}$$

exactly as expected from the definition of the FLRW metric and equation 109, validating the previously determined equations of motion.

4.4 Analysing the Hamiltonian

As shown before, the Hamiltonian contains most information regarding the evolution of a system and its metric through its derivatives. On top of this, the value of the Hamiltonian itself can also contain global information about the system, such as mass and momentum. Before such relations can be considered, however, first the physical meaningfulness of these concepts should be established. In fact, for arbitrary space-times, the notion of a mass or energy does not make any sense [49]. Only in the special case of an asymptotically flat space-time, in which the metric on the hypersurfaces Σ_t reduces asymptotically to a Minkowski metric [58], may quantities such as mass and momentum be defined.

One such definition, based on the value of the previously derived Hamiltonian, is provided by Arnowitt, Deser and Misner [26]. Assuming the matter to be generated by a non-gauge field theory, as is usually the case within classical general relativity, the boundary conditions due to the variation in lapse and shift may be substituted into the bulk Hamiltonian, resulting in it vanishing [71]. Therefore, the value of the Hamiltonian follows purely from the boundary term

$$H_G = -2\oint_{S_t\to\infty}[(k-k_0)N - r_a(K^{ab}-h^{ab}K)N_b]\sqrt{|\sigma|}\mathbf{e}_2, \tag{111}$$

where the lapse and shift can still be arbitrarily chosen. By selecting specific values for these, the total mass, linear and angular momentum in a system can be found. For example, if the tangent t^α to the congruence of curves is set equal to the normal vector to the hypersurfaces Σ_t, i.e. $N = 1$ and $N_a = 0$, the value for the Hamiltonian will be equal to the ADM mass, the relation of which with the energy of a system can be found by rewriting the action in canonical form [46]. Therefore, as found by substituting $N = 1, N_a = 0$ into equation 111, the ADM mass is defined as

$$M_{ADM} \equiv -2\oint_{S_t\to\infty}(k-k_0)\sqrt{|\sigma|}\mathbf{e}. \tag{112}$$

Do note that the value of the ADM mass is completely independent of the shape of the hypersurfaces Σ_t and congruence of curves in the bulk of space-time, as expected, given that mass is a property inherent to the system and Σ_t are arbitrary. Surprisingly, though, the ADM mass is independent of the curvature of space-time in the bulk as well, being fully defined by boundary contributions. Therefore, this definition may be viewed in a similar fashion to Gauss' law for charge, which shows the charge in a volume may be found only knowing the electric field flux through the volume's boundary.

By instead choosing t^α to be asymptotically parallel to a spatial coordinate a, i.e. $N = 0$ and $N_b = \delta^a_b$, the ADM linear momentum in the a-direction is found [58]. Substituting these values for lapse and shift into equation 111, the ADM momentum is found to be

$$P_{ADM} \equiv 2\oint_{S_t\to\infty}(K^{ab}-h^{ab}K)r_bN_a\sqrt{|\sigma|}\mathbf{e}. \tag{113}$$

Similar to the ADM mass, the correlation between the ADM and physical linear momentum can be found by rewriting the action in a canonical shape. Alternatively, the physical meaningfulness of this definition may also be explained using Noether's theorem, which derives an equivalent relation from spatial translation invariance [72].

Finally, the angular momentum can be found analogous to the linear momentum, now defining t^α parallel to a rotational coordinate ϕ, yielding

$$J_{ADM} \equiv -2\oint_{S_t\to\infty}(K^{ab}-h^{ab}K)r_bN_a\sqrt{|\sigma|}\mathbf{e}, \tag{114}$$

where N_a corresponds to a rotational coordinate and the minus sign occurs to ensure consistency with the right-hand rule. Note that, in contrast to the linear momentum, this definition for angular momentum does not transform as a vector under the most general coordinate transformations preserving asymptotic flatness, due to the existence of 'supertranslations' [73]. Therefore, to allow well-definedness of the angular momentum, the coordinate transformations should be restricted beyond preservation of asymptotic flatness, i.e. gauge conditions should be applied. Only after the choice of gauge has been made may the ADM angular momentum be defined.

The validity of the previous two equations can be tested through examples. In appendix VII, the ADM mass for a Schwarzschild metric and ADM angular momentum (within the asymptotically maximal gauge [73]) for a Kerr metric are calculated. The results are

$$M_{ADM} = 16\pi \frac{M \cdot G}{c^2} = 16\pi \frac{M_{\text{Schwarzschild}} \cdot G}{c^2}, \tag{115}$$
$$J_{ADM} = 16\pi \frac{J \cdot G}{c^3} = 16\pi \frac{J_{\text{Kerr}} \cdot G}{c^3}, \tag{116}$$

both constant multiples of the expected value. Therefore, by rescaling the Lagrangian, the ADM mass and angular momentum will be equivalent to the actual mass and angular momentum, confirming the validity of the definitions.

4.5 Symmetries

The elegance of the Hamiltonian and Lagrangian formalism is best expressed through their respective symmetries. Through symmetry arguments, one may argue the Lagrangian formalism to be the most fundamental of the two, given the breaking of Lorentz covariance in the Hamiltonian formalism. Though this is the case, no evidence has been found that the theory of general relativity should inherently be expressed in a covariant formulation, suggesting that a violation of this principle might not carry any consequence. This opinion was already proclaimed by Dirac in the early stages of the development of the Hamiltonian formulation of relativity [25] and has gained traction since then, though multiple views on the matter still exist to the present day.

One such view, supporting the theory of loop quantum gravity, even proclaims that there is one symmetry found in the Hamiltonian which cannot be found in the Lagrangian framework, suggesting the Hamiltonian formalism as the most fundamental [68]. To derive this symmetry, consider applying a Lie bracket on two distinct generators $G(N_1, N_1^\alpha) \equiv t_1^\alpha$ and $G(N_2, N_2^\alpha) \equiv t_2^a$ for the congruence of curves, defined by $t^\alpha = Nn^\alpha + N^a e_a^\alpha$. This generates the new generator:

$$[G(N_1, N_1^a), G(N_2, N_2^a)] = G(\pounds_{M_1} N_2 - \pounds_{M_2} N_1, [M_1, M_2]^\alpha e_\alpha^a - \epsilon h^{ab}(N_1 \partial_b N_2 - N_2 \partial_b N_1)), \tag{117}$$

where $M_1, M_2 \in \mathfrak{X}(M)$ are vector fields generated by N_1^α and N_2^α, respectively [68]. Whereas the first terms are characteristic of a Lie algebra, the final term dependent on the metric is fundamentally different. Due to this additional term, the generators actually constitute a Lie algebroid [74], the link of which with relativity has been only barely researched, though this may hold the key to a canonical theory of (loop) quantum gravity [75]. More importantly for this discussion, though, is the symmetry induced by the presence of the metric-dependent term, which is similar to, but clearly distinct from diffeomorphism invariance, as proven by Hojman, Kuchar and Teitelbohm [76].

Now, consider the effect of quantum corrections on the resulting generator, which is required for a consistent theory of quantum gravity. Any such correction may be incorporated into equation 117 by multiplying the term containing the metric by a certain phase-space function $\beta = \beta(g_{ij}, \pi^{ij})$ [77]. Whereas the

Hamiltonian description of general relativity can account for the function β through the modified form of equation 117, the Lagrangian formalism has no known way of doing so [68], leaving it unable to describe the aforementioned symmetry and inferior to the Hamiltonian formalism. Of course, it may be that, similar to the breaking of Lorentz covariance by the Hamiltonian principle, this symmetry is purely theoretical and has no application in nature, in which case both formalisms should be treated on equal footing.

Apart from the previous two examples, many symmetries are shared by the two frameworks due to their similarity, such as the already discussed diffeomorphism invariance. Though these can give considerable insight into the nature of the formalism and the constraints which accompany them, the in-depth analysis of these lies outside the scope of this report. For the reader interested in delving further into this topic, [27] is recommended as a starting point.

5 Conclusion

In this report, we have discussed both the Lagrangian and Hamiltonian descriptions of Einstein's theory of general relativity using the variables originally introduced by Arnowitt, Deser and Misner, laying a robust foundation to further explore the world of quantum gravity research. First, we adapted the classical variational principle to be suitable for application on fields and identified several vital properties of the variation operator δ. Using this operator, the action corresponding to the Einstein field equations was determined to be the Hilbert action, corrected by a boundary term, a term corresponding to the cosmological constant and a numerical term, yielding the total action

$$S[L] = S_H + S_B + S_\Lambda + S_0 = \int_U (R - 2\Lambda)\sqrt{-g}\mathbf{e} + \int_{\partial U} 2\epsilon(K - K_0)\sqrt{|h|}\mathbf{e}_3. \tag{118}$$

To account for the matter in a system, a matter action $S_M[L_M]$ was introduced, which proved useful in defining the dynamical stress-energy-momentum tensor $T_{\alpha\beta} = -\frac{\partial L_M}{\partial g^{\alpha\beta}} + L_M \frac{1}{2} g_{\alpha\beta}$. It was proven that this definition of the matter tensor is inherently symmetric and locally conserved under covariant differentiation, proving several of Einstein's original assumptions. Another assumption, metric compatibility, was shown to directly follow from the Lagrangian formalism as well, through the variation of the Palatini action instead of the Hilbert action.

Next, before the canonical momentum and thus the Hamiltonian could be derived, the Lorentz covariance of the Lagrangian had to be broken by introducing a 3+1 decomposition, defined by the lapse N and shift N^a. Using the newly defined t-direction and a decomposed form of the action functional, the canonical momenta π^{ab} corresponding to the 3-dimensional metric h_{ab} were derived, which were in turn used to compute the (bulk) Hamiltonian density $\mathcal{H}_B = \pi^{ab}\dot{h_{ab}} - \sqrt{-g}L_B$. From this density, the full Hamiltonian was constructed, which, upon application of the variational principle, yielded the field equations and boundary conditions

$$\begin{cases} \dot{h_{ab}} = \frac{2N}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + 2D_{(b}N_{a)}, \\ \dot{\pi^{ab}} = -\pi^{cb}D_c(N^a) - \pi^{ca}D_c(N^b) - \sqrt{h}D_d(h^{ab}D^d(N) - D^a(N)h^{bd}) + \sqrt{h}D_d(N^d \dfrac{\pi^{ab}}{\sqrt{h}}) \\ \quad - N(\sqrt{h}G^{ab} + \dfrac{1}{\sqrt{h}}(2\pi^{da}\pi_d^b - \pi\pi^{ab}) - \dfrac{1}{2\sqrt{h}}h^{ab}(\pi^{ab}\pi_{ab} - \dfrac{1}{2}\pi^2) + \sqrt{h}\Lambda h^{ab} + (T^{ab} - N^a N^b T^{00})\sqrt{h}), \\ {}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda - 2N^2T^{00} = 0, \\ D_b(K_a^b - h_a^b K) + N(2T^{0a} + 2T^{00}N^a) = 0. \end{cases} \tag{119}$$

To ensure the correctness of these equations, they were verified for the FLRW metric with stress-energy-matter tensor $T = \text{diag}(\rho, p, p, p)$. On top of these field equations, the Hamiltonian was used to define a mass and (angular) momentum within a given space-time as well, the equations for which were validated using a Schwarzschild and Kerr metric, respectively.

Finally, several symmetries within both formalisms were compared, highlighting the elegance of these formulations of general relativity. As for the question which formalism is the most fundamental; only time will provide a definitive answer.

6 Outlook

With this report having provided a basis for exploring the universe of quantum gravity, we can now consider modern, more sophisticated theories. The next prominent step within the canonical approach was taken by Wheeler and DeWitt, who devised a 'Schrödinger equation' for relativistic wave functions [27], which, much like the Hamiltonian discussed in section 4.2, is independent of time. Though revolutionary, the equations met physicists with many infinities, which required great effort to resolve [78]. The real potential of these equations only showed 20 years later, when Ashtekar introduced new canonical variables, different from the metric and its canonical momentum, based on chiral symmetry groups [79, 80]. Using these new variables, several new solutions were found to the Wheeler-DeWitt equations, some of which were based on infinitesimal loops [81]. These solutions inspired Smolin and Rovelli to describe quantum gravity in a loop representation, which allows for exact, non-perturbative solutions [82]. This marks the birth of loop quantum gravity, still one of the most favoured approaches by physicists, although it has faced and still faces many major issues. An important example regards the speed of light, which loop quantum gravity predicts to vary infinitesimally based on wavelength [83], though experiments have yet to confirm this behaviour, leaving the future of this approach uncertain.

