The symplectic 2-form for gravity in terms of free null initial data

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Abstract
A hypersurface $\mathcal{N}$ formed of two null sheets, or ‘light fronts’, swept out by the future null normal geodesics emerging from a common spacelike 2-disc can serve as a Cauchy surface for a region of spacetime. Already in the 1960s, free (unconstrained) initial data for general relativity were found for such hypersurfaces. Here, an expression is obtained for the symplectic 2-form of vacuum general relativity in terms of such free data. This can be done, even though variations of the geometry do not in general preserve the nullness of the initial hypersurface, because of the diffeomorphism gauge invariance of general relativity. The present expression for the symplectic 2-form has been used previously (Reisenberger 2008 Phys. Rev. Lett. 101 211101) to calculate the Poisson brackets of the free data.

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1. Introduction
Free (unconstrained) initial data for general relativity (GR) on certain piecewise null hypersurfaces have been known since the 1960s [Sac62, Dau63, Pen63]. In this work, the symplectic 2-form corresponding to the Einstein–Hilbert action for vacuum GR is expressed in terms of such free data on a so-called double null sheet, a compact hypersurface $\mathcal{N}$, consisting of two null branches, $\mathcal{N}_L$ and $\mathcal{N}_R$, that meet on a spacelike 2-disc $S_0$ as shown in figure 1. $\mathcal{N}_L$ and $\mathcal{N}_R$ are swept out by the two congruences of future null normal geodesics (called generators) emerging from $S_0$, and are truncated on discs $S_L$ and $S_R$ respectively before the generators form caustics. With this symplectic 2-form the space of valuations of the free data becomes a phase space, which, among other things, may serve as a starting point for quantization.

In most initial value formulations of GR, the initial data are subject to constraints, which complicates canonical formulations based on those data. In fact, at present the handling of the constraints absorbs most of the effort invested in canonical approaches to quantum gravity. A canonical formulation based on free initial data is thus of considerable interest.
To be sure, null data are not the only way to obtain a constraint-free canonical theory. York [York72] has identified spacelike free initial data and set up a canonical theory on spacelike hypersurfaces of uniform mean extrinsic curvature in which the most difficult constraint, the scalar constraint, has been eliminated (see [CBY80]).

A canonical framework based on null hypersurfaces is, however, especially suited for addressing certain issues. In particular, the canonical framework obtained here and in [Rei08] seems ideal for attempting a semi-classical proof of Bousso’s formulation of the holographic entropy bound [Bec73, tHoo93, Sus95, Bou99] (provided the generators are not expanding at $S_0$). It also seems a good classical starting point for a search for a quantization of GR respecting this entropy bound; that is, a quantization in which the area of $S_0$ has a discrete spectrum and each eigensubspace is of finite dimension, bounded by the exponential of the maximum entropy of $N_L$ and $N_R$ together according to Bousso’s bound, i.e. by $\exp(Area(S_0)/2\text{Planck area})$. (For Bousso’s bound to apply to both branches of $N$, the generators on both sides of $S_0$ must be non-expanding. Although this seems odd, such $S_0$ are in fact easily constructed even in flat spacetime. For example, take $S_0$ to be a portion of the intersection of two past light cones.)

In [Rei08] and the preprint [Rei07], the symplectic 2-form, $\omega_N$, was used to calculate the Poisson brackets between free initial data on $N$. The main aim of the present work is to provide a detailed derivation of the expression for $\omega_N$ that was used. The symplectic 2-form at a solution metric $g$ takes as arguments two variations $\delta_1$ and $\delta_2$ belonging to the space $L_g$ of smooth solutions to the field equations linearized about $g$. The expression for $\omega_N[\delta_1, \delta_2]$ in terms of free null initial data obtained here is valid for all ‘admissible’ $\delta_1$ and $\delta_2$. Admissible variations preserve the null character of the branches of $N$ and some other structures associated with $N$. Because of diffeomorphism gauge invariance the expression also holds in a slightly indirect way for a much larger class of variations. If $\delta_1, \delta_2 \in L_g$ and $\delta_2 g_{ab}$ vanishes in a spacetime neighbourhood of $\partial N$, then there exist corresponding admissible variations $\delta'_1$ and $\delta'_2$ such that $\omega_N[\delta_1, \delta_2] = \omega_N[\delta'_1, \delta'_2]$. The symplectic form on $\delta_1$ and $\delta_2$ may therefore be expressed in terms of the variations of the free null initial data under $\delta'_1$ and $\delta'_2$. This suffices for the purpose of obtaining a Poisson bracket between the initial data.

