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GROUPOID SYMMETRY AND CONSTRAINTS IN GENERAL RELATIVITY

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To Darryl Holm, for his 64th birthday

Abstract. When the vacuum Einstein equations are cast in the form of hamiltonian evolution equations, the initial data lie in the cotangent bundle of the manifold $\mathcal{M}\Sigma$ of riemannian metrics on a Cauchy hypersurface Σ. As in every lagrangian field theory with symmetries, the initial data must satisfy constraints. But, unlike those of gauge theories, the constraints of general relativity do not arise as momenta of any hamiltonian group action. In this paper, we show that the bracket relations among the constraints of general relativity are identical to the bracket relations in the Lie algebroid of a groupoid consisting of diffeomorphisms between space-like hypersurfaces in spacetimes.

A direct connection is still missing between the constraints themselves, whose definition is closely related to the Einstein equations, and our groupoid, in which the Einstein equations play no role at all. We discuss some of the difficulties involved in making such a connection.

1. Introduction

The vacuum Einstein equations state that the Ricci curvature $\mathrm{Ric}(g)$ of a lorentzian metric g is identically zero. Recast as evolution equations, they become a hamiltonian system on the cotangent bundle of the manifold[1] $\mathcal{M}\Sigma$ of smooth riemannian metrics on a manifold Σ which represents the typical Cauchy hypersurface[2]. Each element of $T^*\mathcal{M}\Sigma$ may be identified with a pair (γ, π), where γ is a riemannian metric and π is a symmetric covariant 2-tensor field.[3]

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[1]In this paper, we will actually treat spaces of smooth functions as diffeological spaces rather than as Fréchet manifolds. In Appendix A, we review the theory of diffeology, concentrating on the aspects which are relevant to our work.

[2]In general relativity, Σ has dimension 3, but that assumption is not necessary for anything we do in this paper.

[3] Strictly speaking, a cotangent vector π to $\mathcal{M}\Sigma$ should be a contravariant symmetric 2-tensor density, but we may use the metric γ and its associated volume element to identify covariant and contravariant tensors, and to identify scalar functions with densities. In addition, we consider π as an endomorphism of the tangent bundle $T\Sigma$ when we form π^2 and take traces.

It has long been known[4] that, for a given γ and π to be admissible as initial conditions for the Einstein equations, they must satisfy a system of constraint equations. These equations may be derived either geometrically from the Gauss-Codazzi equations relating the intrinsic and extrinsic curvatures of a hypersurface, or from a lagrangian formulation of the Einstein equations in terms of the Einstein-Hilbert action. The equations are:

$$\mathbf{C}_{\mathrm{mo}}(\gamma,\pi) := -2\,\mathrm{div}_\gamma\,\pi = 0\,, \tag{1}$$

$$\mathbf{C}_{\mathrm{en}}(\gamma,\pi) := -R(\gamma) + \mathrm{Tr}_\gamma(\pi^2) - \tfrac{1}{\dim\Sigma - 1}(\mathrm{Tr}_\gamma\,\pi)^2 = 0\,. \tag{2}$$

The *momentum constraint*, $\mathbf{C}_{\mathrm{mo}}$, maps $T^*\mathcal{M}\Sigma$ to the space $\mathcal{X}\Sigma$ of vector fields on Σ, while the *energy constraint*, $\mathbf{C}_{\mathrm{en}}$, takes values in the space $\mathcal{F}\Sigma$ of scalar functions on Σ. The constraints may be viewed as those components of the Einstein tensor which involve directions normal to the Cauchy hypersurface. (See Appendix E of [46] for details.)

The *constraint set* $\mathcal{C} \subset T^*\mathcal{M}\Sigma$, where the constraints are all equal to zero, has two properties which always hold for the zero sets of momentum[5] maps of proper hamiltonian group actions.

- The constraint set is coisotropic; i.e., for any two functions vanishing on $\mathcal{C}$, their Poisson bracket vanishes there as well. (This follows from the bracket formulas (4) below.) Consequently, on its regular part, namely those pairs (γ,π) with no common infinitesimal symmetries, $\mathcal{C}$ is foliated by *characteristic submanifolds* whose tangent spaces are spanned by the hamiltonian vector fields whose hamiltonians vanish on $\mathcal{C}$. In the group action setting, these would be the orbits of the symmetry group.
- As shown by Arms, Marsden, and Moncrief [1], the constraint set has quadratic singularities at the points which do admit infinitesimal symmetries. In the group action setting, this would follow from the linearizability of proper actions and the equivariant Darboux theorem.

The aim of the research described in this paper has been to identify the symmetry structure responsible for the constraints and their Poisson bracket relations. What we have found is that the bracket relations, rather than coming from the Lie algebra of a symmetry group, are those of a Lie algebr*oid* which is derived from a group*oid*[6] of diffeomorphisms between space-like hypersurfaces in Lorentz manifolds. Unfortunately, this groupoid, which encodes the arbitrariness in the choice of initial value hypersurface for the Einstein equations as well as of coordinates on this hypersurface, lives over a much larger space than the one where the constraints are defined. It remains to be seen what the relevant structure is which connects our groupoid with the constraints themselves.

Since the constraints $\mathbf{C}_{\mathrm{mo}}$ and $\mathbf{C}_{\mathrm{en}}$ are vector valued, we break them into scalar-valued components to form their Poisson brackets. Following DeWitt [14], we get these components by pairing the constraints by integration against vector fields

[4] See Section 4 below for historical remarks and references.

[5] Note that we are using two meanings of "momentum" in this discussion, first in a slightly extended version of the usual "mass times velocity", and second in the sense used in the theory of hamiltonian actions. In the latter sense, the term "moment" is often used instead. (See the footnote on p. 133 of [33]) for some remarks on the two nomenclatures.)

[6] The definition of groupoid is reviewed briefly in Section A.2. We refer to [32] for a full treatment of Lie algebroids and Lie groupoids.

and functions on Σ, obtaining for each vector field X and function ϕ the following real-valued constraint function on $T^*\mathcal{M}\Sigma$:

$$C_{(X,\phi)}(\gamma,\pi) = \int_\Sigma \big\{\gamma(X, \mathbf{C}_{\mathrm{mo}}(\gamma,\pi)) + \phi\mathbf{C}_{\mathrm{en}}(\gamma,\pi)\big\}\mathrm{vol}_\gamma \, . \tag{3}$$

Since $C_{(X,\phi)}$ is the sum of $C_X \stackrel{\mathrm{def}}{=} C_{(X,0)}$ and $C_\phi \stackrel{\mathrm{def}}{=} C_{(0,\phi)}$, it suffices to write down the Poisson bracket relations among these terms. These were found by DeWitt to be:

$$\begin{aligned} \{C_X, C_Y\} &= C_{[X,Y]} \\ \{C_X, C_\phi\} &= C_{X\cdot\phi} \\ \{C_\phi, C_\psi\} &= C_{\phi \,\mathrm{grad}_\gamma \psi - \psi \,\mathrm{grad}_\gamma \phi} = C_{\gamma^{-1}(\phi d\psi - \psi d\phi)} \, , \end{aligned} \tag{4}$$

where the metric γ is here considered as a bundle map from $T\Sigma$ to $T^*\Sigma$, so that its inverse takes the differentials of functions to their gradients.

The coisotropic property of the constraint set follows immediately from (4) above: the bracket of any two constraint functions vanishes on the constraint set. On the other hand, the dependence of $\{C_\phi, C_\psi\}$ on the metric γ means that the brackets are not those of a fixed Lie algebra structure on $\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma$. Of course, we may freeze the metric γ to some value $\overline{\gamma}$, but then the resulting bracket $\{\ ,\ \}_{\overline{\gamma}}$ will not satisfy the Jacobi identity. The anomaly appears in the jacobiator of a momentum constraint and two energy constraints, namely:

$$\{C_X, \{C_\phi, C_\psi\}_{\overline{\gamma}}\}_{\overline{\gamma}} + \text{circ.perm.} = C_{\mathcal{L}_X(\overline{\gamma}^{-1})(\phi d\psi - \psi d\phi)} \, ,$$

which vanishes only in special cases, such as when X is a Killing vector field for $\overline{\gamma}$.

We must therefore renounce the idea that the constraints should be the momentum map of a symmetry group (such as the group of diffeomorphisms of spacetime). Instead, we use a groupoid.

The objects of our groupoid will be the isometry classes of embeddings of Σ as a cooriented, space-like hypersurface in a lorentzian manifold. We call these Σ-universes. The morphisms of the groupoid, which we call Σ-evolutions, will be the isometry classes of *pairs* of such embeddings into the *same* target lorentzian manifold; they can be identified with diffeomorphisms between the image hypersurfaces. Remarkably, the Lie algebroid of this groupoid is naturally a trivial bundle, and the bracket relations among its constant sections turn out to reproduce precisely the bracket relations (4) among the constraints.