Alongside these advancements within the canonical approach to quantising general relativity, the Feynman and covariant approach developed strongly as well. The former saw its revival taken up by Hawking and his description of black hole radiation [84], which profoundly shaped physicists' understanding of black holes and therefore quantum gravity. Following several alternate derivations confirming his original theory [85], Hawking rewrote Feynman's original propagator to an integral over 4-dimensional metric tensors [86] to further study the motion of particles around the horizon of a black hole. Nevertheless, even after several improvements were made to this theory by Hartle and Hawking [87] in the following years, this 'Euclidean' propagator integral never showed potential surpassing or even matching that of the Wheeler-DeWitt equations [32], leaving this approach to decay over the following decades.

Therefore, the main current contender to loop quantum gravity is the covariant approach, which evolved around 1985 to the well-known (super)string theory [88]. String theory describes a universe filled with minuscule 1-dimensional strings, which form the different particles of the standard model through the excitation of different vibrational modes [89]. The pursuit of string theory over the last decades has been driven by its mathematical beauty and elegance. However, the concepts behind these mathematics are often complex and far from intuitive. For example, for these strings to be able to describe all known particles, they are required to oscillate not only in the three conventional spatial dimensions, but in at least six more dimensions, which should be described by complex Calabi-Yau manifolds [90]. Even more problematic, the only currently known comprehensive framework for string theory is 11-dimensional M-theory, which is not yet well-defined [91]. Although mathematical elegance has led to many great discoveries in the past, the concepts underlying string theory are intricate and difficult to apply practically, leaving the physical viability of this approach uncertain.

Alongside these main theories, many different remarkably interesting ideas have emerged throughout the years, such as spin foams [92, 93], which follow from both the Feynman and canonical approach. Regrettably, the one common factor amongst all these theories is the large number of major unresolved issues after decades of research by many renowned researchers. Therefore, some researchers have suggested a radically different answer to the question of a theory of quantum gravity: a resounding 'no'. This view is supported by a recent new theory led by Oppenheim [94], who even proposes a possible experiment to confirm his theory [95], concerning the measurement of minuscule mass fluctuations - too minuscule for currently available measurement devices.

Until this or another experiment provides a conclusive answer, the future of quantum gravity is uncertain. Unfortunately, this is exactly the main limitation of this research field: a lack of possibilities to experimentally test theories. Due to the low strength of the gravitational field in comparison to other forces [96], alongside the elaborate theoretical schemes proposed by most theories, designing validation experiments poses a considerable challenge to researchers. All tests which have been performed therefore target predictions of theories outside the scope of quantum gravity, such as the varying speed of light within loop quantum gravity.

Very recently, though, two research groups independently devised the same experiment to confirm whether gravity is inherently quantum mechanical [97, 98], nearly simultaneous with the previously mentioned experiment testing the opposite [95], taking a giant leap forwards towards a possible breakthrough. Today, with these new developments, on top of the advent of quantum computers and ever-increasing computing power, computational and experimental potential are reaching unprecedented levels, leaving it just a matter of time and a great amount of enthusiastic, talented physicists before the next breakthrough is made to find the ultimate theory of quantum gravity.

Appendix I: Field Euler-Lagrange equations

Within this appendix, equations analogous to the Euler-Lagrange equations within classical Lagrangian theory will be derived for scalar fields. Recall the definition of the action functional

$$S[L] = \int_M L(\psi, \nabla_\alpha \psi, ..., \nabla_\alpha^k \psi, g_{\alpha\beta}, \partial_\mu g_{\alpha\beta}, ...)\sqrt{-g}\mathbf{e}. \tag{I.1}$$

By minimising the value of the action, the field configuration ψ can be found which is the solution to the field equations, given that S is functionally differentiable. As proven in section 3.1, this is equivalent to requiring that the variation of S, δS, vanishes.

For the sake of simplicity, it will be assumed that the Lagrangian will depend on at most first-order derivatives of the field ψ [64]. For higher orders, similar though more extensive equations can be derived [34]. Additionally, for the same reason, we assume that ψ is a scalar field, implying that it will be independent of g. Under these assumptions, the variation in the action is found to be

$$\begin{aligned}
\delta S &= \int_U \delta\left[L(\psi, \nabla_\mu \psi, g^{\alpha\beta}, \partial_\mu g^{\alpha\beta})\sqrt{-g}\right]\mathbf{e} \\
&= \int_U \left[\frac{\partial L}{\partial \psi}\delta\psi + \frac{\partial L}{\partial(\nabla_\mu \psi)}\delta(\nabla_\mu \psi)\right]\sqrt{-g}\mathbf{e} \\
&= \int_U \left[\frac{\partial L}{\partial \psi}\delta\psi + \frac{\partial L}{\partial(\nabla_\mu \psi)}\nabla_\mu(\delta\psi)\right]\sqrt{-g}\mathbf{e} \\
&= \int_U \left[\frac{\partial L}{\partial \psi}\delta\psi + \nabla_\mu\left(\frac{\partial L}{\partial(\nabla_\mu \psi)}\delta\psi\right) - \nabla_\mu\left(\frac{\partial L}{\partial(\nabla_\mu \psi)}\right)\delta\psi\right]\sqrt{-g}\mathbf{e} \\
&= \int_U \left[\frac{\partial L}{\partial \psi} - \nabla_\mu\left(\frac{\partial L}{\partial(\nabla_\mu \psi)}\right)\right]\delta\psi\sqrt{-g}\mathbf{e} + \oint_{\partial U} \epsilon \frac{\partial L}{\partial(\nabla_\mu \psi)}\delta\psi \cdot n_\mu \sqrt{|h|}\mathbf{e}_3,
\end{aligned} \tag{I.2}$$

using Gauss' theorem, where the latter integral vanishes due to boundary conditions. Equating the final line of equation I.2 to 0 for arbitrary variations in ψ then yields the equations of motion

$$\frac{\partial L}{\partial \psi} - \nabla_\mu\left(\frac{\partial L}{\partial(\nabla_\mu \psi)}\right) = 0. \tag{I.3}$$

Appendix II: Variation of S_H

Recall the Hilbert action from equation 48, $S_H[\mathcal{L}] = \int_U R\sqrt{-g}\mathbf{e}$, where U is a compact manifold embedded in spacetime and R is the Ricci scalar. We will now compute the variation of S_H towards $g^{\alpha\beta}$, after which the equations of motion can be determined. Applying the variation operator δ on S_H yields

$$\begin{aligned}\delta S_H[\mathcal{L}] &= \int_U [\delta R\sqrt{-g} + R\delta\sqrt{-g}]\mathbf{e} \\ &= \int_U [\delta R_{\alpha\beta} g^{\alpha\beta}\sqrt{-g} + R_{\alpha\beta}\delta g^{\alpha\beta}\sqrt{-g} - R\frac{1}{2}\sqrt{-g}g_{\alpha\beta}\delta g^{\alpha\beta}]\mathbf{e} \\ &= \int_U \delta R_{\alpha\beta} g^{\alpha\beta}\sqrt{-g}\mathbf{e} + \int_U [R_{\alpha\beta} - R\frac{1}{2}g_{\alpha\beta}]\delta g^{\alpha\beta}\sqrt{-g}\mathbf{e}.\end{aligned} \tag{II.1}$$

Next, the variation of $R_{\alpha\beta} = \partial_\sigma \Gamma^\sigma_{\alpha\beta} - \partial_\beta \Gamma^\sigma_{\alpha\sigma} + \Gamma^\tau_{\alpha\beta}\Gamma^\sigma_{\tau\sigma} - \Gamma^\tau_{\alpha\sigma}\Gamma^\sigma_{\tau\beta}$ [34] should be determined. Working in a coordinate system in which all connection coefficients at P vanish locally, we find

$$\begin{aligned}\delta R_{\alpha\beta} &= \delta(\partial_\sigma \Gamma^\sigma_{\alpha\beta} - \partial_\beta \Gamma^\sigma_{\alpha\sigma} + \Gamma^\tau_{\alpha\beta}\Gamma^\sigma_{\tau\sigma} - \Gamma^\tau_{\alpha\sigma}\Gamma^\sigma_{\tau\beta}) \\ &= \delta\partial_\sigma \Gamma^\sigma_{\alpha\beta} - \delta\partial_\beta \Gamma^\sigma_{\alpha\sigma} \\ &= \partial_\sigma(\delta\Gamma^\sigma_{\alpha\beta}) - \partial_\beta(\delta\Gamma^\sigma_{\alpha\sigma}) \\ &= \nabla_\sigma(\delta\Gamma^\sigma_{\alpha\beta}) - \nabla_\beta(\delta\Gamma^\sigma_{\alpha\sigma}),\end{aligned} \tag{II.2}$$

where the final step holds due to the vanishing of the connection coefficients, reducing the covariant derivative to a partial derivative and vice versa. As the variation in the connection coefficients is a tensor [99], the final line in equation II.2 is a tensorial equation, which holds true in any coordinate system, even one in which the connection coefficients at P do not vanish. Therefore, the relation holds for all points in U, which may be used to reduce the first integral in equation II.1 as

$$\begin{aligned}\int_U \delta R_{\alpha\beta} g^{\alpha\beta}\sqrt{-g}\mathbf{e} &= \int_U [\nabla_\sigma(\delta\Gamma^\sigma_{\alpha\beta}) - \nabla_\beta(\delta\Gamma^\sigma_{\alpha\sigma})] g^{\alpha\beta}\sqrt{-g}\mathbf{e} \\ &= \int_U \nabla_\beta[\delta\Gamma^\beta_{\alpha\sigma} g^{\alpha\sigma} - \delta\Gamma^\sigma_{\alpha\sigma} g^{\alpha\beta}]\sqrt{-g}\mathbf{e} \\ &= \int_{\partial U} \epsilon n_\beta[\delta\Gamma^\beta_{\alpha\sigma} g^{\alpha\sigma} - \delta\Gamma^\sigma_{\alpha\sigma} g^{\alpha\beta}]\sqrt{|h|}\mathbf{e}_3,\end{aligned} \tag{II.3}$$

using Gauss' theorem. The final step within this derivation will be to evaluate the terms within brackets at the boundary of U, which yields

$$\begin{aligned}\delta\Gamma^\beta_{\alpha\sigma} g^{\alpha\sigma} - \delta\Gamma^\sigma_{\alpha\sigma} g^{\alpha\beta} &= \delta[\frac{1}{2}g^{\beta\rho}(\partial_\alpha g_{\rho\sigma} + \partial_\sigma g_{\alpha\rho} - \partial_\rho g_{\alpha\sigma})]g^{\alpha\sigma} - \delta[\frac{1}{2}g^{\sigma\rho}(\partial_\alpha g_{\rho\sigma} + \partial_\sigma g_{\alpha\rho} - \partial_\rho g_{\alpha\sigma})]g^{\alpha\beta} \\ &= \frac{1}{2}(g^{\beta\rho}\delta[\partial_\alpha g_{\rho\sigma} + \partial_\sigma g_{\alpha\rho} - \partial_\rho g_{\alpha\sigma}]g^{\alpha\sigma} - g^{\sigma\rho}\delta[\partial_\alpha g_{\rho\sigma} + \partial_\sigma g_{\alpha\rho} - \partial_\rho g_{\alpha\sigma}]g^{\alpha\beta}) \\ &= \frac{1}{2}(g^{\beta\alpha}\delta[\partial_\rho g_{\alpha\sigma} + \partial_\sigma g_{\rho\alpha} - \partial_\alpha g_{\rho\sigma}]g^{\rho\sigma} - g^{\sigma\rho}\delta[\partial_\alpha g_{\rho\sigma} + \partial_\sigma g_{\alpha\rho} - \partial_\rho g_{\alpha\sigma}]g^{\alpha\beta}) \\ &= g^{\beta\alpha}g^{\rho\sigma}(\delta[\partial_\rho g_{\alpha\sigma} - \partial_\alpha g_{\rho\sigma}]),\end{aligned} \tag{II.4}$$

where at several points the boundary conditions are used. Using the completeness relation for the metric [46], $g^{\alpha\beta} = \epsilon n^\alpha n^\beta + h^{\alpha\beta}$, the integrand of equation II.3 can be further reduced as

$$\begin{aligned}n_\beta g^{\beta\alpha}g^{\rho\sigma}(\delta[\partial_\rho g_{\alpha\sigma} - \partial_\alpha g_{\rho\sigma}]) &= n^\alpha(\epsilon n^\rho n^\sigma + h^{\rho\sigma})(\delta[\partial_\rho g_{\alpha\sigma} - \partial_\alpha g_{\rho\sigma}]) \\ &= n^\alpha h^{\rho\sigma}(\delta[\partial_\rho g_{\alpha\sigma} - \partial_\alpha g_{\rho\sigma}]),\end{aligned} \tag{II.5}$$

where in the final step we used the fact that the term in the left bracket is symmetric in α and ρ, while the second term is antisymmetric, thus once the summation convention is applied, their contraction vanishes.