To understand this let us briefly review how the Poisson bracket is obtained in [Rei08]. On a finite-dimensional phase space with a non-degenerate symplectic
2-form, the Poisson bracket is determined by the inverse of this 2-form. In the case of initial data for GR on $\mathcal{N}$, subtleties arise, both because $\mathcal{N}$ has boundaries, and because the data have infinitely many degrees of freedom. In an infinite-dimensional phase space, a non-degenerate symplectic 2-form can fail to have an inverse defined on the whole cotangent space because it does not map onto all of this space. This is the case here. The inverse of the symplectic 2-form does not define Poisson brackets between all modes of the initial data. (A point of terminology: in the present work the requirement of non-degeneracy is not part of the definition of the term 'symplectic 2-form'. Pre-symplectic 2-forms are therefore termed symplectic 2-forms here.)

This led the author to look for a new starting point. The Peierls bracket [Pei52] is an alternative expression for the Poisson bracket which does not depend directly on the symplectic 2-form. The Peierls bracket between two functionals of spacetime fields is given by a very simple expression in terms of the first-order perturbations to the solutions of the field equations occasioned by adding these functionals to the action. Its simplicity and its direct relation to the quantum commutator give it a good claim to being a more fundamental definition of the Poisson bracket than the one in terms of the symplectic 2-form. Furthermore, it agrees with the latter definition when both are defined [Pei52, DeW03, Rei07].

Unfortunately, the Peierls bracket between data on $\mathcal{N}$ is ambiguous, because the perturbation generated by a functional of data on a characteristic hypersurface is discontinuous precisely at the hypersurface itself. The Peierls bracket is well defined on what we will call observables, diffeomorphism invariant functionals $F[g]$ of the metric, with smooth functional derivatives $\delta F/\delta g_{ab}$ of compact support contained in the interior of the causal domain of dependence of $\mathcal{N}$.1 (In [Rei07], a wide class of examples of observables in this sense is constructed, which determines the spacetime geometry of the domain of dependence, at least for generic geometries.)

The approach of [Rei08, Rei07] is to look for a Poisson bracket $\{\cdot, \cdot\}_\bullet$ on initial data that reproduces the Peierls brackets between observables. In [Rei07], it is shown that to ensure this match between the $\bullet$ bracket and the Peierls bracket (in a spacetime with metric $g$ satisfying the field equations) it is sufficient to require that

$$\delta A = \omega_{\mathcal{N}}([A, \cdot]_\bullet, \delta), \quad (1)$$

for any observable $A$ and any $\delta$ in the space $L^0_0$ of smooth variations which satisfy the field equations linearized about $g$ and vanish in a spacetime neighbourhood of $\partial \mathcal{N}$.

When both sides of (1) are expressed in terms of the initial data on $\mathcal{N}$ it becomes a condition on the Poisson brackets of these data. (In fact, this condition is nothing but a suitably weakened form of the requirement that the Poisson bracket be inverse to the symplectic 2-form.) To express (1) in terms of initial data, we need an expression for the symplectic 2-form in terms of initial data, but only in the case that one variation, $\delta$, vanishes in a neighbourhood of $\partial \mathcal{N}$. In this case, the symplectic 2-form can be expressed in terms of null initial data. So can the variations of $A$. Thus, (1) does indeed reduce to a condition on the Poisson brackets of null initial data.