To facilitate computations with the rather abstractly defined spaces of isometry classes, we will use the fact that each Σ-universe has near the image of Σ a unique gaussian representative, i.e. a metric near (in the appropriate sense) $\Sigma\times\{0\}$ on $\Sigma\times\mathbb{R}$ for which the paths $t \mapsto (x,t)$ for each $x \in \Sigma$ are time-like geodesics parametrized by (negative) arc-length and normal to $\Sigma \times \{0\}$.

As an aside, we will show that the groupoid of Σ-evolutions is equivalent in a precise sense to the groupoid of isometries between those Lorentz manifolds which admit a cooriented, space-like hypersurface diffeomorphic to Σ.

There remains a significant gap between our results and a satisfactory geometric explanation of the relations (4) among the constraints, since our Lie algebroid lies over a space much bigger than the phase space $T^*\mathcal{M}\Sigma$ on which the constraints live. The latter space may be identified, via a natural riemannian metric on $\mathcal{M}\Sigma$, with the tangent bundle $T\mathcal{M}\Sigma$, and this tangent bundle may be in turn identified with the space of 1-jets around Σ of Σ-universes. Differentiation by tangent vectors based along Σ gives a natural projection from the Σ-universes to the 1-jets. Unfortunately, it does not seem to be possible to make our Lie algebroid descend along this projection.

To end this introduction, we note that Teitelboim [45] already gave an argument leading to the Poisson bracket relations among the constraints using pure geometry, without any appeal to Einstein's equations. In some sense, the accomplishment of our paper is to put Teitelboim's argument in its proper mathematical context, that of groupoids and Lie algebroids.

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2. Universes

We turn now to the construction of a groupoid whose Lie algebroid is a trivial bundle with fibre $\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma$, such that the bracket of constant sections is given by (4).

2.1. Σ-universes.

A connected lorentzian manifold M will be called a **spacetime**[7] (whether or not its dimension is 4). M will be called Σ-**adapted** if it admits a cooriented (i.e. with an orientation of the normal bundle), proper embedding of Σ as a space-like hypersurface; such an embedding will be called a Σ-**space** in M, and a pair consisting of a spacetime and a Σ-space in it will be called a Σ-**spacetime.**

Since the identity of specific points in the ambient spacetime is irrelevant[8] to the evolution of metrics on a manifold Σ, it is natural to make Definition 2.2 below.

Notation 2.1. For better compatibility with composition, we will often represent mappings by arrows going from right to left; hence we write $C^\infty(X, Y)$ for the smooth mappings *to X from Y*.

Definition 2.2. *A* Σ-**universe** *is an equivalence class of* Σ*-spacetimes, where* $M \overset{i}{\hookleftarrow} \Sigma$ *and* $M' \overset{i'}{\hookleftarrow} \Sigma$ *are equivalent if there is an isometry* $M' \overset{\psi}{\leftarrow} M$ *which is consistent*

[7]Note that any such manifold satisfies an Einstein equation of the form $\mathrm{Ric}(g) = T$ if the energy-momentum tensor T is simply defined by that equation.

[8]Dirac [16] wrote, "I am inclined to believe . . . that four-dimensional symmetry is not a fundamental property of the physical world." Pirani [36], reviewing Dirac's paper, "finds it difficult to concur".

with the coorientations and which satisfies $\psi \circ i = i'$ *. We will denote the set*[9] *of all* Σ*-universes by* $\mathcal{U}\Sigma$*.*

To define a diffeology on $\mathcal{U}\Sigma$, since different Σ-universes may be represented by different lorentzian manifolds, we follow the pattern described in Appendix A for functional diffeologies on spaces of mappings with varying domains. Namely, we stipulate that a parametrization $\mathcal{U}\Sigma \xleftarrow{\phi} P$ is smooth if:

(1) each point of P has a neighborhood $\mathcal{U}$ for which there is a fixed manifold M such that the Σ-universes $\phi(p)$, $p \in \mathcal{U}$, are represented by Σ-spacetimes $M_p \overset{i_p}{\hookleftarrow} \Sigma$, where all the M_p are open subsets of M;
(2) $i_p \hookleftarrow p$ is a smooth map $C^\infty(M, \Sigma) \leftarrow P$.
(3) $M_{\text{tot}} = \{(x, p) | p \in P \text{ and } x \in M_p\}$ is open in $M \times P$;
(4) the lorentzian structures on the fibres are the restrictions of a smooth section over M_{tot} of the bundle of symmetric fibrewise 2-forms;

The following proposition gives a first description of the tangent bundle of $\mathcal{U}\Sigma$. A more explicit description will follow the introduction of gaussian splittings.

Proposition 2.3. *The tangent cone to* $\mathcal{U}\Sigma$ *at a* Σ*-universe* $[(M, g) \overset{i}{\hookleftarrow} \Sigma]$ *is a vector space which may be identified with the quotient of the space* $\Gamma(S^2(T^*M))$ *of symmetric 2-forms on* M *by the image of the map* $\Gamma(S^2(T^*M)) \xleftarrow{\mathcal{L}g} \mathcal{X}_{i(\Sigma)}M$ *taking each vector field* Z *defined on* M *and vanishing on* $i(\Sigma)$ *to the Lie derivative* $\mathcal{L}_Z g$*.*

Proof. A tangent vector to $\mathcal{U}\Sigma$ is represented by a 1-parameter family $(M_s, g_s) \overset{i_s}{\hookleftarrow} \Sigma$ of embeddings, where $M_0 = M$, M_s are open subsets of a fixed manifold $\overline{M}$, and g_s are lorentzian metrics depending smoothly upon s.

We will simplify the representative by fixing M_s and the embeddings, so that it is only g which varies. To do this, let ξ_s be the vector field $di_s/ds = \xi_s$ along i_s. Since i_s is a proper embedding for each s, we may "extend" the family ξ_s over $\overline{M}$, i.e. we may choose a smooth family σ_s of vector fields on $\overline{M}$ such that $\xi_s = \sigma_s \circ i_s$ for all s. This family may not be complete, but we may integrate it as far as is possible. The result is a family of open sets $M'_s \subset \overline{M}$ and a family of open embeddings $M_s \xleftarrow{\psi_s} M'_s$ defining a smooth path in $C^\infty(\overline{M}, [\overline{M}])_{\text{open}}$ such that $M'_0 = M_0$, ψ_0 is the identity on M_0, and $d\psi_s/ds = \sigma_s \circ \psi_s$. Since $\xi_s = \sigma_s \circ i_s$, $\psi_s \circ i_0 = i_s$. (In particular, M'_s contains $i_0(\Sigma)$ for all s.) We obtain a new family $(M'_s, g'_s) \overset{i'_s}{\hookleftarrow} \Sigma$ of embeddings by setting $g'_s = \psi_s^*(g_s)$ and $i'_s = i_s \circ \psi_s^{-1} = i_0$. This family is not quite equivalent to the original one, since the domains M'_s are not mapped by ψ_s to all of M_s, but they do agree at $s = 0$. According to the observation in Appendix A that tangent vectors are insensitive to variations of domain, this insures that the paths in $\mathcal{U}\Sigma$ represented by $(M_s, g_s) \overset{i_s}{\hookleftarrow} \Sigma$ and $(M'_s, g'_s) \overset{i'_s}{\hookleftarrow} \Sigma$ represent the same tangent vector to $\mathcal{U}\Sigma$ at $[(M, g) \overset{i_0}{\hookleftarrow} \Sigma]$, where the latter path has constant embedding i_0. We may keep M'_s constant as well, in which case the only object varying with s is the lorentzian metric g_s. Its derivative with respect to s at $s = 0$ is the required smooth section of $S^2(T^*M)$.

[9]The collection of all Σ-spacetimes is, like the collection of all sets, a "class" in the set-theoretic sense rather than a set. But the Σ-universes $\mathcal{U}\Sigma$ do form a set because every connected manifold is diffeomorphic to a submanifold of some $\mathbb{R}^n$.

Our representative of the tangent vector is not unique, since we may apply an arbitrary family of diffeomorphisms of M which fix $i(\Sigma)$ and the normal orientation there. (This freedom corresponds, essentially, to the freedom which we had in extending ξ_s to σ_s.) The only such diffeomorphism which can preserve a lorentzian metric on (connected) M is the identity. The infinitesimal action of these diffeomorphisms, i.e. the map $\mathcal{L}_\xi g \leftarrow\!\shortmid \xi$, is therefore injective, and the tangent space to $\mathcal{U}\Sigma$ at $[i]$ is the quotient of $S^2(T^*M)$ by the image of that map. ☐

2.2. **Σ-evolutions.** The relative positions of pairs of Σ-spaces in the same spacetime, up to equivalence, form a groupoid over $\mathcal{U}\Sigma$ which will be our fundamental symmetry structure.