Finally, due to the fact that $\delta g_{\alpha\beta} = 0$ on the boundary, all derivatives tangential to the boundary must vanish as well, thus $h^{\rho\sigma}\partial_\rho \delta g_{\alpha\sigma} = 0$. Concluding, the integral from equation II.3 can be reduced to

$$\int_U \delta R_{\alpha\beta} g^{\alpha\beta} \sqrt{-g}\mathbf{e} = -\int_{\partial U} \epsilon n^\alpha h^{\rho\sigma} \delta(\partial_\alpha g_{\rho\sigma}) \sqrt{|h|}\mathbf{e}_3, \tag{II.6}$$

yielding the total variation of the action

$$\delta S_H[\mathcal{L}] = \int_U (R_{\alpha\beta} - R\frac{1}{2} g_{\alpha\beta}) \delta g^{\alpha\beta} \sqrt{-g}\mathbf{e} - \int_{\partial U} \epsilon n^\alpha h^{\rho\sigma} \delta(\partial_\alpha g_{\rho\sigma}) \sqrt{|h|}\mathbf{e}_3. \tag{II.7}$$

Appendix III: Relations between boundary surfaces

To define the boundary of the compact space U, the surfaces Σ_t with their boundaries S_t as well as the timelike boundary B have been introduced. Between these different surfaces, several important relations can be derived regarding their coordinates, metric and extrinsic curvature, many of which will be required for derivations within the Hamiltonian formalism of general relativity. Therefore, all relations will be summarized concisely within this appendix, for further reference.

Within section 4.1, the surface Σ_t has already been embedded into general space-time. Therefore, to be able to properly embed S_t into space-time, it should first be embedded into Σ_t. The boundary S_t may be defined by the relation $\Phi_t(y^a)|_{S_t} = \text{constant}$, where $\Phi_t : \Sigma_t \to \mathbb{R}$ is an arbitrary function defined on Σ_t for any $t \in [t_1, t_2]$. The surface S_t has its own coordinates $\theta^A \in \mathbb{R}^2$ and a normal vector r^α, which can be used to define a metric and extrinsic curvature similar to the hypersurfaces Σ_t. Finally, adding a completeness relation leads to a set of relations between S_t and Σ_t given by

$$\begin{cases} \Phi_t(y^a)|_{S_t} = \text{constant}, \\ e^a_A = \frac{\partial y^a}{\partial \theta^A}, \\ \sigma_{AB} = h_{ab} e^a_A e^b_B, \\ k_{AB} = (D_b r_a) e^a_A e^b_B, \\ h^{ab} = r^a r^b + \sigma^{AB} e^a_A e^b_B, \end{cases} \tag{III.1}$$

where D_b is the intrinsic covariant derivative as defined in section 2.2. If the previous relations are combined with those embedding Σ_t into space-time, given by equation 74, S_t can be embedded into space-time through the relations

$$\begin{cases} \Psi(x^\alpha)|_{S_t} = \text{constant}, \\ e^\alpha_A = \frac{\partial x^\alpha}{\partial \theta^A} = \frac{\partial x^\alpha}{\partial y^A} \frac{\partial y^a}{\partial \theta^A} = e^\alpha_a e^a_A, \\ \sigma_{AB} = g_{\alpha\beta} e^\alpha_a e^\beta_b e^a_A e^b_B = g_{\alpha\beta} e^\alpha_A e^\beta_B, \\ k_{AB} = (\nabla_\beta r_\alpha) e^\alpha_A e^\beta_B, \\ g^{\alpha\beta} = -n^\alpha n^\beta + r^\alpha r^\beta + \sigma^{AB} e^\alpha_A e^\beta_B. \end{cases} \tag{III.2}$$

Here $\Psi : U \to \mathbb{R}$ is again an arbitrary function, where $\Psi(x^\alpha) = \text{constant}$ is equivalent to $\Phi_t(x^\alpha e^a_\alpha) = \text{constant}$ & $t(x^\alpha) = \text{constant}$.

Currently, there is no relationship between the coordinates θ^A on the different surfaces S_t, though for later convenience, it will be beneficial to introduce such a relationship. Analogous to the congruence of curves $\gamma_m(t)$, define a new congruence of timelike curves with parameter t, such that the curves intersect each surface S_t at the same coordinates θ^A. These curves may be defined to intersect each surface S_t orthogonally, as the introduction of a lapse and shift does not provide any advantages here. The tangent vector to these curves is therefore proportional to n^α, the unit normal vector to the surfaces Σ_t.

Finally, using the previously found relations for S_t, the spatial boundary B can be embedded in space-time. The surface B is again defined by an equation $\Xi(x^\alpha) = \text{constant}$, with $\Xi : U \to \mathbb{R}$ an arbitrary function defined on the whole of space-time. The previously defined congruence of curves of constant θ^A naturally gives rise to a set of coordinates on B: $z^i = (t, \theta^A)$. Additionally, it can be easily seen that the normal vectors to S_t and B are the same, which can be used together with the coordinates to define a metric and extrinsic curvature, yielding the set of relations

$$\begin{cases} \Xi(x^\alpha)|_B = \text{constant}, \\ e_i^\alpha = \frac{\partial x^\alpha}{\partial z^i}, \\ \gamma_{ij} = g_{\alpha\beta} e_i^\alpha e_j^\beta, \\ \mathcal{K}_{ij} = (\nabla_\beta r_\alpha) e_i^\alpha e_j^\beta, \\ g^{\alpha\beta} = r^\alpha r^\beta + \gamma^{ij} e_i^\alpha e_j^\beta. \end{cases} \tag{III.3}$$

To close, it may be proven that $\sqrt{|\gamma|} = N\sqrt{|\sigma|}$ in a way fully analogous to the derivation of the relation $\sqrt{-g} = N\sqrt{h}$, reinforcing the notion that the surfaces S_t form a foliation of B.

Appendix IV: 3+1 decomposition of the vacuum action

Recall the definition of the action for the vacuum field equations,

$$S = S_H + S_B + S_\Lambda + S_0 = \int_U (R - 2\Lambda)\sqrt{-g}\mathbf{e} + \int_{\partial U} 2\epsilon(K - K_0)\sqrt{|h|}\mathbf{e}_3. \tag{IV.1}$$

To be able to apply a time derivative, which is vital to the Hamiltonian formalism, all quantities should be decomposed into a time and space component. One such quantity is the action functional, which is written as a 4-dimensional integral over 4-dimensional quantities. Both the integrals and quantities need to be split to allow the full action functional to be decomposed.

Before initiating the decomposition, the S_0 term is considered. In section 3.3, this term was added to the action to ensure finite values for the action on a cylinder in flat space-time. The term has no other significant physical meaning and will therefore be ignored in the following discussion, to be reintroduced into the equations at the end.

First, the 4-dimensional Ricci scalar will be reduced to lower dimensional quantities. Using only quantities defined on Σ_t for an arbitrary value of $t \in \mathbb{R}$, the Ricci scalar can be decomposed as

$$R = {}^3R + K^{ab}K_{ab} - K^2 - 2\nabla_\alpha[(\nabla_\beta n^\alpha)n^\beta - (\nabla_\beta n^\beta)n^\alpha], \tag{IV.2}$$

where n^α is the normal vector to Σ_t [46]. With this information and using Gauss' theorem, the bulk integral within the action can be rewritten as

$$\int_U (R-2\Lambda)\sqrt{-g}\mathbf{e} = \int_U ({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)\sqrt{-g}\mathbf{e} - 2\oint_{\partial U} \epsilon[(\nabla_\beta n^\alpha)n^\beta - (\nabla_\beta n^\beta)n^\alpha]r_\alpha\sqrt{|h|}\mathbf{e}_3, \tag{IV.3}$$

where r_α is the normal vector to the surface ∂U. The first integral in the previous equation already contains solely spatial quantities, such that only the second term should be further reduced. To do so, the integral can be split over the three different surfaces ∂U consists of: $-\Sigma_{t_1}$, Σ_{t_2} and B. The surface Σ_{t_1} is denoted with a negative sign, as the normal vector is future-directed, whereas the normal vector to ∂U is past-directed. Incorporating this additional minus sign, the boundary integral over Σ_{t_1} reduces as

$$\begin{aligned}\oint_{\Sigma_{t_1}} -\epsilon[(\nabla_\beta n^\alpha)n^\beta - (\nabla_\beta n^\beta)n^\alpha]n_\alpha\sqrt{h}\mathbf{e}_3 &= \oint_{\Sigma_{t_1}} \epsilon^2(\nabla_\beta n^\beta)\sqrt{h}\mathbf{e}_3 \\ &= \oint_{\Sigma_{t_1}} g^{\alpha\beta}(\nabla_\beta n_\alpha)\sqrt{h}\mathbf{e}_3 \\ &= \oint_{\Sigma_{t_1}} (-n^\alpha n^\beta + h^{ab}e^\alpha_a e^\beta_b)(\nabla_\beta n_\alpha)\sqrt{h}\mathbf{e}_3 \\ &= \oint_{\Sigma_{t_1}} K\sqrt{h}\mathbf{e}_3,\end{aligned} \tag{IV.4}$$

using that the covariant derivative of the normal vector and the normal vector itself are orthogonal, i.e. $2\nabla_\beta(n^\alpha)n_\alpha = \nabla_\beta(n^\alpha)n_\alpha + \nabla_\beta(n_\alpha)n^\alpha = \nabla_\beta(n^\alpha n_\alpha) = 0$. Similarly for the surface Σ_{t_2},

$$\oint_{\Sigma_{t_2}} \epsilon[(\nabla_\beta n^\alpha)n^\beta - (\nabla_\beta n^\beta)n^\alpha]n_\alpha\sqrt{h}\mathbf{e}_3 = -\oint_{\Sigma_{t_2}} K\sqrt{h}\mathbf{e}_3, \tag{IV.5}$$

where the minus sign occurs due to the opposite orientation of the normal vector on Σ_{t_2} with respect to the normal vector of Σ_{t_1}. These terms exactly cancel with the original boundary terms of the action, as