Sachs [Sac62] and Dautcourt [Dau63] showed formally that any valuation of their null initial data on $\mathcal{N}$ determines a matching solution which is unique up to diffeomorphisms. This is the basis of their claim that their data, which are equivalent to the data we will use, are free and complete. And, of course, it is the basis of the program of canonical GR in terms of these null initial data. Because their analyses do not address convergence issues these do not give a

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1 The causal domain of dependence $D[S]$ of a set $S$ in a Lorentzian signature spacetime is the set of all points $p$ such that every inextendible causal curve through $p$ intersects $S$. In relativistic field theories, in which signals travel no faster than light, one expects that initial data on a closed achronal hypersurface $S$ determines the solution in $D[S]$. See [Wald84].
clear indication of the domain on which the solution exists or is unique. It seems reasonable to expect that the data in fact determine a maximal Cauchy development of \( \mathcal{N} \), but what has been demonstrated rigorously so far is that a solution matching the data exists and is unique in some neighbourhood of \( S_0 \) in the future of \( \mathcal{N} \). It has not been established that there is always a development of all of \( \mathcal{N} \).

It is therefore worth noting that the existence and uniqueness of Cauchy developments of the data is not strictly necessary for the results of this work. The space of data, the symplectic 2-form, and the Poisson bracket on the data found in [Rei08], are all defined independently of Cauchy developments. Indeed, it is possible, and perhaps fruitful, to define a phase space of initial data on just a single branch of \( \mathcal{N} \), even though the data on a single branch cannot by itself define a Cauchy development.

Given that free null initial data for GR have been available for such a long time the question arises as to why a canonical framework based on such data was not developed sooner. In fact, canonical GR using constrained data on double null sheets has been developed by several researchers [Tor85, GRS92, GS95, d’ILV06], and an expression for the symplectic 2-form that was important for the development of this work was given by Epp [Epp95]. Also, partial results have been obtained on the Poisson brackets of free data [GR78, GS95]. In [GR78], Gambini and Restuccia give perturbation series in Newton’s constant for the brackets of free data living on the bulk of \( \mathcal{N} \), but no brackets for other (necessary) data that live on the intersection surface \( S_0 \). Their results are consistent with the present work and were indeed crucial for its genesis. In [GS95], Goldberg and Soteriou present distinct free data on the bulk of \( \mathcal{N} \), which are claimed to form a canonically conjugate pair on the basis of a machine calculation of their Dirac brackets. It would be interesting to see if they are conjugate according to the symplectic structure obtained here.

There is however a conceptual issue which seems to have discouraged many researchers from trying to develop null canonical theory. Namely the problem of generator crossings and caustics. This problem is actually much less serious than it seems. Let us briefly examine the problem and its solution. Although it is not relevant to the main task of this paper, which is to express the symplectic 2-form in terms of free initial data, it is relevant to the viability of the over-all program of developing a canonical formulation of GR based on these free null initial data.

The problem is the following. Suppose a double null sheet \( \mathcal{N} \) is constructed in a given solution spacetime \( M \). It can easily happen that the generators that sweep out \( \mathcal{N} \) pass through a caustic and/or cross if extended far enough. See figure 2. Once this occurs the generators enter the chronological future of \( \mathcal{N} \) (see [Wald84] theorem 9.3.8). In fact, the segments of the generators beyond caustic or crossing points enter the interior of the domain of dependence of \( \mathcal{N} \). The portion of \( \mathcal{N} \) composed of these segments lies in the domain of dependence of the remainder of \( \mathcal{N} \). See appendix B of [Rei07]. The initial data on part of \( \mathcal{N} \) will thus be determined by the solution defined by the data on the rest of \( \mathcal{N} \), which constitutes a highly complex constraint on data which were supposed to be free. (This argument supposes that the solution matching the data is unique on the whole domain of dependence, which has not been established. However, the solutions to the linearized field equations are certainly unique on this domain, and this already precludes independent continuous variations of the data on the part of \( \mathcal{N} \) lying in the interior of the domain of dependence.)