Definition 2.4. *A* Σ**-evolution** *is an equivalence class of pairs (i_1, i_0) of Σ-spaces in the same spacetime, where a pair (i_1, i_0) in M is equivalent to (i'_1, i'_0) in M' if there is a single isometry $M' \xleftarrow{\psi} M$ which is consistent with the coorientations and which satisfies both $\psi \circ i_1 = i'_1$ and $\psi \circ i_0 = i'_0$. We will denote the set of all Σ-evolutions by $\mathcal{E}\Sigma$.*

The Σ-evolutions form a diffeological groupoid over the Σ-universes with the diffeology on $\mathcal{E}\Sigma$, like that on $\mathcal{U}\Sigma$, defined in terms of representatives. The groupoid structure has as target and source the projections $[i_1, i_0] \xleftarrow{l} [i_1]$ and $[i_1, i_0] \xleftarrow{r} [i_0]$ (square brackets denoting equivalence classes); the composition law is $[i_2, i_1][i_1, i_0] = [i_2, i_0]$; and the inversion rule $[i_1, i_0]^{-1} = [i_0, i_1]$.

We will show in Section 2.7 that $\mathcal{E}\Sigma$ is Morita equivalent to the isometry groupoid $\mathcal{I}\Sigma$ of Σ-adapted spacetimes. This implies that the orbits of $\mathcal{E}\Sigma$ are in bijection with the orbits of $\mathcal{I}\Sigma$, which are the isometry classes of Σ-adapted spacetimes.

The isotropy group of $[i]$ consists of all pairs $([i_1, i_0])$ such that $[i_1] = [i_0] = [i]$. For such a pair, $M \xhookleftarrow{i_1} \Sigma$ and $M \xhookleftarrow{i_0} \Sigma$ are equivalent, which means that there is an isometry ψ from M to itself such that $i_1 = \psi \circ i_0$. Such an isometry is unique, if it exists, which implies that the isotropy group of $[i]$ is isomorphic to the isometry group of its target spacetime.

Remark 2.5. Each (i_1, i_0) corresponds to a diffeomorphism $i_1 \circ i_0^{-1}$ between Σ-spaces in the same spacetime, and composition in $\mathcal{E}\Sigma$ corresponds to composition of diffeomorphisms.

Elements of the Lie algebroid of $\mathcal{E}\Sigma$ are infinitesimal Σ-evolutions and may be parametrized by triples consisting of Σ-universes, "shift" vector fields on Σ, and "lapse" functions on Σ, per the following proposition.

Proposition 2.6. *The Lie algebroid $A\mathcal{E}\Sigma \to \mathcal{U}\Sigma$ is isomorphic as a vector bundle to the trivial bundle $\mathcal{U}\Sigma \times (\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma)$.*

Proof. An element of $A\mathcal{E}\Sigma$ at the base point $[i_0] \in \mathcal{U}\Sigma$ is a tangent vector to a smooth path in $\mathcal{E}\Sigma$ whose image is contained in the r-fibre of $[i_0]$ starting at the unit $[i_0, i_0]$. Such a path is represented by a smooth family (i_s, i_0) defined on an interval containing $s = 0$, and its tangent vector at $s = 0$ corresponds to a vector field along i_0. (Note that the i_s may all be chosen to have the same target; the Lie algebroid fibres are thus simpler to analyze than the tangent spaces to $\mathcal{U}\Sigma$ to which the anchor projects them.) Using the lorentzian metric on the target manifold to decompose this vector field into its tangential and normal components, and dividing the latter by the unit future normal field $\mathbf{n}$, we obtain a vector field X and smooth function ϕ on Σ which correspond to the Lie algebroid element given by the path.

Each fibre of $A\mathcal{E}\Sigma$ is now identified with the fixed space $\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma$. We omit here the verification that this identification depends smoothly on the base point in $\mathcal{U}\Sigma$. $\square$

2.3. **Gaussian normal form.** To compute the bracket and anchor of the Lie algebroid $A\mathcal{E}\Sigma \to \mathcal{U}\Sigma$, we may work in a neighborhood of the units $[i,i]$. There, we may use the simplified representation of each Σ-universe $[i]$ near $S = i(\Sigma)$ given by the following gaussian normal form. Using the metric g on the target of the cooriented embedding $M \overset{i}{\hookleftarrow} \Sigma$, we first extend the unit future normal field along S by parallel translation along the geodesics normal to S to obtain a time-like vector field $\mathbf{n}$ on a neighborhood U of S in M; this extension will satisfy the equations $g(\mathbf{n}, TS) = 0$, $g(\mathbf{n}, \mathbf{n}) = -1$, and $\nabla_{\mathbf{n}}\mathbf{n} = 0$, where ∇ is the Levi-Civita connection of g. Transporting S along the flow $\Phi^{\mathbf{n}}_s$ of $\mathbf{n}$ produces a codimension-1 foliation on a neighborhood of S with space-like leaves which are everywhere orthogonal to $\mathbf{n}$. We call the leaves of this foliation the **gaussian time slices**. This construction induces a canonical isometry to a neighborhood of S in M from a neighborhood of $\Sigma \times \{0\}$ in $\Sigma \times \mathbb{R}$ on which the metric has the gaussian form

$$\frac{1}{2}(\gamma_{ij}(x,t)dx^i dx^j - dt^2)\,, \tag{5}$$

where x^i are coordinates on Σ. Replacing the former neighborhood by the latter, we have established the following normal form result.

Proposition 2.7. *Every Σ-universe has a representative $M \overset{i}{\hookleftarrow} \Sigma$ in which a neighborhood U of $i(\Sigma)$ in M is equal to a neighborhood of $\Sigma \times \{0\}$ in $\Sigma \times \mathbb{R}$, $i(x) = (x, 0)$, and the metric on U has the gaussian form* (5). *This gaussian metric is uniquely determined by* $[i]$.

Similarly, any tangent vector to $\mathcal{U}\Sigma$ has a unique representation in the form

$$\frac{1}{2}\alpha_{ij}(x,t)dx^i dx^j\,. \tag{6}$$

When Σ is compact (and sometimes when it is not), one can take U to be a product $\Sigma \times I$ for some open interval I containing zero. We will call such a Σ-universe *cylindrical.* The "spatial" component $\frac{1}{2}\gamma_{ij}(x,t)dx^i dx^j$ of the gaussian metric is then a 1-parameter family of riemannian metrics on Σ. Thus we may parametrize the cylindrical Σ-universes by paths of metrics, and the tangent vectors to them by paths of symmetric covariant 2-tensors (not necessarily positive definite) on Σ.

For noncompact Σ, we may have to take U to consist of pairs (x,t) with $|t| < \epsilon(x)$ for a smooth positive function ϵ on Σ. In any case, on a neighborhood of any compact subset of Σ, a Σ-universe is defined by a path of metrics and a tangent vector to the Σ-universes by a path of symmetric covariant 2-tensors.

2.4. **Gaussian vector fields.** To use the gaussian normal form in our computations, we must deal with the fact that a slicing which is gaussian for one embedding of Σ is not gaussian for most others. The following lemma about diffeomorphisms will lead us to its infinitesimal version about vector fields, which is all we need to use.

Lemma 2.8. *Every diffeomorphism $S \to S'$ between space-like, cooriented hypersurfaces in spacetimes (M, g) and (M', g') extends to a diffeomorphism $\psi : U \to U'$ between neighborhoods of S and S' respectively which respects the gaussian time-splittings, i.e. which intertwines the (local) gaussian time flows:*

$$\psi \circ \Phi_t^{\boldsymbol{n}} = \Phi_t^{\boldsymbol{n}'} \circ \psi \,. \tag{7}$$

The diffeomorphism is unique up to the choice of (connected relative to S) U.

We note that (7) holds if and only if ψ preserves inner products with the unit normal, i.e. $g(\mathbf{n}, w) = (\psi^* g')(\mathbf{n}, w)$ for all vector fields w. By letting $(M, g) = (M', g')$ and defining ψ in the domain of a flow Φ_s^v generated by some vector field v on M, and differentiating with respect to s, we obtain the following infinitesimal version of Eq. (7).

Definition 2.9. *Let U be a neighborhood of a hypersurface S as in Lemma 2.8. A vector field v on U is called g-*gaussian *if it satisfies*

$$(\mathcal{L}_v g)(\mathbf{n}, w) = 0 \tag{8}$$

for all vector fields w.