$\epsilon = -1$ for both spacelike surfaces. This only leaves the contribution of the timelike boundary B, which is found to be

$$
\begin{aligned}
\oint_B \epsilon[(\nabla_\beta n^\alpha)n^\beta - (\nabla_\beta n^\beta)n^\alpha]r_\alpha\sqrt{|\gamma|}\mathbf{e}_3 &= \oint_B \epsilon(\nabla_\beta n^\alpha)n^\beta r_\alpha\sqrt{|\gamma|}\mathbf{e}_3 \\
&= \oint_B \epsilon[\nabla_\beta(n^\alpha n^\beta r_\alpha\sqrt{|\gamma|}) - n^\alpha\nabla_\beta(n^\beta r_\alpha\sqrt{|\gamma|})]\mathbf{e}_3 \\
&= -\oint_B \epsilon[n^\alpha\nabla_\beta(n^\beta)r_\alpha\sqrt{|\gamma|} + n^\alpha n^\beta\nabla_\beta(r_\alpha)\sqrt{|\gamma|}]\mathbf{e}_3 \\
&= -\oint_B \epsilon n^\alpha n^\beta(\nabla_\beta r_\alpha)\sqrt{|\gamma|}\mathbf{e}_3,
\end{aligned}
\tag{IV.6}
$$

where in multiple steps it was used that n_α and r_α are orthogonal, i.e. $n^\alpha r_\alpha = 0$. Combining all previous derivations, it is found that

$$
S = \int_U ({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)\sqrt{-g}\mathbf{e} + 2\oint_B (\mathcal{K} + \epsilon n^\alpha n^\beta\nabla_\beta r_\alpha)\sqrt{|\gamma|}\mathbf{e}_3, \tag{IV.7}
$$

where $\epsilon = 1$ on the timelike hypersurface B. As the bulk integrand already consists solely of 3-dimensional quantities, the final step towards the decomposition of the action is to further reduce the boundary integral. To this end, expand the extrinsic curvature $\mathcal{K}$ as

$$
\begin{aligned}
\mathcal{K} &= \gamma^{ij}\mathcal{K}_{ij} \\
&= \gamma^{ij}(\nabla_\beta r_\alpha)e_i^\alpha e_j^\beta \\
&= (\nabla_\beta r_\alpha)(g^{\alpha\beta} - r^\alpha r^\beta),
\end{aligned}
\tag{IV.8}
$$

which may be combined with the other part of the integrand to find

$$
\begin{aligned}
\mathcal{K} + n^\alpha n^\beta(\nabla_\beta r_\alpha) &= (\nabla_\beta r_\alpha)(g^{\alpha\beta} - r^\alpha r^\beta) + n^\alpha n^\beta(\nabla_\beta r_\alpha) \\
&= (\nabla_\beta r_\alpha)(g^{\alpha\beta} - r^\alpha r^\beta + n^\alpha n^\beta) \\
&= (\nabla_\beta r_\alpha)\sigma^{AB}e_A^\alpha e_B^\beta \\
&= k_{AB}\sigma^{AB} \\
&= k.
\end{aligned}
\tag{IV.9}
$$

By substituting this back into equation IV.7, the action is found to be

$$
S = \int_U ({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)\sqrt{-g}\mathbf{e} + 2\oint_B k\sqrt{|\gamma|}\mathbf{e}_3, \tag{IV.10}
$$

which may be fully decomposed as

$$
S = \int_{t_i}^{t_f}\left(\int_{\Sigma_t}({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)N\sqrt{h}\mathbf{e}_3 + 2\oint_{\mathcal{S}_t} kN\sqrt{|\sigma|}\mathbf{e}_2\right)dt. \tag{IV.11}
$$

Finally, consider the contribution of S_0, a boundary term which should cancel the current boundary term in the case of a flat space-time, to the decomposed action. By defining k_0 as the curvature of the surface S_t in flat space-time and adding $S_0 = -2\oint_B k_0\sqrt{|\gamma|}\mathbf{e}_3$ to S, the required behaviour can be achieved, ultimately yielding the full decomposed action

$$
S = \int_{t_i}^{t_f}\left(\int_{\Sigma_t}({}^3R + K^{ab}K_{ab} - K^2 - 2\Lambda)N\sqrt{h}\mathbf{e}_3 + 2\oint_{\mathcal{S}_t}(k - k_0)N\sqrt{|\sigma|}\mathbf{e}_2\right)dt. \tag{IV.12}
$$

Appendix V: Variation of the vacuum Hamiltonian

Recall the definition of the Hamiltonian,

$$H_G = \int_{\Sigma_t} [-2D_a(K^{ab}-h^{ab}K)N_b - N(^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)]\sqrt{h}\mathbf{e}_3 - 2\oint_{S_t}[(k-k_0)N - r_a(K^{ab}-h^{ab}K)N_b]\sqrt{|\sigma|}\mathbf{e}_2. \tag{V.1}$$

The Hamiltonian depends on 4 different variables which can vary independently: N, N_a, π^{ab} and h_{ab}. Firstly, the variation of the Hamiltonian is analysed when the lapse and shift are varied, after which the variation operator as defined in equation 75 is applied to find the functional derivative of the Hamiltonian towards the metric and canonical momenta. These variations are restricted by the boundary conditions $\eth N|_{S_t} = \eth N_a|_{S_t} = \delta h_{ab}|_{S_t} = 0$, as mentioned in section 4.1, where $\eth N$ and $\eth N_a$ describe the variation in the lapse and shift, respectively.

Variation towards lapse and shift

The variation of the Hamiltonian towards the lapse and shift can swiftly be found to be

$$\int_{\Sigma_t} [-2D_a(K^a_b - h^a_b K)\eth N^b - \eth N(^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)]\sqrt{h}\mathbf{e}_3 - 2\oint_{S_t}[(k-k_0)\eth N - r_a(K^{ab}-h^{ab}K)\eth N_b]\sqrt{|\sigma|}\mathbf{e}_2. \tag{V.2}$$

Due to the boundary conditions, the boundary integrand vanishes, leaving only the bulk integral as

$$\int_{\Sigma_t} [-2D_a(K^a_b - h^a_b K)\eth N^b - \eth N(^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)]\sqrt{h}\mathbf{e}_3 \equiv \int_{\Sigma_t}[-2C_b\eth N^b - C\eth N]\mathbf{e}_3, \tag{V.3}$$

where $C_b = \sqrt{h}D_a(K^a_b - h^a_b K)$ and $C = (^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)\sqrt{h}$.

Variation towards canonical momenta

Next, the variation operator is applied to the Hamiltonian, where we first focus on the variation towards the canonical momenta π^{ab}. Firstly, the Hamiltonian will be rewritten to a function of the metric and canonical momenta instead of the extrinsic curvature. Recall that by equation 93, $K^{ab} - h^{ab}K = \frac{\pi^{ab}}{\sqrt{h}}$, which implies that

$$K^{ab}K_{ab} - K^2 = K_{ab}(K^{ab} - h^{ab}K) = K_{ab}\frac{\pi^{ab}}{\sqrt{h}}. \tag{V.4}$$

Using the relation $\pi = \pi^{ab}h_{ab} = \sqrt{h}(K^{ab} - h^{ab}K)h_{ab} = -2\sqrt{h}K$, it is found that

$$K_{ab} = h_{ab}K + \frac{\pi_{ab}}{\sqrt{h}} = \frac{1}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}). \tag{V.5}$$

Using these relations between the extrinsic curvature and the metric and canonical momenta, as well as the final lines in equation 95, the Hamiltonian can be rewritten as

$$\begin{aligned} &\int_{\Sigma_t}\left[-2D_a(\frac{\pi^{ab}}{\sqrt{h}})N_b - N(^3R - \frac{1}{h}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - 2\Lambda)\right]\sqrt{h}\mathbf{e}_3 - 2\oint_{S_t}\left[(k-k_0)N - r_a\frac{\pi^{ab}}{\sqrt{h}}N_b\right]\sqrt{|\sigma|}\mathbf{e}_2 \\ &\qquad = \int_{\Sigma_t}\left[2\frac{\pi^{ab}}{\sqrt{h}}D_a(N_b) - N(^3R - \frac{1}{h}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - 2\Lambda)\right]\sqrt{h}\mathbf{e}_3 - 2\oint_{S_t}\left[(k-k_0)N\right]\sqrt{|\sigma|}\mathbf{e}_2. \end{aligned} \tag{V.6}$$

By noting that the 3-dimensional Ricci scalar and curvature of the surfaces S_t are independent of the canonical momenta, the variation of the Hamiltonian towards the canonical momenta can be found to be

$$\begin{aligned}
\delta H_G &= \delta \int_{\Sigma_t} \left[2\frac{\pi^{ab}}{\sqrt{h}} D_a(N_b) - N({}^3R - \frac{1}{h}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - 2\Lambda) \right] \sqrt{h}\mathbf{e}_3 - 2\delta \oint_{S_t} \left[(k-k_0)N \right] \sqrt{|\sigma|}\mathbf{e}_2 \\
&= \delta \int_{\Sigma_t} \left[2\frac{\pi^{ab}}{\sqrt{h}} D_a(N_b) + N(\frac{1}{h}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2)) \right] \sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} \left[2\frac{\delta\pi^{ab}}{\sqrt{h}} D_a(N_b) + \frac{N}{h}\delta(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) \right] \sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} \left[2\frac{\delta\pi^{ab}}{\sqrt{h}} D_a(N_b) + \frac{N}{h}(\pi_{ab}\delta\pi^{ab} + \pi^{ab}\delta\pi_{ab} - \pi\delta\pi) \right] \sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} \left[2\frac{\delta\pi^{ab}}{\sqrt{h}} D_a(N_b) + \frac{N}{h}(\pi_{ab}\delta\pi^{ab} + \delta(h_{ac}h_{bd}\pi^{cd})\pi^{ab} - \pi\delta(h_{ab}\pi^{ab})) \right] \sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} \left[2\frac{\delta\pi^{ab}}{\sqrt{h}} D_a(N_b) + \frac{N}{h}(\pi_{ab}\delta\pi^{ab} + h_{ac}h_{bd}\delta(\pi^{cd})\pi^{ab} - \pi h_{ab}\delta\pi^{ab}) \right] \sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} \left[2\frac{\delta\pi^{ab}}{\sqrt{h}} D_a(N_b) + \frac{N}{h}(\pi_{ab}\delta\pi^{ab} + \pi_{ab}\delta\pi^{ab} - \pi h_{ab}\delta\pi^{ab}) \right] \sqrt{h}\mathbf{e}_3 \\
&= 2\int_{\Sigma_t} \left[\frac{N}{h}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + \frac{1}{\sqrt{h}} D_a(N_b) \right] \delta\pi^{ab}\sqrt{h}\mathbf{e}_3 \\
&\equiv \int_{\Sigma_t} \mathcal{H}_{ab}\delta\pi^{ab}\mathbf{e}_3,
\end{aligned} \tag{V.7}$$

where $\mathcal{H}_{ab} = \frac{2N}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + 2D_a(N_b)$.