Thus, one would apparently wish to exclude initial data corresponding to hypersurfaces containing caustics and crossings from the phase space. A condition excluding caustics is easily found, but it seems to be much more difficult to exclude non-caustic crossing points. One could imagine imposing some sort of non-local inequality, which would of course rob the phase space of free initial data of its simplicity.
Figure 2. (a) A simple example of a caustic and intersections of generators in \(2+1\) Minkowski space: \(S_0\) is a spacelike curve having the shape of a half racetrack—a semicircle extended at each end by a tangent straight line. The congruence of null geodesics normal to \(S_0\) and directed inward and to the future sweep out \(N_R\), which takes the form of a ridge roof, terminated by a half-cone over the semicircle. The generators from the semicircle form a caustic at the vertex of the cone. There neighbouring generators intersect. On the other hand, generators from the two straight segments of \(S_0\) cross on a line (the ridge of the roof) starting at the caustic, but the generators that cross there are not neighbours at \(S_0\). Clearly, the generator segments beyond the crossing points enter the interior of the domain of dependence of \(N\). (b) The double null sheet defined by \(S_0\) in the covering space is shown, with the points that are identified in the original spacetime indicated.

In fact this is unnecessary. Once caustics have been excluded from \(N\) any further crossing points can be ‘unidentified’ because there exists an isometric covering spacetime in which the generators do not cross, formed by pulling the metric back to the normal bundle of \(S_0\) via the exponential map. (See appendix B of [Rei07].) In this new spacetime, no constraint forbids the independent variation of the free initial data on all parts of \(\mathcal{N}\). Of course, once the data are changed there is no guarantee that the spacetime regions that were unidentified in going to the covering spacetime are still isometric, so it may no longer be possible to identify them. The complicated constraints arising from generator crossings in the original spacetime are precisely the conditions that must be met in order that the isometry of these regions be maintained. They are not constraints that must be satisfied in order that a solution matching the data exists.

(It is worth noting that the same issue arises in the spacelike Cauchy problem, and is resolved in the same way. Spacelike hypersurfaces that enter the interior of their own domains of dependence are easily constructed in any solution spacetime \(M\). But the unique maximal Cauchy development of the initial data induced from \(M\) on such a hypersurface is a covering manifold of the original domain of dependence, in which the hypersurface is achronal.)

We are thus led to the following simple and plausible picture. Any valuation of the free data without caustics on \(\mathcal{N}\) possesses a Cauchy development satisfying Einstein’s equations. The Cauchy developments of a subset of valuations of the initial data, which satisfy certain complicated conditions, have isometries which allow the identification of regions so that the generators of \(\mathcal{N}\) cross in the resulting spacetime. Note that we have not proved that this picture is correct. That requires a proof of the existence of solutions matching the free data throughout \(\mathcal{N}\), which is not yet available. What has been shown is that the possibility of generator crossings does not represent an obstruction to this picture, nor even an argument against it.

This resolution of the problem of generator crossings suffices for the development of a simple and meaningful canonical theory based on null initial data. However, it does not mean
that generator crossings are always to be regarded as unphysical. In many applications, one surely would have to deal with them. But even in such cases a canonical framework based on Cauchy developments in which all generator crossings have been unidentified might provide a useful perspective.

A different conceptual issue, which is directly relevant to the calculation of the symplectic 2-form, is the following. The symplectic 2-form is a bilinear on perturbations of the metric satisfying the linearized field equations. Generically, such perturbations do not preserve the null character of the branches of \( \mathcal{N} \). (In our formalism, \( \mathcal{N} \) is a fixed hypersurface in spacetime, the branches of which are null according to the unperturbed metric but of course not, in general, with other metrics.) How then are these perturbations to be represented by the variations of null initial data? The key is the diffeomorphism gauge invariance of GR. Roughly speaking, to each perturbation there corresponds a gauge equivalent one which does preserves the nullness of the branches of \( \mathcal{N} \), and so can be expressed in terms of the variations of null initial data. This is only approximately correct. As we shall see, the precise resolution of the problem is rather delicate because not all diffeomorphisms are gauge in the sense of being degeneracy vectors of the symplectic 2-form.