The following infinitesimal version of Lemma 2.8 will be proven by a purely infinitesimal computation.

Proposition 2.10. *Every vector field v_0 with values in TM defined on a hypersurface S as in Lemma 2.8 extends to a g-gaussian vector field v defined on a neighborhood of S.*

Proof. Condition (8) can be rewritten as

$$\begin{aligned} 0 = i_{\mathbf{n}} \mathcal{L}_v g &= (\mathcal{L}_v i_{\mathbf{n}} + i_{[\mathbf{n},v]}) g = (d i_v + i_v d) i_{\mathbf{n}} g + i_{[\mathbf{n},v]} g \\ &= d(i_v i_{\mathbf{n}} g) + i_{[\mathbf{n},v]} g \,, \end{aligned}$$

where we have used the fact that $i_{\mathbf{n}} g = -dt$ so that $d i_{\mathbf{n}} g = 0$. Equivalently,

$$[\mathbf{n}, v] = -\operatorname{grad}_g (g(\mathbf{n}, v)) \,, \tag{9}$$

where grad_g is the gradient with respect to g.

Splitting the vector field $v = X + \phi \mathbf{n}$ into components orthogonal and parallel to $\mathbf{n}$ and observing that $[\mathbf{n}, v] = \nabla_{\mathbf{n}} v - \nabla_v \mathbf{n} = \nabla_{\mathbf{n}} v - \nabla_X \mathbf{n}$ because $\nabla_{\mathbf{n}} \mathbf{n} = 0$, and that $g(\mathbf{n}, v) = -\phi$ because $g(\mathbf{n}, \mathbf{n}) = -1$, we obtain the equivalent condition

$$\nabla_{\mathbf{n}} v = \nabla_X \mathbf{n} + \operatorname{grad}_g \phi \,.$$

If we now take the inner product with $\mathbf{n}$, use the facts that $g(\nabla_{\mathbf{n}} X, \mathbf{n}) = 0$ and $g(\nabla_{\mathbf{n}} \phi \mathbf{n}, \mathbf{n}) = -\mathbf{n} \cdot \phi$, then we obtain the condition $\mathbf{n} \cdot \phi = 0$. In in other words, the gradient $\operatorname{grad}_g \phi$ does not have a normal component, i.e. $\operatorname{grad}_g \phi = \operatorname{grad}_\gamma \phi$, where the "spatial gradient" $\operatorname{grad}_\gamma \phi$ is defined as $\operatorname{grad}_g \phi + (\mathbf{n} \cdot \phi)\mathbf{n}$. (Note the sign again.)

This implies that that Eq. (9) splits into components orthogonal and parallel to $\mathbf{n}$ as

$$[\mathbf{n}, X] = \operatorname{grad}_\gamma \phi \,, \qquad \mathbf{n} \cdot \phi = 0 \,. \tag{10}$$

In local coordinates these equations read

$$\frac{\partial X}{\partial t} = \operatorname{grad}_\gamma \phi \tag{11}$$

$$\frac{\partial \phi}{\partial t} = 0. \tag{12}$$

Using the boundary conditions $X_{t=0} = X_0$ and $\phi_{t=0} = \phi_0$, we see that the g-gaussian extension $v = X + \phi\mathbf{n}$ of the vector field $v_0 = X_0 + \phi_0\mathbf{n}$ exists and is uniquely determined in a very simple way by the initial values of X and ϕ. □

We will denote the g-gaussian extension of $X_0 + \phi_0\mathbf{n}$ by $G_g(X_0, \phi_0)$. Furthermore, we will abuse notation by omitting the zero subscripts for the initial values when the context distinguishes them from their extensions.

For future reference, we write below an explicit formula for the gaussian extension, to first order in t.

$$G_g(X_0, \phi_0) = X_0 + t \operatorname{grad}_{\gamma_0} \phi_0 + \phi_0\mathbf{n} + O(t^2). \tag{13}$$

2.5. **The action of g-gaussian vector fields on symmetric 2-forms.** To compute the anchor $A\mathcal{E}\Sigma \to T\mathcal{U}\Sigma$ of our Lie algebroid, we need to express, in terms of the space/time splitting on the ambient manifold, the Lie derivative of a symmetric 2-form of the type

$$\alpha = \frac{1}{2}\alpha_{ij}(x,t)dx^i dx^j$$

by a g-gaussian vector field $v = X + \phi\mathbf{n}$.

The pull-back of the Lie derivative on the ambient manifold to the gaussian time slices is

$$\mathcal{L}_v^\top \alpha := \mathcal{L}_v\alpha - (i_\mathbf{n}\mathcal{L}_v\alpha)dt = \mathcal{L}_v\alpha - (i_{[\mathbf{n},v]}\alpha)dt\,.$$

If $v = X + \phi\mathbf{n}$ is g-gaussian we have $[\mathbf{n}, v] = \operatorname{grad}_\gamma \phi$. Writing $\mathcal{L}_\mathbf{n}\alpha = \mathcal{L}_\mathbf{n}^\top\alpha = \frac{1}{2}\phi\,\dot\alpha_{ij}dx^i dx^j =: \dot\alpha$, we obtain

$$\mathcal{L}_v\alpha = \mathcal{L}_X^\top\alpha + \phi\,\dot\alpha + (i_{\operatorname{grad}_\gamma \phi}\alpha)dt\,,$$

where $\mathcal{L}_X^\top\alpha = \mathcal{L}_{X(t)}^\top\alpha(t)$ is the Lie derivative on the time slice at t. We will drop the superscript of $\mathcal{L}_X^\top$ if it is clear from the context what $\mathcal{L}_X$ denotes.

Using the last equation, we can compute the action of v on the metric,

$$\begin{aligned}\mathcal{L}_v g = \mathcal{L}_v(\gamma - \tfrac{1}{2}dt^2) &= \mathcal{L}_X\gamma + \phi\,\dot\gamma + (i_{\operatorname{grad}_\gamma \phi}\gamma)dt - d\phi\,dt \\ &= \mathcal{L}_X\gamma + \phi\,\dot\gamma\,.\end{aligned}$$

Note that the terms containing derivatives of ϕ cancel. Furthermore, we have

$$\mathcal{L}_\mathbf{n} g = -2K\,,$$

where $K(X,Y) = g(\nabla_X Y, \mathbf{n})$ is the second fundamental form with respect to $\mathbf{n}$ of the time slice at t. (See Section 9.3 of [46], but note that Wald's "extrinsic curvature" is the negative of the second fundamental form.) Thus, the Lie derivative of the metric with respect to a g-gaussian vector field is given by

$$\mathcal{L}_{X+\phi\mathbf{n}}g = \mathcal{L}_X\gamma + \phi\dot\gamma = \mathcal{L}_X\gamma - 2\phi K\,. \tag{14}$$

2.6. **The bracket and the anchor.** We can now make explicit the Lie algebroid structure on $A\mathcal{E}\Sigma \to \mathcal{U}\Sigma$ in terms of the trivialization $A\mathcal{E}\Sigma \approx \mathcal{U}\Sigma \times (\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma)$ given by gaussian extension.

Using (10), we find the Lie bracket of two g-gaussian vector fields to be:

$$[X + \phi\mathbf{n}, Y + \psi\mathbf{n}] = [X, Y] + \phi \operatorname{grad}_\gamma \psi - \psi \operatorname{grad}_\gamma \phi + (X \cdot \psi - Y \cdot \phi)\mathbf{n}\,, \tag{15}$$

which corresponds exactly to (4).

As for any bracket of vector fields, the jacobiator $[u, [v, w]] + [v, [w, u]] + [w, [u, v]]$ of three g-gaussian vector fields u, v, and w vanishes. However, the bracket of two g-gaussian vector fields is in general not g-gaussian, as the following proposition shows.