Variation towards 3-dimensional metric

Finally, the variation of the Hamiltonian towards the metric h_{ab} will be determined, by analysing the variation of each individual term in the last line of equation V.6. For the first term, it is found that

$$\delta \int_{\Sigma_t} 2\frac{\pi^{ab}}{\sqrt{h}} D_a(N_b)\sqrt{h}\mathbf{e}_3 = \delta \int_{\Sigma_t} 2\pi^{ab} D_a(N_b)\mathbf{e}_3 = 2\int_{\Sigma_t} \pi^{ab}\delta(D_a(N_b))\mathbf{e}_3, \tag{V.8}$$

where the variation in the intrinsic covariant derivative of the shift can be further reduced as

$$\begin{aligned}
\delta(D_a(N_b)) &= \delta(D_a(N^c h_{bc})) \\
&= \delta(D_a(N^c)h_{bc}) \\
&= D_a(N^c)\delta h_{bc} + \delta(D_a(N^c))h_{bc} \\
&= D_a(N^c)\delta h_{bc} + \delta(\partial_a(N^c) + \Gamma^c_{ad}N^d)h_{bc} \\
&= D_a(N^c)\delta h_{bc} + (\partial_a(\delta N^c) + \delta(\Gamma^c_{ad})N^d + \Gamma^c_{ad}\delta N^d)h_{bc} \\
&= D_a(N^c)\delta h_{bc} + \delta(\Gamma^c_{ad})N^d h_{bc}.
\end{aligned} \tag{V.9}$$

Secondly, the term containing the 3-dimensional Ricci scalar is considered. The variation of the 4-dimensional variant has already been determined in equations II.1 and II.2 which can easily be reduced to three dimensions as

$$\begin{aligned}
\delta({}^3R\sqrt{h}) &= -\sqrt{h}(R^{ab} - R\frac{1}{2}h^{ab})\delta h_{ab} + \sqrt{h}(D_c(h^{ab}\delta\Gamma^c_{ab}) - D_b(h^{ab}\delta\Gamma^c_{ac})) \\
&= -\sqrt{h}G^{ab}\delta h_{ab} + \sqrt{h}h^{ab}(D_c(\delta\Gamma^c_{ab}) - D_b(\delta\Gamma^c_{ac})),
\end{aligned} \tag{V.10}$$

where $G^{ab} \equiv R^{ab} - R\frac{1}{2}h^{ab}$ is the 3-dimensional Einstein tensor and where the minus sign occurs due to the opposite signs of h and g. Then the third and fourth terms are reduced, the final terms of the bulk integral over the hypersurface Σ_t. It was assumed that π^{ab} and h_{ab} vary independently, such that the variation in the first part of the third term becomes

$$\begin{aligned}
\delta(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) &= \delta(\pi^{ab}\pi_{ab}) - \pi\delta\pi \\
&= \pi^{ab}\delta\pi_{ab} - \pi\delta(h_{ab}\pi^{ab}) \\
&= \pi^{ab}\delta(\pi^{cd}h_{ac}h_{bd}) - \pi\pi^{ab}\delta h_{ab} \\
&= \pi^{ab}\pi^{cd}(h_{bd}\delta h_{ac} + h_{ac}\delta h_{bd}) - \pi\pi^{ab}\delta h_{ab} \\
&= (\pi^{ba}\pi^{d}_{a} + \pi^{ab}\pi^{d}_{a})\delta h_{bd} - \pi\pi^{ab}\delta h_{ab} \\
&= (2\pi^{da}\pi^{b}_{d} - \pi\pi^{ab})\delta h_{ab}.
\end{aligned} \tag{V.11}$$

The second part of this term, as well as the fourth term, consist of a power of the determinant of the 3-dimensional metric tensor h, of which the variation can be found using Jacobi's formula, similar to equation 42, yielding

$$\delta\sqrt{h} = \frac{1}{2}\sqrt{h}h^{ab}\delta h_{ab}. \tag{V.12}$$

Using this relation, the variation of the term $\sqrt{h}^{-1}$ can easily be found, as

$$\delta\sqrt{h}^{-1} = -\frac{1}{2}h^{-3/2}\delta h = -h^{-1}(\frac{1}{2}\sqrt{h}^{-1/2}\delta h) = -h^{-1}\delta\sqrt{h}. \tag{V.13}$$

Finally, the variation in the boundary term is found by determining the variation of the 2-dimensional extrinsic curvature k. The variation in this curvature can be derived equivalently to the derivation displayed in equation 50, reducing by a dimension to find

$$\delta k = \frac{1}{2}h^{ab}\delta(\partial_c h_{ab})r^c. \tag{V.14}$$

All previous steps can be combined to find the variation in the Hamiltonian towards the metric to be

$$\begin{aligned}
\delta H_G = \delta \int_{\Sigma_t} &\left[2\frac{\pi^{ab}}{\sqrt{h}}D_a(N_b) - N({}^3R - \frac{1}{h}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - 2\Lambda)\right]\sqrt{h}\mathbf{e}_3 - 2\delta\oint_{S_t}\left[(k-k_0)N\right]\sqrt{|\sigma|}\mathbf{e}_2 \\
= \int_{\Sigma_t} &\Bigg[2\frac{\pi^{ab}}{\sqrt{h}}(D_a(N^c)\delta h_{bc} + N^d h_{bc}\delta\Gamma^c_{ad}) - N((-G^{ab}\delta h_{ab} + D_c(h^{ab}\delta\Gamma^c_{ab}) - D_b(h^{ab}\delta\Gamma^c_{ac})) \\
&\quad - \frac{1}{h}(2\pi^{da}\pi^b_d - \pi\pi^{ab})\delta h_{ab} + \frac{1}{h}(\frac{1}{2}h^{ab}\delta h_{ab})(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - \Lambda h^{ab}\delta h_{ab})\Bigg]\sqrt{h}\mathbf{e}_3 \\
&\quad - \oint_{S_t}\left[h^{ab}\delta(\partial_c h_{ab})r^c N\right]\sqrt{|\sigma|}\mathbf{e}_2 \\
= \int_{\Sigma_t} &\Bigg[(2\frac{\pi^{cb}}{\sqrt{h}}D_c(N^a) - N(-G^{ab} - \frac{1}{h}(2\pi^{da}\pi^b_d - \pi\pi^{ab}) + \frac{1}{2h}h^{ab}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) - \Lambda h^{ab}))\delta h_{ab} \\
&\quad - ND_b(h^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac}) + 2\delta\Gamma^c_{ad}N^d h_{bc}\frac{\pi^{ab}}{\sqrt{h}}\Bigg]\sqrt{h}\mathbf{e}_3 - \oint_{S_t}\left[h^{ab}\delta(\partial_c h_{ab})r^c N\right]\sqrt{|\sigma|}\mathbf{e}_2 \\
\equiv \int_{\Sigma_t} &\left[\mathcal{G}^{ab}\delta h_{ab} - ND_b(h^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac}) + 2\delta\Gamma^c_{ad}N^d h_{bc}\frac{\pi^{ab}}{\sqrt{h}}\right]\sqrt{h}\mathbf{e}_3 - \oint_{S_t}\left[h^{ab}\delta(\partial_c h_{ab})r^c N\right]\sqrt{|\sigma|}\mathbf{e}_2.
\end{aligned} \tag{V.15}$$

All terms in the above equation which contain variations of terms which are not the metric h_{ab} should be further reduced. First, consider the variation in the Christoffel symbols, which is present in several terms within the bulk integral. To this end, consider the intrinsic covariant derivative of the variation in the metric, which can be expanded as

$$\begin{aligned}
D_a(\delta h_{bc}) &= \nabla_\alpha(\delta h_{\beta\gamma})e^\alpha_a e^\beta_b e^\gamma_c \\
&= (\partial_\alpha(\delta h_{\beta\gamma}) - \Gamma^d_{\alpha\beta}\delta h_{d\gamma} - \Gamma^d_{\alpha\gamma}\delta h_{\beta d})e^\alpha_a e^\beta_b e^\gamma_c \\
&= (\delta\partial_\alpha(h_{\beta\gamma}) - \Gamma^d_{\alpha\beta}\delta h_{d\gamma} - \Gamma^d_{\alpha\gamma}\delta h_{\beta d})e^\alpha_a e^\beta_b e^\gamma_c \\
&= (\delta(\partial_\alpha h_{\beta\gamma} - \Gamma^d_{\alpha\beta}h_{d\gamma} - \Gamma^d_{\alpha\gamma}h_{\beta d}) + \delta\Gamma^d_{\alpha\beta}h_{d\gamma} + \delta\Gamma^d_{\alpha\gamma}h_{\beta d})e^\alpha_a e^\beta_b e^\gamma_c \\
&= (\delta(\nabla_\alpha h_{\beta\gamma}) + \delta\Gamma^d_{\alpha\beta}h_{d\gamma} + \delta\Gamma^d_{\alpha\gamma}h_{\beta d})e^\alpha_a e^\beta_b e^\gamma_c \\
&= (\delta\Gamma^d_{\alpha\beta}h_{d\gamma} + \delta\Gamma^d_{\alpha\gamma}h_{\beta d})e^\alpha_a e^\beta_b e^\gamma_c \\
&= \delta\Gamma^d_{ab}h_{dc} + \delta\Gamma^d_{ac}h_{bd}.
\end{aligned} \tag{V.16}$$

By cyclically permuting the found relation over the indices a, b and c, similarly to the derivation of the Levi-Civita connection, it is found that

$$\begin{aligned}
D_a(\delta h_{bc}) + D_b(\delta h_{ca}) - D_c(\delta h_{ab}) &= (\delta\Gamma^d_{ab}h_{dc} + \delta\Gamma^d_{ac}h_{bd}) + (\delta\Gamma^d_{bc}h_{da} + \delta\Gamma^d_{ba}h_{cd}) - (\delta\Gamma^d_{ca}h_{db} + \delta\Gamma^d_{cb}h_{ad}) \\
&= (\delta\Gamma^d_{ab}h_{dc} + \delta\Gamma^d_{ac}h_{bd}) + (\delta\Gamma^d_{bc}h_{da} + \delta\Gamma^d_{ba}h_{cd}) - (\delta\Gamma^d_{ac}h_{bd} + \delta\Gamma^d_{bc}h_{da}) \\
&= \delta\Gamma^d_{ab}h_{dc} + \delta\Gamma^d_{ba}h_{cd} \\
&= 2\delta\Gamma^d_{ab}h_{cd},
\end{aligned} \tag{V.17}$$

By contracting the previous equation with h^{ce} and relabeling indices, the variation in a Christoffel symbol is found to be

$$\delta\Gamma^d_{ab} = \frac{1}{2}h^{cd}(D_a(\delta h_{bc}) + D_b(\delta h_{ca}) - D_c(\delta h_{ab})). \tag{V.18}$$

This relation can directly be used to reduce the last bulk integrand as

$$\begin{aligned}
\int_{\Sigma_t}\left[2\delta\Gamma^c_{ad}N^d h_{bc}\frac{\pi^{ab}}{\sqrt{h}}\right]\sqrt{h}\mathbf{e}_3 &= \int_{\Sigma_t} 2\left[\frac{1}{2}h^{cf}(D_a(\delta h_{fd}) + D_d(\delta h_{af}) - D_f(\delta h_{ad}))N^d h_{bc}\frac{\pi^{ab}}{\sqrt{h}}\right]\sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t}\left[(D_a(\delta h_{fd}) + D_d(\delta h_{af}) - D_f(\delta h_{ad}))N^d\frac{\pi^{af}}{\sqrt{h}}\right]\sqrt{h}\mathbf{e}_3 \\
&\overset{*}{=} \int_{\Sigma_t} D_d\left(\delta h_{ab}\right)N^d\frac{\pi^{ab}}{\sqrt{h}}\sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} D_d\left(\delta h_{ab}N^d\frac{\pi^{ab}}{\sqrt{h}}\right)\sqrt{h}\mathbf{e}_3 - \int_{\Sigma_t}\delta h_{ab}D_d\left(N^d\frac{\pi^{ab}}{\sqrt{h}}\right)\sqrt{h}\mathbf{e}_3 \\
&= \oint_{S_t}\epsilon r_d\delta h_{ab}N^d\frac{\pi^{ab}}{\sqrt{h}}\sqrt{|\sigma|}\mathbf{e}_2 - \int_{\Sigma_t}\delta h_{ab}D_d\left(N^d\frac{\pi^{ab}}{\sqrt{h}}\right)\sqrt{h}\mathbf{e}_3 \\
&= -\int_{\Sigma_t}\delta h_{ab}D_d\left(N^d\frac{\pi^{ab}}{\sqrt{h}}\right)\sqrt{h}\mathbf{e}_3,
\end{aligned} \tag{V.19}$$

where the boundary term vanishes due to the boundary conditions and equation $(*)$ holds due to the symmetry of π^{af}, such that the antisymmetric part in a and f between brackets drops out. Next, the term containing the intrinsic covariant derivatives of the variation of Christoffel symbols will be reduced.