The remainder of the paper is organized as follows. In the following section, the free initial data that will be used are defined using a convenient chart on each of the branches of \( \mathcal{N} \). These data are shown to be equivalent to Sachs’s data, and thus free and complete to the extent that Sachs’s is. In section 3, an expression for the symplectic 2-form on an arbitrary hypersurface corresponding to the Einstein–Hilbert action is obtained in terms of the 4-metric and its variations. A large class of infinitesimal diffeomorphisms is shown to be gauge in subsection 3.1. Section 4 is dedicated to expressing the symplectic 2-form in terms of the null initial data. In subsection 4.1, it is shown how diffeomorphism gauge invariance can be exploited to express the symplectic 2-form in terms of null initial data, on the class of variations that enter in the calculation of the Poisson bracket, and indeed to express all of equation (1) defining the bracket in terms of null initial data. Subsection 4.2 is a discussion of the role of the so-called diffeomorphism data. In subsection 4.3, some important charts are defined. In subsection 4.4, the symplectic potential is expressed in terms of the free null initial data. Finally, in subsection 4.5 the symplectic 2-form is obtained in terms of these data. An appendix treats variations in fixed and moving charts.

2. The free data

2.1. Coordinates on \( \mathcal{N} \)

A special chart \((v^A, \theta^1, \theta^2)\) will be used on each branch \( \mathcal{N}_A \) (\( A = L \) or \( R \)) of \( \mathcal{N} \). In this chart, \( v^A \) is a parameter along the generators and \( \theta^p \) (\( p = 1, 2 \)) is constant along these. Since \( \partial_{v^A} \) is tangent to the generators it is null and normal to \( \mathcal{N}_A \). The line element on \( \mathcal{N}_A \) thus takes the form

\[
\text{d}s^2 = h_{pq} \text{d}\theta^p \text{d}\theta^q, \tag{3}
\]

Proof. Suppose \( t \) is tangent to \( \mathcal{N}_A \) at \( p \in \mathcal{N}_A \). Then, \( t \) may be Lie dragged along \( n_A = \partial_{v^A} \) to the whole generator through \( p \), staying always tangent to \( \mathcal{N}_A \). The resulting field satisfies

\[
\partial_{v^A}(n_A \cdot t) = [V_{v^A}t] \cdot n_A + [V_{\partial_{v^A}}n_A] \cdot t. \tag{2}
\]

The first term on the right vanishes since \([V_{v^A}t] \cdot n_A = [V_{\partial_{v^A}}n_A] \cdot n_A = 1/2V_{\partial_{v^A}}^2 = 0\), and, because the generators are geodesics, the second term reduces to \( \alpha n_A \cdot t \) with \( \alpha \) a scalar measuring the non-affineness (i.e. acceleration) of the parameter \( v^A \). Thus, \( \partial_{v^A}(n_A \cdot t) = \alpha n_A \cdot t \). But \( n_A \cdot t \) vanishes at \( S_0 \), since there \( t \) is a linear combination of \( n_A \) and a tangent to \( S_0 \), which are both normal to \( n_A \)—the normal null to \( S_0 \). It follows that \( n_A \cdot t \) vanishes also at \( p \). \( \square \)
with no \( dv \) terms. The coordinate \( v^A \) is taken proportional to the square root of \( \rho \equiv \sqrt{\text{det} h_{\theta\theta}} \), the area density in \( \theta \) coordinates on 2D cross sections of \( N_A \), and normalized to 1 at \( S_0 \). Thus, \( \rho = \rho_0 (\theta^1, \theta^2) v^2 \), with \( \rho_0 \) being the area density on \( S_0 \). We will call \( v \) the area parameter. (The index \( A \) specifying the branch \( N_A \) of \( N \) to which a quantity belongs will often be dropped when there is little risk of confusion.)

Note that \( h_{pq} = \rho_0 v^2 e_{pq} \), with \( e_{pq} = h_{pq}/\rho \) being a symmetric, unit determinant, \( 2 \times 2 \) matrix. This matrix will be called the conformal 2-metric, and will be our principal free initial datum.