Proposition 2.11. *The bracket (15) of two g-gaussian vector fields is not always g-gaussian.*

Proof. We have

$$\begin{aligned}
i_{\mathbf{n}}\mathcal{L}_{[v,w]}g &= \mathcal{L}_{[v,w]}i_{\mathbf{n}}g + i_{[\mathbf{n},[v,w]]}g\\
&= d(g([v, w], \mathbf{n})) + i_{[v,[\mathbf{n},w]]}g + i_{[[\mathbf{n},v],w]}g\\
&= -d(X \cdot \psi - Y \cdot \phi) + i_{[v,\operatorname{grad}_\gamma \psi]}g - i_{[w,\operatorname{grad}_\gamma \phi]}g\\
&= -d(X \cdot \psi - Y \cdot \phi) + (\mathcal{L}_v i_{\operatorname{grad}_\gamma \psi} - i_{\operatorname{grad}_\gamma \psi}\mathcal{L}_v)g - (\mathcal{L}_w i_{\operatorname{grad}_\gamma \phi} - i_{\operatorname{grad}_\gamma \phi}\mathcal{L}_w)g\\
&= -d(X \cdot \psi - Y \cdot \phi) + \mathcal{L}_v d\psi - \mathcal{L}_w d\phi + i_{\operatorname{grad}_\gamma \phi}\mathcal{L}_w g - i_{\operatorname{grad}_\gamma \psi}\mathcal{L}_v g\\
&= i_{\operatorname{grad}_\gamma \phi}(\mathcal{L}_Y\gamma - 2\psi K) - i_{\operatorname{grad}_\gamma \psi}(\mathcal{L}_X\gamma - 2\phi K)\\
&= i_{\operatorname{grad}_\gamma \phi}\mathcal{L}_Y\gamma - i_{\operatorname{grad}_\gamma \psi}\mathcal{L}_X\gamma + 2i_{(\phi \operatorname{grad}_\gamma \psi - \psi \operatorname{grad}_\gamma \phi)}K\,.
\end{aligned}$$

In the second step, we have used that $i_{\mathbf{n}}g = -dt$. On the hypersurface $\Sigma \times \{0\}$, we may choose X, ϕ, Y, and ψ arbitrarily. For $X = Y = 0$ there, the right hand side of the last equation is the second fundamental form contracted with $\psi \operatorname{grad}_\gamma \phi - \phi \operatorname{grad}_\gamma \psi$, which is generally not zero. ☐

The anchor $A\mathcal{E}\Sigma \xrightarrow{\rho} T\mathcal{U}\Sigma$ of our Lie algebroid is given, up to a sign by the action computed in the previous section:

$$\rho(X, \phi, g) := -\mathcal{L}_{X(t)+\phi\mathbf{n}}g = -\mathcal{L}_{G_g(X,\phi)}\gamma - \phi\,\dot{\gamma}\,, \tag{16}$$

where $g = \gamma(t) - \frac{1}{2}dt^2$ is a gaussian metric on $\Sigma \times \mathbb{R}$ and $G_g(X, \phi) = X(t) + \phi\mathbf{n}$ is the g-gaussian extension of $X + \phi\mathbf{n}$. This Lie derivative represents the change in the "appearance" of the metric on the ambient manifold as the "viewpoint" changes according to a vector field $X + \phi\mathbf{n}$ along a space-like embedding. Note that the anchors of two constant sections are applied consecutively to a metric as $\rho(X, \phi)\rho(Y, \psi)(g) = \mathcal{L}_{G_g(Y,\psi)}\mathcal{L}_{G_g(X,\phi)}g$, that is, by applying the Lie derivatives of the gaussian extensions in reverse order. This takes care of the negative signs in Eq. (16).

The kernel of ρ consists of those (X, ϕ) whose g-gaussian extension is a Killing vector field. It follows that the dimension of this kernel is zero[10] over an open dense subset of $\mathcal{U}\Sigma$, since any Σ-universe is contained in a 1-parameter family whose generic members have no isometries. (Local perturbations of the lorentzian metric suffice to achieve this; deeper results in the riemannian case go back at least as far

[10]The dimension of the kernel of ρ is always finite; it is at most $\frac{1}{2}(n + 1)n + n + 1$, where $n = \dim \Sigma$, with equality only when g has constant sectional curvature.

as [17].) It follows immediately that the bracket on sections of the Lie algebroid $A\mathcal{E}\Sigma$ is determined by that on their images under the anchor (16). In particular, the bracket of constant sections (X, ϕ) and (Y, ψ) of the trivial bundle must be that given by given by Eq. (15):

$$[(X, \phi), (Y, \psi)] = ([X, Y] + \phi \operatorname{grad}_\gamma \psi - \psi \operatorname{grad}_\gamma \phi, X \cdot \psi - Y \cdot \phi)\,, \tag{17}$$

where we now evaluate X and ϕ at $t = 0$. Together with the anchor (16), this bracket determines the Lie algebroid structure on $A\mathcal{U}\Sigma$. To summarize, we have:

Theorem 2.12. *The Σ-evolutions $\mathcal{E}\Sigma$ form a groupoid over the Σ-universes $\mathcal{U}\Sigma$. Each orbit of this groupoid consists of all Σ-universes which are represented by Σ-spaces in a fixed spacetime (M, g). The Lie algebroid $A\mathcal{E}\Sigma$ has a natural identification with the trivial bundle $\mathcal{U}\Sigma \times (\mathcal{X}\Sigma \oplus \mathcal{F}\Sigma)$. Under this identification, in the gaussian representation of ambient metrics, the anchor is the Lie derivative by gaussian extensions: $\rho(X, \phi, g) = \mathcal{L}_{G_g(X,\phi)} g$. The bracket of constant sections is given by (17).*

2.7. **An equivalent groupoid and the moduli stack of spacetimes.** This section is peripheral to the main argument of this paper, but it suggests another point of view toward the groupoid $\mathcal{E}\Sigma$ of Σ-evolutions.

We have just seen that the orbits of $\mathcal{E}\Sigma$ are in one-to-one correspondence with isometry classes of Σ-adapted spacetimes, while the isotropy groups in $\mathcal{E}\Sigma$ are just the isometry groups of those spacetimes. It turns out that $\mathcal{E}\Sigma$ is equivalent to another groupoid in which Σ plays a much less central role. We only require that the spacetimes be Σ-adapted, without ever specifying the placement of Σ. For the notion of equivalence of groupoids, we refer to [10] and [34].

Definition 2.13. *The groupoid $\mathcal{I}\Sigma$ is defined to be that in which the objects are Σ-adapted spacetimes, and the morphisms are isometries between these spacetimes.*

Remark 2.14. Strictly speaking, $\mathcal{I}\Sigma$ is not a groupoid, since the spacetimes do not form a set. But it is equivalent to its wide subgroupoid consisting of isometries between those spacetimes whose underlying manifolds are submanifolds of euclidean spaces.

$\mathcal{I}\Sigma$ may be identified with an action groupoid whose objects are the elements of the collection $\mathcal{S}\Sigma$ of all Σ-adapted spacetimes (or, alternatively, a set as in the remark above). The groupoid acting on $\mathcal{S}\Sigma$ consists of the diffeomorphisms between these objects. If (M_1, g_1) is a Σ-adapted spacetime and Φ is a diffeomorphism to a manifold M_0 from M_1, then the result of acting on (M_1, g_1) by Φ is defined to be the spacetime $(M_0, (\Phi^{-1})^* g_1)$. Φ then becomes an isometry and so may be considered as a morphism in $\mathcal{I}\Sigma$.

Proposition 2.15. *The groupoids $\mathcal{I}\Sigma$ and $\mathcal{E}\Sigma$ are equivalent.*

Proof. An equivalence between groupoids is given by a biprincipal bundle, i.e. a space on which the groupoids have commuting free actions, with the fibres of the moment map[11] of each one being the orbits of the other. Such a bibundle induces

[11] An action of a groupoid G over G_0 on a space X includes as part of its data a map $G_0 \leftarrow X$ which determines which groupoid elements act on which elements of X. This map is sometimes called the **moment map** of the action.

bijections between the orbit spaces of the two groupoids and between the isotropy groups of corresponding objects.

To get an equivalence between $\mathcal{I}\Sigma$ and $\mathcal{E}\Sigma$, we take as total space of our bundle the collection $\mathcal{H}\Sigma$ of all Σ-spaces in all possible spacetimes.

The moment map for the left action of $\mathcal{I}\Sigma$ forgets the embedding and remembers only the target. The typical morphism in $\mathcal{I}\Sigma$ is an isometry $M' \xleftarrow{\psi} M$ between spacetimes. It acts on any Σ-space $M \overset{i}{\hookleftarrow} \Sigma$ to give the (equivalent) embedding $M' \overset{\psi\circ i}{\hookleftarrow} M$. This action is free because an isometry of a connected manifold which fixes a hypersurface and its normal bundle must be the identity.

The moment map for the right action of $\mathcal{E}\Sigma$ takes each $M' \overset{\psi}{\hookleftarrow} M$ to its equivalence class $[i]$. If $i \in \mathcal{HL}$ and $[i_1, i_0]$ are such that $[i] = [i_1]$, then we define the right action of $[i_1, i_0]$ on i as follows. The equivalence between $M \overset{i}{\hookleftarrow} \Sigma$ and $M' \overset{i'}{\hookleftarrow} \Sigma$ is realized by a unique isometry $M' \xleftarrow{\psi} M$ such that $\psi \circ i_1 = i$. Then $i \cdot [i_1, i_0]$ is defined to be the embedding $M' \overset{\psi\circ i_0}{\hookleftarrow} \Sigma$. To see that this action is free, suppose that $i \cdot [i_1, i_0] = i$. Then $M = M'$ and $\psi \circ i_0 = i = \psi \circ i_1$, so $i_1 = i_0$, and $[i_1, i_0]$ is an identity morphism.