By applying Gauss' theorem, it is found that

$$\begin{aligned}
&-\int_{\Sigma_t} ND_b(h^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac})\sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} D_b(N)\cdot(h^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac})\sqrt{h}\mathbf{e}_3 - \int_{\Sigma_t} D_b(Nh^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac})\sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} D_b(N)\cdot\frac{1}{2}(h^{ac}h^{bd} - h^{ab}h^{cd})(D_a(\delta h_{dc}) + D_c(\delta h_{ad}) - D_d(\delta h_{ac}))\sqrt{h}\mathbf{e}_3 - \oint_{S_t} \epsilon r_b(Nh^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac})\sqrt{|\sigma|}\mathbf{e}_2 \\
&\overset{*}{=} \int_{\Sigma_t} -D_b(N)\cdot(h^{ac}h^{bd} - h^{ab}h^{cd})D_d(\delta h_{ac})\sqrt{h}\mathbf{e}_3 - \oint_{S_t} \epsilon r_b(Nh^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac})\sqrt{|\sigma|}\mathbf{e}_2 \\
&\overset{**}{=} \int_{\Sigma_t} -D_b(N)\cdot(h^{ac}h^{bd} - h^{ab}h^{cd})D_d(\delta h_{ac})\sqrt{h}\mathbf{e}_3 + \oint_{S_t} \epsilon r^a N(h^{dc}\delta\partial_a h_{dc})\sqrt{|\sigma|}\mathbf{e}_2 \\
&= \int_{\Sigma_t} -(h^{ac}D^d(N) - D^a(N)h^{cd})D_d(\delta h_{ac})\sqrt{h}\mathbf{e}_3 + \oint_{S_t} r^c N(h^{ab}\delta\partial_c h_{ab})\sqrt{|\sigma|}\mathbf{e}_2.
\end{aligned} \tag{V.20}$$

Here, equation $(*)$ holds due to the antisymmetry in a and d of the left term, such that the symmetric term $D_c(\delta h_{ad})$ drops out and $D_a(\delta h_{dc})$ can be replaced by $-D_d(\delta h_{ac})$. Additionally, equation $(**)$ holds due to a three-dimensional equivalent of equations II.4 and II.5. Finally, as r^c is spacelike, $\epsilon = 1$ in the last step. Note that the boundary integral above is equivalent to the boundary term of equation V.15, though with opposite sign. Therefore, these terms will cancel. The bulk integral is further reduced through integration by parts, as

$$\begin{aligned}
&-\int_{\Sigma_t} (h^{ac}D^d(N) - D^a(N)h^{cd})D_d(\delta h_{ac})\sqrt{h}\mathbf{e}_3 \\
&= -\int_{\Sigma_t} D_d(h^{ac}D^d(N) - D^a(N)h^{cd}\delta h_{ac})\sqrt{h}\mathbf{e}_3 + \int_{\Sigma_t} D_d(h^{ac}D^d(N) - D^a(N)h^{cd})\delta h_{ac}\sqrt{h}\mathbf{e}_3 \\
&= -\oint_{S_t} \epsilon r_d(h^{ac}D^d(N) - D^a(N)h^{cd})\delta h_{ac}\sqrt{|\sigma|}\mathbf{e}_2 + \int_{\Sigma_t} D_d(h^{ac}D^d(N) - D^a(N)h^{cd})\delta h_{ac}\sqrt{h}\mathbf{e}_3 \\
&= \int_{\Sigma_t} D_d(h^{ac}D^d(N) - D^a(N)h^{cd})\delta h_{ac}\sqrt{h}\mathbf{e}_3,
\end{aligned} \tag{V.21}$$

where the boundary term vanishes due to the boundary conditions. Combining all previous derivations with equation V.15, the variation in the Hamiltonian with respect to the metric can be concluded to be

$$\begin{aligned}
\delta H_G &= \int_{\Sigma_t} [\mathcal{G}^{ab}\delta h_{ab} - ND_b(h^{ac}\delta\Gamma^b_{ac} - h^{ab}\delta\Gamma^c_{ac}) + 2\delta\Gamma^c_{ad}N^d h_{bc}\frac{\pi^{ab}}{\sqrt{h}})]\sqrt{h}\mathbf{e}_3 - \oint_{S_t} [h^{ab}\delta(\partial_c h_{ab})r^c N]\sqrt{|\sigma|}\mathbf{e}_2 \\
&= \int_{\Sigma_t} [\mathcal{G}^{ab}\delta h_{ab} + D_d(h^{ac}D^d(N) - D^a(N)h^{cd})\delta h_{ac} - \delta h_{ab}D_d(N^d\frac{\pi^{ab}}{\sqrt{h}})]\sqrt{h}\mathbf{e}_3 \\
&\equiv \int_{\Sigma_t} \mathcal{P}^{ab}\delta h_{ab}\mathbf{e}_3.
\end{aligned} \tag{V.22}$$

As δh_{ab} is symmetric, the antisymmetric part of $\mathcal{P}^{ab}$ will vanish when applying the summation convention. Therefore, $\mathcal{P}^{ab}$ may be symmetrized to find

$$\begin{aligned}
\mathcal{P}^{ab} &= \pi^{cb}D_c(N^a) + \pi^{ca}D_c(N^b) + \sqrt{h}D_d(h^{ab}D^d(N) - D^a(N)h^{bd}) - \sqrt{h}D_d(N^d\frac{\pi^{ab}}{\sqrt{h}}) \\
&\quad + N(\sqrt{h}G^{ab} + \frac{1}{\sqrt{h}}(2\pi^{da}\pi^b_d - \pi\pi^{ab}) - \frac{1}{2\sqrt{h}}h^{ab}(\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2) + \sqrt{h}\Lambda h^{ab}).
\end{aligned} \tag{V.23}$$

Combining all previous derivations, the total variation in the Hamiltonian, including variations in the lapse and shift, is found to be

$$\begin{cases} \delta H_G = \int_{\Sigma_t} (\mathcal{P}^{ab}\delta h_{ab} + \mathbb{H}_{ab}\delta\pi^{ab} - \mathcal{C}\delta N - 2\mathcal{C}_a\delta N^a)\mathbf{e}_3, \\ \mathcal{P}^{ab} = \pi^{cb}D_c(N^a) + \pi^{ca}D_c(N^b) + \sqrt{h}D_d(h^{ab}D^d(N) - D^a(N)h^{bd}) - \sqrt{h}D_d(N^d\dfrac{\pi^{ab}}{\sqrt{h}}) \\ \qquad\qquad + N(\sqrt{h}G^{ab} + \dfrac{1}{\sqrt{h}}(2\pi^{da}\pi^b_d - \pi\pi^{ab}) - \dfrac{1}{2\sqrt{h}}h^{ab}(\pi^{ab}\pi_{ab} - \dfrac{1}{2}\pi^2) + \sqrt{h}\Lambda h^{ab}), \\ \mathbb{H}_{ab} = \frac{2N}{\sqrt{h}}(\pi_{ab} - \frac{1}{2}\pi h_{ab}) + 2D_{(b}N_{a)}, \\ \mathcal{C} = ({}^3R - K^{ab}K_{ab} + K^2 - 2\Lambda)\sqrt{h}, \\ \mathcal{C}_a = D_b(K^b_a - h^b_a K)\sqrt{h}, \end{cases} \tag{V.24}$$

Appendix VI: Code to evaluate the Hamiltonian equations of motion

Clear all variables and define the number of dimensions, as well as the coordinates.

```
In[1]:= Clear[density, pressure, ξ, coord, metric, inversemetric, metric3,
  inversemetric3, α, affine, shift, lapse, Kmatrix, Kscalar, sqrth, pimatrix,
  inversepimatrix, piscalar, affine3, riemann3, ricci3, ricciscalar3,
  einstein3, inverseeinstein3, CurlyH, CurlyP, hmatrix, pmatrix, r, θ, ϕ, t]
$Assumptions = {α > 0, δ > 0, θ > 0, θ < π, m > 0, r > 0,
   α[t] > 0, t > 0, χ > 0, Im[θ] == 0, c > 0, Im[v] == 0, Im[u] == 0}
n = 4;
coord = {r, θ, ϕ, t};

Out[2]= {α > 0, δ > 0, θ > 0, θ < π, m > 0, r > 0, α[t] > 0,
  t > 0, χ > 0, Im[θ] == 0, c > 0, Im[v] == 0, Im[u] == 0}
```

Define the density and the pressure, which are the independent components of the stress-energy-matter tensor.

```
In[5]:= (* Result of Einstein Field Equations*)
```

$$\text{density} = \frac{3}{\chi\text{^}4}\left(\frac{\alpha'[t]\text{^}2}{\alpha[t]\text{^}2} + \frac{\delta*\chi\text{^}2}{\alpha[t]\text{^}2}\right);$$

$$\text{pressure} = \frac{-1}{\chi\text{^}2}\left(\frac{2\,\alpha''[t]}{\alpha[t]} + \frac{\alpha'[t]\text{^}2}{\alpha[t]\text{^}2} + \frac{\delta*\chi\text{^}2}{\alpha[t]\text{^}2}\right);$$

Define the metric, as well as the inverse and the three dimensional metric.

$$\text{In[7]:= metric} = \left\{\left\{\frac{\alpha[t]\text{^}2}{1-\delta*r\text{^}2}, 0, 0, 0\right\}, \{0, \alpha[t]\text{^}2*r\text{^}2, 0, 0\},\ \{0, 0, \alpha[t]\text{^}2*r\text{^}2\,\text{Sin}[\theta]\text{^}2, 0\}, \{0, 0, 0, -\chi\text{^}2\}\right\};$$

```
(* Calculate the metric inverse g^{α, β} *)
inversemetric = Simplify[Inverse[metric]];

(* Calculate the 3-metric, its inverse and the root of its determinant,
which will be required later *)
metric3 = Drop[metric, 0, {n}][[1 ;; n - 1]];
inversemetric3 = Simplify[Inverse[metric3]];
sqrth = Sqrt[Det[metric3]];
Print["Metric = ", metric // MatrixForm]
```

$$\text{Metric} = \begin{pmatrix} \frac{\alpha[t]^2}{1-r^2\delta} & 0 & 0 & 0 \\ 0 & r^2\alpha[t]^2 & 0 & 0 \\ 0 & 0 & r^2\,\text{Sin}[\theta]^2\alpha[t]^2 & 0 \\ 0 & 0 & 0 & -\chi^2 \end{pmatrix}$$

Define the affine connection coefficients.

```
In[13]:= affine := Simplify[Table[(1 / 2) * Sum[(inversemetric⟦i, s⟧) *
        (D[metric⟦s, j⟧, coord⟦k⟧] +
          D[metric⟦s, k⟧, coord⟦j⟧] - D[metric⟦j, k⟧, coord⟦s⟧]), {s, 1, n}],
     {i, 1, n}, {j, 1, n}, {k, 1, n}]]
  listaffine :=
   Table[If[UnsameQ[affine⟦i, j, k⟧, 0], {ToString[Γ[i, j, k]], affine⟦i, j, k⟧}] ,
    {i, 1, n}, {j, 1, n}, {k, 1, j}]
  TableForm[Partition[DeleteCases[Flatten[listaffine], Null], 2], TableSpacing → {2, 2}]
```

Out[15]//TableForm=

Γ[1, 1, 1]	$\frac{r\,\delta}{1-r^2\,\delta}$
Γ[1, 2, 2]	$r\left(-1+r^2\,\delta\right)$
Γ[1, 3, 3]	$r\left(-1+r^2\,\delta\right)\text{Sin}[\theta]^2$
Γ[1, 4, 1]	$\frac{\alpha'[t]}{\alpha[t]}$
Γ[2, 2, 1]	$\frac{1}{r}$
Γ[2, 3, 3]	$-\text{Cos}[\theta]\,\text{Sin}[\theta]$
Γ[2, 4, 2]	$\frac{\alpha'[t]}{\alpha[t]}$
Γ[3, 3, 1]	$\frac{1}{r}$
Γ[3, 3, 2]	$\text{Cot}[\theta]$
Γ[3, 4, 3]	$\frac{\alpha'[t]}{\alpha[t]}$
Γ[4, 1, 1]	$\frac{\alpha[t]\,\alpha'[t]}{\left(1-r^2\,\delta\right)\chi^2}$
Γ[4, 2, 2]	$\frac{r^2\,\alpha[t]\,\alpha'[t]}{\chi^2}$
Γ[4, 3, 3]	$\frac{r^2\,\text{Sin}[\theta]^2\,\alpha[t]\,\alpha'[t]}{\chi^2}$

From the metric, calculate the lapse and shift functions. Here, we define Σ_t as surfaces of constant t and S_t as surfaces of constant r and t.

```
In[16]:= gtcol = metric⟦4, 1 ;; n - 1⟧;
  shift = LinearSolve[metric3, gtcol] // Simplify;
  Nshift[a_] := shift⟦a⟧;
  lapse = Sqrt[ shiftᵀ.metric3.shift - metric⟦n, n⟧] // Simplify;
  lapse = χ;
  Print["Lapse = ", lapse]
  Print["Shift = " , shift]
```

Lapse = χ

Shift = {0, 0, 0}

Define the extrinsic curvature and extrinsic curvature scalar, as well as the canonical momentum in covariant and contravariant form.