The transitivity of the left action on the right moment fibres is just a restatement of the definition of equivalence used in defining the Σ-universes. Transitivity of the right action on the left moment fibres is obvious, since the morphisms in $\mathcal{E}\Sigma$ are (equivalence classes) of pairs of embeddings into the same target. $\square$

Remark 2.16. The notion of **stack** was introduced in algebraic geometry and has recently migrated to differential geometry [6]; the purpose of the notion is to provide a description of spaces of equivalence classes when it is important to keep track of the multiple ways in which objects can be equivalent and thereby to overcome difficulties related to singular behavior of quotient spaces. One way to understand stacks is to see them as **presented** by groupoids, where equivalent groupoids determine "the same" stack in the same sense that a given manifold may be described in different ways by overlapping families of coordinate charts.

The equivalence between $\mathcal{E}\Sigma$ and $\mathcal{I}\Sigma$ which we have just proven shows that we may consider $\mathcal{E}\Sigma$ as a presentation of the moduli stack of Σ-adapted spacetimes, i.e. the isometry classes (including information about self-isometries) of spacetimes admitting Σ as an "instantaneous space", or "initial condition". (Note that this is a purely "kinematic" construction, as we have not imposed any dynamical condition such as the vacuum Einstein equations.)

3. Discussion: the descent problem

We have constructed a groupoid over $\mathcal{U}\Sigma$ whose Lie algebroid bracket, for constant sections in a natural local trivialization, exactly matches the bracket relations on the constraints for Einstein's equations. To establish a more direct relation with the constraints themselves, we would need to find similar structures on the phase space $T^*\mathcal{M}\Sigma$.

There is a natural projection $\mathcal{P}$ to $T\mathcal{M}\Sigma$ from $\mathcal{U}\Sigma$, assigning to every Σ-universe the 1-jet with respect to t at $t = 0$ of its gaussian representation as a path in $\mathcal{M}\Sigma$. (Note that this is well defined even if the Σ-universe is not cylindrical.) But there is no way to push our Lie algebroid forward under this projection, essentially because the value of the anchor at a given 1-jet would have to depend on the 2-jet.

To surmount this difficulty, we tried to use a second-order evolution equation on $\mathcal{M}\Sigma$, i.e. a rule which expresses 2-jets in terms of 1-jets, such as the Einstein evolution equations themselves. But the resulting anchor was not consistent with the bracket relations.

We also tried "reverse engineering", *defining* the anchor so that it would take constant sections to the hamiltonian vector fields of the constraint functions. But the anchor so-defined, when applied to two constant sections associated to functions ϕ and ψ on M, generally takes their bracket as defined by the metric-dependent relations (4) to a vector field which is not even hamiltonian.

4. Some history

A hamiltonian formulation of general relativity can be found in the work of Pirani and Schild [37], aimed at the quantization of Einstein's gravitational field equations. These authors, as well as Bergmann, Penfield, Schiller, and Zatzkis [9] consider a physical state at a certain time to be given by data on a space-like hypersurface, which must in some sense be arbitrary in order to maintain four-dimensional covariance.

Bergmann [7] had by then already begun a systematic study of covariant field theories of general type, addressing the problem of bringing general relativity into the canonical form as a preliminary step to quantization. While canonical quantization of field theories was being developed, it soon became clear that general relativity posed additional difficulties connected with the degeneracy of the lagrangian which was a consequence of four-dimensional diffeomorphism invariance. In fact, Dirac's original work [15] on constrained dynamics was inspired in large part by this problem.

It was noted by Pirani, Schild, and Skinner [38] and not long after by Dirac [16] and Arnowitt, Deser, and Misner (ADM) [3] that great simplifications could be made at the expense of giving up four-dimensional symmetry. Such simplifications became possible by fixing a foliation of spacetime by space-like hypersurfaces, with the physical states living on these surfaces. Such a spacetime decomposition leads to the decomposition of vectors along each hypersurface into their normal and tangential components, and the metric tensor itself may be presented in the form

$$g^{(4)}_{\mu\nu} = \begin{pmatrix} N^2 + N_s N^s & N_n \\ N_m & g_{mn} \end{pmatrix},$$

where the lapse function N and the shift 3-vector N^n describe the variation of the time and space coordinates on infinitesimally close space-like hypersurfaces. The lapse and shift can be chosen arbitrarily but enter in the constraint equations, which arise from the degeneracy of the lagrangian and are given by time components of the Einstein field equations $G^{0\mu} = 0$. It had already been realized by Dirac and many others that the shift functions N_n generated coordinate transformations on the hypersurfaces, whereas the lapse N was related to time translation. In this sense, lapse and shift could be viewed as gauge potentials that had to be fixed in order to solve the initial value problem. The lapse and shift functions were first introduced in [2]. Their geometrical meaning was explained in [47] and in more global terms by Fischer and Marsden [18], who were perhaps the first authors to suggest that the constraints should be seen as something like a momentum map.

Still in search of avoiding the shortcomings of coordinate-dependent language, Kuchař [28] argued that field dynamics does not take place in spacetime, or along a single foliation of hypersurfaces but in what he called hyperspace, an infinite-dimensional manifold consisting of all the spacelike hypersurfaces in a given spacetime.

After the appearance of [16], Katz [26] found the formulas for the Poisson brackets of the constraint functions. In their space-integrated form, the brackets were first computed by DeWitt [14]. While the computation of the brackets was straightforward, their geometric interpretation was not satisfactory. A number of authors have tried to give a more conceptual derivation, e.g., by studying hypersurface deformations [45], as a method to guarantee the path-independence of geometrodynamical evolution [27], or by generalizing the concept of transformation groups [8] [47]. In particular, Teitelboim [45] was perhaps the first to show that the Poisson bracket relations are purely a consequence of the geometry of hypersurfaces in a riemannian or lorentzian manifold, independent of any particular field theory. In a sense, our paper may be seen as setting Teitelboim's argument in its proper mathematical setting, that of groupoids and Lie algebroids.

The most ambitious approaches aimed at recovering diffeomorphism covariance of the initial value problem [21] [24] [25] [29]. Parallel developments were also made by Wheeler [47]. Inspired by the dynamical description of the electromagnetic field in terms of the vector potential, he proposed to describe the dynamics of three-space metrics through the propagation of the intrinsic metric of space-like hypersurfaces with respect to a time coordinate. Such a time parameter would label the leaves the dynamically produced spacetime. In this approach the extrinsic curvature of these hypersurfaces corresponds to the canonical momenta. The configuration space of this theory is known as Wheeler's superspace. Trajectories of metrics in this space produce four-dimensional spacetime geometries.

Since the bracket of constraint functions is metric dependent, this suggested to Bergmann and Komar [8] that the associated symmetries could be metric-dependent as well. Their paper contains many ideas which are very close to ours, although the language is somewhat different. In particular, we would say that their "Q-type transformations" are precisely the bisections of the action groupoid (essentially our $\mathcal{I}\Sigma$, but without a specific choice of Σ), associated to the diffeomorphisms of a 4-manifold M acting on the function space of lorentzian metrics on M. Their infinitesimal transformations are the sections of the action Lie algebroid; their equation (3.1) is precisely the formula for the bracket of sections in this Lie algebroid! Bergmann and Komar also observe that the orbits are isometry classes and that the action fails to be faithful in the presence of isometries.

Bergmann and Komar even make the tantalizing statement, "That these transformations form a group, or at least a groupoid, is seen from their definition." Unfortunately, groupoids do not reappear anywhere in the paper, and it is not clear what notion of groupoid the authors had in mind. In particular, although [8] includes a discussion of the set of diffeomorphisms between hypersurfaces in spacetime (the infinitesimal transformations being 4-vector fields along these hypersurfaces), there is no suggestion that these form a groupoid.

The idea of associating the Q-type transformations with diffeomorphism invariance of general relativity appeared also in [11] where these transformations arise from "field dependent" gauge generators. These field dependent generators appeared also in [39], [40], [41], and [42], and more recently in [35].

Hojman, Kuchař, and Teitelboim [21] look at space-like embeddings into a fixed lorentzian manifold and find what is more or less the Lie algebroid bracket for the Lie algebroid of the groupoid of diffeomorphisms between hypersurfaces.

Finally, we should at least mention the immense analysis literature on existence theory, both local and global, for the Einstein initial value problem, beginning with fundamental work of Lichnerowicz [31] and Fourès-Bruhat (= Choquet-Bruhat) [19] and continuing to this day. (See [13] for a fairly recent survey.) We hope that our work provides new geometric understanding which may contribute to both the analysis and the quantization of the Einstein field equations.

Appendix A. Diffeology

Although some of the infinite-dimensional spaces of smooth mappings in this paper may be considered as Fréchet manifolds, this analytical structure is not necessary for formal computations. Instead, we work in the framework of diffeological spaces. These objects were introduced[12] by Souriau [43] and developed extensively by Iglesias [22] and others. We give a brief introduction to diffeology here and refer to [20], [30], and the work-in-progress [23] for further details. Similar notions in the topological setting are discussed in [4].

Roughly speaking, we can do a great deal of differential geometry on a set X once we know what it means for a family of elements of X to depend smoothly on parameters.

Definition A.1. *A* **parameter space** *is an open subset of $\mathbb{R}^n$ for some n, and a* **parametrization** *of a set X is a map to X from some parameter space P. A* **diffeology** *on X is a set $\mathcal{D}$ of parametrizations of X which contains all constant maps, which is closed under composition on the right with smooth (in the usual sense) maps between parameter spaces, and which is locally defined in the sense that a parametrization is in $\mathcal{D}$ if and only if its restrictions to all the sets in some open covering are. The elements of $\mathcal{D}$ are called* **plots***, or* **smooth parametrizations***. $(X, \mathcal{D})$ is called a* **diffeological space***; we denote it simply by X when it is clear what diffeology is being used. A plot $X \xleftarrow{\phi} P$ with $x = \phi(0)$ is called a* **plot at** *x.*

Remark A.2. In the language of sheaf theory, a diffeological space is a concrete sheaf on the site of open subsets of euclidean spaces [5]. This point of view is particularly well suited to show that the category of diffeological spaces has small limits (taken point-wise), small colimits (first taken point-wise, then sheafified), and exponential objects (given by the universal property), thus allowing for constructions such as quotient spaces, pull-backs, mapping spaces, etc. that generally fail to exist for smooth manifolds. For our purposes, however, we will need to give the explicit descriptions of these constructions.

Just as in topology, every set X carries the **discrete** diffeology, for which only the locally constant maps are plots, and the **coarse** diffeology, for which every parametrization is smooth. If X is a (finite-dimensional) manifold, the usual smooth maps to X from parameter spaces form the "standard" diffeology.

Diffeological spaces are the objects of a category in which the morphisms are the smooth maps, defined as follows.

[12] A very similar notion was introduced by Chen [12], and different notions of "smootheology" are compared in [44]

Definition A.3. *A map $X \xleftarrow{f} Y$ between diffeological spaces is a* **smooth map** *if $f \circ \phi$ is a plot for X whenever ϕ is a plot for Y. We denote the set of all such smooth maps by $C^\infty(X, Y)$. (Note that many authors denote it by $C^\infty(Y, X)$.) A smooth map with a smooth inverse is a* **diffeomorphism**.

A smooth map between manifolds with the standard diffeologies is just a smooth map in the usual sense. The parametrizations of any diffeological space which are smooth are just the plots, so the term "smooth parametrization" has an unambiguous meaning.

Any diffeological space $(X, \mathcal{D})$ carries the $\mathcal{D}$-topology, defined as the finest topology for which all plots are continuous; i.e., a subset $U \subseteq X$ is open [closed] if and only if $\phi^{-1}(U)$ is open [closed] for every plot ϕ. Smooth maps are always $\mathcal{D}$-continuous.

A product $X \times Y$ of diffeological spaces carries a **product diffeology**, whose plots are the parametrizations whose compositions with the projections to X and Y are smooth. Each subset of a diffeological space has a natural **subspace diffeology** in which the plots are those parametrizations whose composition with the inclusion is smooth. The restriction of a smooth map to any subset with the subspace diffeology is again smooth.

Any set $\mathcal{D}_0$ of maps to X from diffeological spaces **generates** the diffeology $\overline{\mathcal{D}_0}$ consisting of all those parametrizations which are locally compositions of the form $\phi \circ s$, where ϕ is in $\mathcal{D}_0$ and s is a parametrization of the domain of ϕ, together with all constant maps from parameter spaces. (The latter are already included if the images of the elements of $\mathcal{D}_0$ cover X.)

If $\mathcal{D}_0$ consists of a single surjective map $X \leftarrow Y$ from a diffeological space Y, the diffeology which it generates is called the **quotient diffeology**. Conversely, any diffeology is the quotient diffeology for the union of all its plots, considered as a single map defined on the disjoint union of the domains of the plots.

If X and Y are diffeological spaces, the **functional diffeology** on $C^\infty(X, Y)$ is that for which a parametrization $C^\infty(X, Y) \xleftarrow{\phi} P$ is a plot if and only if the corresponding evaluation map $X \leftarrow Y \times P$ is smooth. The "exponential law" $C^\infty(C^\infty(X, Y), Z)) \cong C^\infty(X, Y \times Z)$ then holds for all X, Y, and Z, not just in the defining case where Z is a parameter space, and the composition operations $C^\infty(X, Z) \leftarrow C^\infty(X, Y) \times C^\infty(Y, Z)$ are smooth.

The subspace diffeology construction produces diffeologies on spaces of mappings satisfying extra conditions, such as spaces of diffeomorphisms or embeddings, spaces of sections of smooth bundles (e.g. tensors), and solution spaces of ordinary or partial differential equations.

We can also define diffeologies on spaces of mappings with variable domains. For simplicity, we let these domains be subsets of a fixed space. Let $[Y]$ be some collection of subsets of a diffeological space Y (for instance the open subsets, if Y carries a topology), and let $C^\infty(X, [Y])$ be the set of all mappings to X whose domains belong to $[Y]$. Thinking of a parametrization $C^\infty(X, [Y]) \leftarrow P$ as a family $X \xleftarrow{f_p} Y_p$ of maps parametrized by $p \in P$, we call it a plot when the evaluation map $X \leftarrow D \subseteq Y \times P$ is smooth, where the domain $D = \{(y, p) | y \in Y_p)\}$ carries the subspace diffeology. When Y is a manifold and $[Y]$ consists of the open subsets, it may be appropriate to restrict the diffeology to consist of those families for which the domain D is open in $Y \times P$, so that we are always dealing with maps defined on manifolds. In this case, we denote the space of mappings by $C^\infty(X, Y_{\mathrm{open}})$. In particular, if X is a single point, we obtain a diffeology on the set of open subsets of Y.

Example A.4. If Σ is any manifold, the space $\mathcal{M}\Sigma$ of riemannian metrics on Σ carries a functional diffeology. So does $\mathcal{M}\Sigma_{\text{open}}$, the metrics defined on open subsets of Σ.

If the diffeological space Y carries a topology (not necessarily the $\mathcal{D}$-topology), $C^\infty(X,Y)$ also carries the "finer" **compact functional diffeology** in which the plots $C^\infty(X,Y) \overset{\phi}{\leftarrow} P$ are required to satisfy the additional condition that each $p \in P$ has a neighborhood $\mathcal{V}$ for which all the maps in $\phi(\mathcal{V})$ agree outside some compact subset of Y. $C^\infty(X,Y)$ with this diffeology is denoted by $C_c^\infty(X,Y)$.

A.1. **Jets and tangent vectors.** To define jets in diffeology, we start with the basic case of parameter spaces. For $k = 0, 1, 2, \ldots, \infty$, and smooth maps s and t to $\mathbb{R}^n$ from a parameter space P containing 0, s and t are defined to have the same k-jet at 0 if $s(0) = t(0)$ and if their partial derivatives through order k match at 0. Plots f and g to a diffeological space X from P will be said to have the same k-jet at 0 if there is a plot $X \overset{h}{\leftarrow} Q$ such that $f = h \circ s$ and $g = h \circ t$, where s and t are plots for Q the same k-jet at 0. Finally, for any diffeological spaces X and Y, two maps $X \leftarrow Y$ have the same k-jet at $y \in Y$ if their compositions with any plot at y have the same k-jet at 0. (It is easy to see that, if X and Y are parameter spaces, this coincides with the original definition.)

Having the same k-jet at y is an equivalence relation $\sim_y^k$, and two maps with the same germ at y have the same k-jet there for any k. We thus obtain an equivalence relation on germs, and we define the space $J^k(X,Y)$ of k-jets of maps to X from Y to be the set of pairs $(j_y^k f, y)$, where f is the germ of a map to X from some neighborhood of y in y, and $j_y^k f$ is the equivalence class of f for $\sim_y^k$.

If $K \subset Y$, we say that $f \sim_K^k g$ if f and g have the same k-jet at all points of K, and we call the equivalence classes for this relation k-jets along k. If X is a bundle over Y, we may refer to the k-jets of those maps $Y \leftarrow X$ which happen to be sections of the bundle as k-jets of sections.