In[23]:=
```
(* Covariant derivative of first order contravariant tensors *)
CovD[β_, α_, x_] := D[x[α], coord[[β]]] - Sum[affine[[c, α, β]] * x[c], {c, 1, n}]

(* Covariant derivative of first order covariant tensors *)
InverseCovD[β_, α_, x_] :=
 D[x[α], coord[[β]]] + Sum[affine[[α, c, β]] * x[c], {c, 1, n - 1}]

(* Calculate the extrinsic curvature tensor and scalar *)
x[a_] := -lapse * D[coord[[4]], coord[[a]]];
K[a_, b_] := CovD[b, a, x];
Kmatrix = Table[K[a, b], {a, 1, n - 1}, {b, 1, n - 1}];
Kscalar = Sum[Kmatrix[[i, j]] * inversemetric3[[i, j]], {i, 1, n - 1}, {j, 1 , n - 1}];

(* Calculate the canonical momentum tensor and the corresponding scalar *)
pi[a_, b_] := (Kmatrix[[a, b]] - Kscalar * metric3[[a, b]]) * sqrth // Simplify;
pimatrix = Table[pi[a, b], {a, 1, n - 1}, {b, 1, n - 1}];
inversepimatrix := inversemetric3.pimatrix.inversemetric3;
inversepi[a_, b_] := inversepimatrix[[a, b]];
piscalar = Sum[pi[i, j] * inversemetric3[[i, j]], {i, 1, n - 1}, {j, 1 , n - 1}];

listpik := Table[{ToString[Π[i, j]], pimatrix[[i, j]],
   ToString["         K"[i, j]], Kmatrix[[i, j]]} , {i, 1, n - 1}, {j, 1, n - 1}]
TableForm[Partition[Flatten[listpik], 4], TableSpacing → {2, 2}]
```

Out[35]//TableForm=

Π[1, 1]	$\frac{2\, r^2 \sqrt{\frac{1}{1-r^2\,\delta}}\, \mathrm{Sin}[\theta]\, \alpha[t]^4\, \alpha'[t]}{-\chi+r^2\,\delta\,\chi}$	K[1, 1]	$\frac{\alpha[t]\, \alpha'[t]}{(1-r^2\,\delta)\,\chi}$
Π[1, 2]	0	K[1, 2]	0
Π[1, 3]	0	K[1, 3]	0
Π[2, 1]	0	K[2, 1]	0
Π[2, 2]	$-\frac{2\, r^4 \sqrt{\frac{1}{1-r^2\,\delta}}\, \mathrm{Sin}[\theta]\, \alpha[t]^4\, \alpha'[t]}{\chi}$	K[2, 2]	$\frac{r^2\, \alpha[t]\, \alpha'[t]}{\chi}$
Π[2, 3]	0	K[2, 3]	0
Π[3, 1]	0	K[3, 1]	0
Π[3, 2]	0	K[3, 2]	0
Π[3, 3]	$-\frac{2\, r^4 \sqrt{\frac{1}{1-r^2\,\delta}}\, \mathrm{Sin}[\theta]^3\, \alpha[t]^4\, \alpha'[t]}{\chi}$	K[3, 3]	$\frac{r^2\, \mathrm{Sin}[\theta]^2\, \alpha[t]\, \alpha'[t]}{\chi}$

Calculate the 3-dimensional Einstein tensor, by calculating the 3-dimensional affine connection coefficients and Riemann tensor.

```
In[36]:= affine3 := affine3 = Simplify[Table[(1 / 2) * Sum[(inversemetric[[i, s]]) *
          (D[metric[[s, j]], coord[[k]] ] +
            D[metric[[s, k]], coord[[j]] ] - D[metric[[j, k]], coord[[s]] ]), {s, 1, n - 1}],
      {i, 1, n - 1}, {j, 1, n - 1}, {k, 1, n - 1}] ]
riemann3 := riemann3 = Simplify[Table[
      D[affine3[[i, j, l]], coord[[k]] ] - D[affine3[[i, j, k]], coord[[l]] ] +
       Sum[affine3[[s, j, l]] × affine3[[i, k, s]] - affine3[[s, j, k]] × affine3[[i, l, s]],
        {s, 1, n - 1}],
      {i, 1, n - 1}, {j, 1, n - 1}, {k, 1, n - 1}, {l, 1, n - 1}] ];
ricci3 =
  Simplify[Table[Sum[riemann3[[i, j, i, l]], {i, 1, n - 1}], {j, 1, n - 1}, {l, 1, n - 1}] ];
ricciscalar3 = Simplify[Sum[inversemetric3[[i, j]] × ricci3[[i, j]],
    {i, 1, n - 1}, {j, 1, n - 1}] ];
einstein3[a_, b_] := Simplify[ricci3[[a, b]] - (1 / 2) ricciscalar3 * metric3[[a, b]]];
inverseeinstein3[a_, b_] :=
 Sum[einstein3[c, d] * inversemetric3[[a, c]] * inversemetric3[[b, d]],
  {c, 1, n - 1}, {d, 1, n - 1}]
```

Define the functions for curly H and curly P, which should be equal to the Lie derivative in the time direction of the metric and canonical momenta, respectively.

```
In[42]:= CurlyH[a_, b_] := Simplify[2 * lapse * 1/sqrth (pi[a, b] - 1/2 piscalar * metric3[[a, b]]) +
    InverseCovD[b, a, Nshift] + InverseCovD[a, b, Nshift], TimeConstraint → Infinity]
CurlyP[a_, b_] := Simplify[lapse * sqrth * inverseeinstein3[a, b] - 1/(2 * sqrth) * lapse *
    (Sum[pi[i, j] * inversepi[i, j], {i, 1, n - 1}, {j, 1 , n - 1}] - 1/2 piscalar^2) ×
     inversemetric3[[a, b]] + 2 * lapse * 1/sqrth
     ((Sum[(inversemetric3.pimatrix)[[a, d]] * inversepi[b, d], {d, 1, n - 1}]) -
       1/2 * piscalar * inversepi[a, b]) - sqrth *
     (D[D[lapse, coord[[b]]], coord[[a]]] - inversemetric3[[a, b]] * Sum[inversemetric3[[c, d]] *
          D[D[lapse, coord[[c]]], coord[[d]]], {c, 1, n - 1}, {d, 1, n - 1}]) -
    sqrth * (Sum[D[1/sqrth * inversepi[a, b] * Nshift[c], coord[[c]]] +
        1/sqrth Sum[affine[[a, c, d]] * inversepi[d, b] * Nshift[c] +
           affine[[b, c, d]] * inversepi[a, d] * Nshift[c] + affine[[c, c, d]] *
            inversepi[a, b] * Nshift[d], {d, 1, n - 1}], {c, 1, n - 1}]] +
    Sum[inversepi[c, a] * InverseCovD[c, b, Nshift], {c, 1, n - 1}] +
    Sum[inversepi[c, b] * InverseCovD[c, a, Nshift], {c, 1, n - 1}] -
    lapse * sqrth * (inversemetric3[[a, b]] * pressure + shift[[a]] * shift[[b]] * density),
   TimeConstraint → Infinity]
```

Display the results of the previously defined equations alongside the results of directly taking the (partial) derivative.

In[44]:=
```
(* Results for the 3-metric*)
hmatrix = Table[CurlyH[a, b], {a, 1, n - 1}, {b, 1, a}];
metric3derivative[a_, b_] := D[metric3[[a, b]], t] // Simplify
listhdot := Table[
  {ToString[h[i, j]], metric3derivative[i, j], hmatrix[[i, j]]} , {i, 1, n - 1}, {j, 1, i}]
TableForm[Partition[Flatten[listhdot], 3], TableSpacing → {3, 3}]
```

Out[47]//TableForm=

h[1, 1]	$\frac{2\alpha[t]\,\alpha'[t]}{1-r^2\delta}$	$\frac{2\alpha[t]\,\alpha'[t]}{1-r^2\delta}$
h[2, 1]	0	0
h[2, 2]	$2r^2\alpha[t]\,\alpha'[t]$	$2r^2\alpha[t]\,\alpha'[t]$
h[3, 1]	0	0
h[3, 2]	0	0
h[3, 3]	$2r^2\mathrm{Sin}[\theta]^2\alpha[t]\,\alpha'[t]$	$2r^2\mathrm{Sin}[\theta]^2\alpha[t]\,\alpha'[t]$

In[48]:=
```
(* Results for the corresponding canonical momenta *)
pmatrix = Table[CurlyP[a, b], {a, 1, n - 1}, {b, 1, a}];
inversepiderivative[i_, j_] := D[inversepimatrix[[i, j]], t] // Simplify
listpidot := Table[{ToString[Π[i, j]], -pmatrix[[i, j]] // Simplify,
   inversepiderivative[i, j]} , {i, 1, n - 1}, {j, 1, i}]
TableForm[Partition[Flatten[listpidot], 3], TableSpacing → {3, 3}]
```

Out[51]//TableForm=

Π[1, 1]	$-\frac{2r^2\mathrm{Sin}[\theta]\,\alpha''[t]}{\sqrt{\frac{1}{1-r^2\delta}}\,\chi}$	$-\frac{2r^2\mathrm{Sin}[\theta]\,\alpha''[t]}{\sqrt{\frac{1}{1-r^2\delta}}\,\chi}$
Π[2, 1]	0	0
Π[2, 2]	$-\frac{2\sqrt{\frac{1}{1-r^2\delta}}\,\mathrm{Sin}[\theta]\,\alpha''[t]}{\chi}$	$-\frac{2\sqrt{\frac{1}{1-r^2\delta}}\,\mathrm{Sin}[\theta]\,\alpha''[t]}{\chi}$
Π[3, 1]	0	0
Π[3, 2]	0	0
Π[3, 3]	$-\frac{2\sqrt{\frac{1}{1-r^2\delta}}\,\mathrm{Csc}[\theta]\,\alpha''[t]}{\chi}$	$-\frac{2\sqrt{\frac{1}{1-r^2\delta}}\,\mathrm{Csc}[\theta]\,\alpha''[t]}{\chi}$

Calculate the value of the four constraint equations and check whether these equal zero.

```
In[52]:= (* Calculate the mixed tensor component of the extrinsic curvature *)
Kmixed[a_, b_] := Sum[K[a, c] * inversemetric[[c, b]], {c, 1, n}];

(* Calculate the term K^{a b}K_{a b} *)
kabkab =
  Sum[Kmatrix[[a, b]] * Kmatrix[[c, d]] * inversemetric3[[a, c]] * inversemetric3[[b, d]],
   {a, 1, n - 1}, {b, 1, n - 1}, {c, 1, n - 1}, {d, 1, n - 1}] // FullSimplify;

(* Calculate the value of the constraint equations *)
C0 = ricciscalar3 + Kscalar^2 - kabkab - 2 * lapse^2 * density;
Ca[a_] := Sum[D[Kmixed[a, b] - Kscalar * KroneckerDelta[a, b], coord[[b]]] + Sum[
     affine[[γ, b, a]] * (Kmixed[γ, b] - Kscalar * KroneckerDelta[γ, b]) - affine[[b, γ, b]] *
      (Kmixed[a, γ] - Kscalar * KroneckerDelta[a, γ]), {γ, 1, n - 1}], {b, 1, n - 1}]
C0 // Simplify
Ca[1] // Simplify
Ca[2] // Simplify
Ca[3] // Simplify

Out[56]= 0

Out[57]= 0

Out[58]= 0

Out[59]= 0
```

Appendix VII: Verification ADM formulae

In section 4.4, the formulae for the ADM mass and (angular) momentum are derived, stating

$$\begin{cases} M_{ADM} = -2 \oint_{S_t \to \infty} (k - k_0) \sqrt{|\sigma|} \mathbf{e}, \\ P_{ADM} = 2 \oint_{S_t \to \infty} (K^{ab} - h^{ab} K) r_b N_a \sqrt{|\sigma|} \mathbf{e}. \end{cases} \tag{VII.1}$$

These will be verified for a stationary Schwarzschild metric and rotating Kerr metric, respectively, to ensure physical meaningfulness of the definitions.