We define diffeological structures on jet bundles by considering them as quotients of spaecs of mappings, using the functional diffeology. When $k = \infty$ and X and Y are manifolds, the sheaf diffeology is also interesting, since the smooth maps are maps into the leaves of a foliation.

Since constant maps are always smooth, and the 0-jets of maps are just their values, there is a natural identification of $J^0(X,Y)$ with $X \times Y$. There are also natural maps $J^k(X,Y) \leftarrow J^l(X,Y)$ for $k \le l$. For $k = 0$, this gives natural projections of the jet spaces to X and Y. That the infinite jet space $J^\infty(X,Y)$ is the inverse limit of the jet spaces for finite k.

Jets of mappings into mapping spaces are mappings into jet bundles. If X, Y, and Z are manifolds, smooth maps $C^\infty(X,Y) \overset{f}{\leftarrow} Z$ correspond to smooth maps $X \overset{F}{\leftarrow} Y \times Z$. It follows that $J^k(C^\infty(X,Y),Z) = C^\infty(J^k(X,Z),Y)$.

Of special importance are the 1-jets at 0 of maps to X from neighborhoods of 0 in $\mathbb{R}$; these are the tangent vectors. We denote the set of all tangent vectors to X by TX and call it the **tangent cone bundle** of X. It is the disjoint union of tangent cones T_xX at the points of X, which are cones because reparametrization of curves by the action of the multiplicative group $\mathbb{R}\backslash\{0\}$ on $\mathbb{R}$ leads to a natural action of this group on the tangent spaces. TX has a diffeological structure and projection to X inherited from those on $J^1(X, \mathbb{R})$.

For mapping spaces between manifolds, the general result above on jet bundles gives, with $Z = \mathbb{R}$ and $k = 1$, $TC^\infty(X, Y) = C^\infty(TX, Y)$. The tangent bundle projection $C^\infty(X, Y) \leftarrow TC^\infty(X, Y)$ is just composition with the projection $X \leftarrow TX$.

Two warnings are in order. First of all, the action of $\mathbb{R}\backslash\{0\}$ on the tangent cone may not be faithful. For instance, if X is the half-line $[0, \infty)$ viewed as $\mathbb{R}/\mathbb{Z}_2$ with the quotient diffeology, its tangent cone at 0 is also a half-line on which multiplication by -1 is the identity. Second, it is generally not possible to add 1-jets of curves. If it were, we would find that adding a vector v at 0 in $\mathbb{R}/\mathbb{Z}_2$ to itself would give both $2v$ and 0. Another example where addition is not possible is the tangent cone at 0 to the union of the coordinate axes in $\mathbb{R}^2$ with the subspace diffeology.

An example where all the tangent cones are zero is the space $[Y]_{\text{open}} = C^\infty(\{p\}, [Y])_{\text{open}}$ of open subsets of a manifold Y. A path in $[Y]_{\text{open}}$ is just an open subset of $I \times Y$ for some interval I of real numbers. If U_s is any such path defined around $s = 0$, it has the same tangent vector as the constant path through U_0. In fact, they factor via curves tangent at 0 through the plot on $I \times \mathbb{R}$ defined by $U_{(s,0)} = U_s$, $U_{(s,s^2)} = U_0$, and $U_{(s,s')} = Y$ elsewhere. Similarly, tangent vectors to spaces $C^\infty(X, [Y])_{\text{open}}$ are insensitive to the variation of domain with s and may all be represented by families of functions with unchanging domains. The same arguments apply to jets of any order.

Example A.5. For the space $\mathcal{M}\Sigma_{\text{open}}$ of riemannian metrics defined on open subsets of Σ, the tangent space at a metric g defined on all of Σ consists of the smooth symmetric covariant 2-forms on Σ, even though the domain of a path through g may shrink as the path parameter varies.

It is possible to define a tangent vector *space* at each point of a diffeological space by taking formal linear combinations of 1-jets of curves, as in [20], but it is then necessary to introduce further relations, so that, for instance, the tangent space at the conical singular point 0 of the space $\mathbb{R}/\mathbb{Z}_2$ reduces to zero, while the tangent cone does not. (On the other hand, the tangent space at the intersection point in the union of the coordinate axes in the plane is two-dimensional.)

For a diffeological group, group multiplication induces a a vector space structure on each tangent cone [30].

Cotangent spaces to diffeological spaces may be defined as spaces of 1-jets of smooth mappings to $\mathbb{R}$; these all have vector space structures derived from that on $\mathbb{R}$. The composition of real-valued functions with curves defines a natural pairing (which can be degenerate) between tangent and cotangent spaces.

If N and E are manifolds and p is a submersion, then the finite jet spaces $J^k(Y, E)$ are also smooth manifolds with submersions to Y, and the infinite jet space $J^\infty(Y, E)$ carries the projective limit diffeology in which a map into it is smooth if all of the compositions with projections into finite jet spaces are smooth.

A.2. **Diffeological groupoids.** Diffeological groupoids are defined like topological groupoids [22][23]. Recall that a category C consists of a collection C_0 of objects and a collection C_1 of morphisms, with target and source maps l and r to C_0 from C_1, a unit inclusion map $C_1 \xleftarrow{\epsilon} C_0$, and a composition map to C_1 from $C_2 = \{(f, g) \in$

$C_1 \times C_1 | r(f) = l(g)\}$, satisfying the usual axioms for associativity and units. A **groupoid** is a category[13] in which every morphism is invertible.

If C_0 and C_1 are diffeological spaces, we give $C_2 \subseteq C_1 \times C_1$ the subspace diffeology. If all of the structure maps are smooth, we say that C is a diffeological category. If C is, in addition, a groupoid, and the map ι which takes each morphism to its inverse is smooth, then C is a **diffeological groupoid**. Note that we do not require l and r to be submersions; in fact, this notion is better replaced with that of "subduction" [23] in the diffeological case. But if a diffeological groupoid C is a manifold and l and r are submersions, then C is a Lie groupoid in the usual sense.

Defining the Lie algebroid of a Lie groupoid is not so simple, even when C_0 is a single point, in which case C_1 is a diffeological group. A "Lie algebra" bracket for such a group G is defined in [20] using the conjugation operation of G on itself. It is a bilinear operation on the tangent (vector) space T_eG at the identity, but antisymmetry and the Jacobi identity have been established in [30] under some extra assumptions on T_eG, holding for example in the case where G is the group of diffeomorphisms of a manifold M with the functional diffeology. In this case, T_eG is, as expected, the space $\mathcal{X}M$ of vector fields on M, and the bracket is the usual Lie algebra bracket.

If we replace M above by a diffeological space X, it is no longer even clear that inversion is smooth in the group of diffeomorphisms, though this is the case for many X. We can always define a stronger diffeology by admitting as plots only those whose composition with inversion is a plot in the functional diffeology. The tangent space at the identity may be identified with those vector fields which are tangent to paths of diffeomorphisms.

Let G be a diffeological groupoid, and let $B(G)$ be its group of bisections, i.e. smooth sections γ of r for which $l \circ \gamma$ is a diffeomorphism. We give $B(G)$ the diffeology in which the plots are those plots for the subspace-functional diffeology for which composition with inversion is also a plot. The tangent space to the identity then consists of smooth maps $TG_1 \xleftarrow{a} G_0$ lifting the unit section ϵ which are tangent to smooth paths through the identity in $B(G)$. The values of a are tangent to the r-fibres, so it is natural to consider them as sections of the "bundle" $A(G)$ over G_0 which is the pullback by ϵ of $\ker Tr$. Without further assumptions, $A(G)$ is not a vector bundle, but it should still play the role of the Lie algebroid. To get a bracket operation, we follow [20] and [30] and use the natural action of the group $B(G)$ on $A(G)$. Its derivative at the identity with respect to the first variable gives a binary operation $[a, b]$ on sections of $A(G)$, defined *a priori* only when a is **admissible** in the sense of being tangent to a path in $B(G)$. In addition, there is an anchor which takes admissible sections of $A(G)$ to admissible vector fields, i.e. admissible sections of TG_0.

Since the action of $B(G)$ preserves all the structures in sight, the operation of bracketing on the left by an admissible section is a derivation with respect to both the bracket itself and multiplication by functions. In other words, we have: $[a, fb] = f[a, b] + (\rho(a)f)b$ for admissible a, functions f, and all sections b, and $[a, [b, c]] = [[a, b], c] + [b, [a, c]]$ for admissible a, b, and c.

[13] Many authors require a groupoid to be a **small** category, in the sense the morphisms and objects form sets rather than just collections. We will not make this assumption, but will occasionally point out how to replace "large" groupoids by small ones.

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