ADM mass for a Schwarzschild metric

The Schwarzschild metric, describing a massive, spherically symmetric, static object, is defined by the line element

$$ds^2 = -(1 - 2\frac{\mu}{r})dt^2 + \frac{1}{1 - 2\frac{\mu}{r}} dr^2 + r^2 d\Omega^2, \tag{VII.2}$$

where $\mu = \frac{GM}{c^2}$ and $d\Omega^2 = d\theta^2 + \sin(\theta)^2 d\phi^2$. To determine the ADM mass of this object, first the surfaces Σ_t should be defined, after which the extrinsic curvatures k and k_0 can be calculated. Let Σ_t be hypersurfaces of constant t with boundaries S_t, surfaces of constant t and r with normal vector $r_\alpha = \sqrt{h_{rr}} \partial_\alpha r = \sqrt{\frac{1}{1-2\frac{\mu}{r}}} \partial_\alpha r$. Then, using this normal vector, the extrinsic curvature tensor of S_t, k_{AB}, may be computed to be

$$\begin{aligned} k_{AB} &= \nabla_\alpha r_\beta e^\beta_B e^\alpha_A \\ &= \left(\partial_\alpha r_\beta - \Gamma^\gamma_{\alpha\beta} r_\gamma \right) e^\beta_B e^\alpha_A \\ &= \left(\partial_\alpha \left(\sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \partial_\beta r \right) - \Gamma^\gamma_{\alpha\beta} \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \partial_\gamma r \right) e^\beta_B e^\alpha_A \\ &= \left(\partial_A \left(\sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \partial_B r \right) - \Gamma^r_{AB} \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \right) \\ &= -\Gamma^r_{AB} \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}}. \end{aligned} \tag{VII.3}$$

By contracting the previous expression with σ^{AB} and substituting the values of the affine connection coefficients as derived in [63], the extrinsic curvature scalar is found to be

$$\begin{aligned} k &= k_{AB} \sigma^{AB} \\ &= -\Gamma^r_{AB} \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \sigma^{AB} \\ &= -\sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} (\Gamma^r_{\theta\theta} \sigma^{\theta\theta} + \Gamma^r_{\phi\phi} \sigma^{\phi\phi}) \\ &= \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \left((r - 2\mu) * \frac{1}{r^2} + (r - 2\mu) * \sin(\theta)^2 * \frac{1}{r^2 * \sin(\theta)} \right) \\ &= \sqrt{\frac{1}{1 - 2\frac{\mu}{r}}} \left(2(r - 2\mu) * \frac{1}{r^2} \right) \\ &= \sqrt{r(r - 2\mu)} \frac{2}{r^2}. \end{aligned} \tag{VII.4}$$

The extrinsic curvature scalar of the hypersurface S_t in flat space-time, k_0, can be derived similarly using a Minkowski metric and the connection coefficients related to polar coordinates [63], yielding $k_0 = \frac{2}{r}$. These values for the extrinsic curvature scalars are then substituted into equation VII.1, finding the ADM mass to be

$$\begin{aligned} M_{ADM} &= -2\oint_{S_t\to\infty}(k-k_0)\sqrt{|\sigma|}\mathbf{e} \\ &= -4\oint_{S_t\to\infty}(\sqrt{r(r-2\mu)}-r)\frac{1}{r^2}\sqrt{|\sigma|}\mathbf{e} \\ &= -4\int_0^{2\pi}\int_0^{\pi}\lim_{R\to\infty}(\sqrt{R(R-2\mu)}-R)\frac{1}{R^2}R^2\sin(\theta)d\theta d\phi \\ &= -8\pi\int_0^{\pi}\lim_{R\to\infty}(\sqrt{R(R-2\mu)}-R)\sin(\theta)d\theta \\ &= \lim_{R\to\infty}16\pi(R-\sqrt{R(R-2\mu)}) \\ &= \lim_{R\to\infty}16\pi R(1-(1-\frac{\mu}{R})) \\ &= 16\pi\mu \\ &= 16\pi\frac{G\cdot M}{c^2}, \end{aligned} \tag{VII.5}$$

a constant multiple of the physical mass M. Therefore, as the Lagrangian may be adapted by dividing out the constant, the ADM mass corresponds exactly to the physical mass M, proving its validity.

ADM angular momentum for a Kerr metric

To verify the definition for the ADM angular momentum, the Schwarzschild metric is of little use, as it describes a stationary space-time, implying a vanishing momentum. The most logical next step is to consider the Kerr metric, with length element in Boyer-Lindquist coordinates

$$ds^2 = -(1-\frac{r_s r}{\Sigma})c^2dt^2 + \frac{\Sigma}{\Delta}dr^2 + \Sigma d\theta^2 + (r^2+a^2+\frac{r_s r a^2}{\Sigma}\sin(\theta)^2)\sin(\theta)^2 d\phi^2 - \frac{2r_s r a\sin(\theta)^2}{\Sigma}cdtd\phi, \tag{VII.6}$$

where $\Sigma = r^2 + a^2\cos(\theta)^2$, $\Delta = r^2 - r_s r + a^2$, $a = \frac{J}{mc}$ and $r_s = \frac{2Gm}{c^2}$ is the Schwarzschild radius. This metric describes a massive, spherically symmetric object rotating around the ϕ-axis, implying $\phi^i = \delta^i_\phi$ as an obvious choice for the shift. Similar to the analysis of the Schwarzschild metric, Σ_t are chosen to be the hypersurfaces of constant t and S_t are hypersurfaces of constant r and t, again with normal vector $r_\alpha = \sqrt{h_{rr}}\partial_\alpha r = \sqrt{\frac{\Sigma}{\Delta}}\partial_\alpha r$. Additionally, as noted in section 4.4, the angular momentum may only be defined within a certain gauge, which in this case is chosen to be the asymptotically maximal gauge [73]. Therefore, the following results will only hold in this gauge.

The equations to determine the integrand $K^{ab} - h^{ab}K$ are significant in size, hence Wolfram Mathematica is utilised for this. As the canonical momenta and the integrand are directly related as $\frac{\pi^{ab}}{\sqrt{h}} = K^{ab} - h^{ab}K$, the code in appendix VI may be reused, yielding

$$\begin{cases} \pi^{23} = \pi^{32} = \frac{a^3 r r_s\cos(\theta)\sin(\theta)^4}{(r^2+a^2)\Sigma^2+a^2 r r_s\sin(\theta)^2\Sigma}, \\ \pi^{13} = \pi^{31} = \frac{a r_s\sin(\theta)^3(a^2(a^2-r^2)\cos(\theta)^2-r^2(a^2+3r^2))}{\sin(\theta)^2(2(r^2+a^2)\Sigma^2+2a^2 r r_s\sin(\theta)^2\Sigma)}, \end{cases} \tag{VII.7}$$

as the non-vanishing components of the canonical momenta. Instead of dividing these equations by $\sqrt{h}$ and directly substituting the result into equation VII.1, it will be beneficial to first consider the expression $(K^{ab} - h^{ab}K)\sqrt{|\sigma|} = \pi^{ab}\frac{\sqrt{|\sigma|}}{\sqrt{h}}$. As the determinant of the 3-metric h_{ab} is given by $h =$

$h_{rr} \cdot (h_{\theta\theta} \cdot h_{\phi\phi} - h_{\theta\phi} \cdot h_{\phi\theta})$ and the determinant of the 2-metric is $\sigma = \sigma_{\theta\theta} \cdot \sigma_{\phi\phi} - \sigma_{\theta\phi} \cdot \sigma_{\phi\theta} = h_{\theta\theta} \cdot h_{\phi\phi} - h_{\theta\phi} \cdot h_{\phi\theta}$, this fraction is found to be

$$\frac{\pi^{ab}\sqrt{|\sigma|}}{\sqrt{|h|}} = \frac{\pi^{ab}}{\sqrt{|h_{rr}|}} = \pi^{ab}\sqrt{\frac{\Delta}{\Sigma}}, \tag{VII.8}$$

a significantly simpler expression than would have been found by dividing the canonical momenta by $\sqrt{h}$. Substituting this result into equation VII.1, the ADM angular momentum is found to be

$$\begin{aligned}
P_{ADM} &= 2\oint_{S_t\to\infty} (K^{ab} - h^{ab}K) r_b N_a \sqrt{|\sigma|}\mathbf{e} \\
&= 2\oint_{S_t\to\infty} (\frac{\pi^{13}}{\sqrt{|h|}} r_1\phi_3 + \frac{\pi^{23}}{\sqrt{|h|}} r_2\phi_3)\sqrt{|\sigma|}\mathbf{e} \\
&\overset{*}{=} 2\oint_{S_t\to\infty} h_{\phi\phi}\sqrt{\frac{\Delta}{\Sigma}}(\pi^{13}r_1 + \pi^{23}r_2)\mathbf{e} \\
&= 2\oint_{S_t\to\infty} h_{\phi\phi}\sqrt{\frac{\Delta}{\Sigma}}(\pi^{13}\sqrt{\frac{\Sigma}{\Delta}}\partial_r r + \pi^{23}\sqrt{\frac{\Sigma}{\Delta}}\partial_\theta r)\mathbf{e} \\
&= 2\oint_{S_t\to\infty} h_{\phi\phi}\pi^{13}\mathbf{e} \\
&= 2\oint_{S_t\to\infty} (r^2 + a^2 + \frac{r_s r a^2}{\Sigma}\sin(\theta)^2)\cdot\sin(\theta)^2\cdot\frac{a r_s \sin(\theta)^3(a^2(a^2-r^2)\cos(\theta)^2 - r^2(a^2+3r^2))}{\sin(\theta)^2(2(r^2+a^2)\Sigma^2 + 2a^2 r r_s \sin(\theta)^2\Sigma)}\mathbf{e} \\
&= 2\oint_{S_t\to\infty} \frac{a r_s \sin(\theta)^3(a^2(a^2-r^2)\cos(\theta)^2 - r^2(a^2+3r^2))}{2\Sigma^2}\mathbf{e} \\
&= 2\int_0^{2\pi}\int_0^{\pi} \lim_{r\to\infty} \frac{a r_s \sin(\theta)^3(a^2(a^2-r^2)\cos(\theta)^2 - r^2(a^2+3r^2))}{2\Sigma^2} d\theta d\phi \\
&= 4\pi\int_0^{\pi} \lim_{r\to\infty} \frac{a r_s \sin(\theta)^3 \cdot -3r^4}{2r^4} d\theta \\
&= -6\pi\int_0^{\pi} a r_s \sin(\theta)^3 d\theta \\
&= -8\pi a r_s \\
&= -16\pi\frac{J\cdot G}{c^3} \\
&= -J_{ADM},
\end{aligned} \tag{VII.9}$$

where equation ($*$) holds as $\phi_i = \phi^j h_{ij} = \phi^i h_{ii}$. The final equality shows that $J_{ADM} = 16\pi\frac{J\cdot G}{c^3}$, again a constant multiple of the physical angular momentum of the system. Therefore, rescaling the Lagrangian will align the ADM angular momentum with the physical angular momentum (within the asymptotically maximal gauge), verifying equation VII.1.

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