The area parameter is related to affine parameters on the generators by the vacuum Einstein equation contracted with the tangents of the generators, \( R_{\theta\theta} = R[\partial_\theta, \partial_\theta] = 0 \). Suppose \( \eta \) is an affine parameter along the generators of \( N_A \). Then, because of this field equation and because the generators are surface forming, the Raychaudhuri equation ([Wald84], equation (9.2.32)) reduces to the focusing equation
\[
\frac{d}{d\eta} \left( \frac{\rho}{\rho_0} v^2 \right) = -\frac{1}{2} \left( \frac{\rho}{\rho_0} v^2 \right)^2 - \sigma_{pq} \sigma_{pq},
\]
(4)
where \( \sigma_{pq} = \frac{1}{\rho^2} e_{pq} \sigma_{\theta\theta} = -\frac{1}{2 \rho} \frac{\partial}{\partial \eta} e_{pq} \), (5)
and that
\[
\sigma_{pq} = h_{pq} h^{st} \sigma_{st} = -\frac{1}{2 \rho} \frac{\partial}{\partial \eta} e_{pq},
\]
where \( e_{pq} \) is the inverse of \( e_{pq} \), not \( e_{pq} \) with indices raised using \( h \). Substituting these expressions into (4) one finds
\[
\frac{\partial^2}{\partial \eta^2} \ln v + \left( \frac{\partial}{\partial \eta} \ln v \right)^2 = \frac{1}{2} \frac{\partial}{\partial \eta} e_{pq} \frac{\partial}{\partial \eta} e_{pq}.
\]
Finally, changing the variable of differentiation to \( v \) we obtain
\[
\frac{d}{dv} \ln \frac{d\eta}{dv} = -\frac{v}{8} \frac{\partial}{\partial \eta} e_{pq} \frac{\partial}{\partial \eta} e_{pq}.
\]
This is the key equation that relates our initial data to Sachs’ [Sac62] free initial data.

Using \( v \) as a coordinate makes avoiding caustics easy. At caustic points \( v^2 = \rho / \rho_0 \) vanishes, so the caustic free \( N \) are represented by initial data on coordinate domains in which \( v > 0 \).

On the other hand, \( v \) is not always a good parameter on the generators. For instance, it fails in the important special case in which \( N_A \) is a null hyperplane in Minkowski space, because the generators neither converge nor diverge, resulting in a \( v \) that is constant on each generator. Nevertheless, for generic \( N \) in generic spacetimes \( v \) is good enough. Indeed, in the case of greatest interest from the point of view of the holographic entropy bound, in which the generators are converging everywhere on \( S_0 \) (\( v \) decreasing away from \( S_0 \)), the focusing equation (8) ensures that \( v \) continues to decrease until a caustic is reached. Since the generator segments in \( N \) are truncated before reaching a caustic, this implies that \( v \) is a good parameter on \( N \).

The area parameter \( v \) is also a good parameter if the generators are diverging at \( S_0 \), provided they are truncated before they begin to reconverge. If the generators converge on some parts of \( S_0 \) and diverge on others, then our methods may still be used. Suppose \( \rho \) is a point on \( S_0 \) at which the expansion of both the \( R \) and the \( L \) future null normals is non-zero
(and suppose both the spacetime geometry and \( S_0 \) are smooth\(^3\)); then, this will also be true throughout a small disc \( S'_0 \subset S_0 \) about \( p \). The chart \((v^A, \theta^q)\) is thus good on each branch of a double null sheet \( N' \subset N \) swept out by the generators emerging from \( S'_0 \). The symplectic 2-form may be computed on \( N' \), and from it the Poisson brackets between the data on \( N' \).

Causality requires that these in fact be all the non-zero Poisson bracket of the data on the generators through \( p \). The only points of \( N \) that are causally connected to a point on these generators are the points of these generators themselves, all others are ‘spacelike separated’ from them (see appendix B of [Rei07]), so data on distinct generators should have vanishing Poisson brackets. Indeed, this is what is found when the brackets are computed [Rei08] on double null sheets on which \( v \) is a good parameter.

In the following, we shall assume, without great loss of generality according to the preceding arguments, that \( v \) is a good parameter throughout each branch of \( N \).

Ultimately, in order to define a phase space of the gravitational field in terms of initial data we have to express all limitations on admissible solutions and coordinates as restrictions on the initial data (expressed as functions of the coordinates). Points at which the parameter \( v \) is stationary, and thus not a good parameter, turn out to be detectable in the field \( e_{pq} \) on \( N' \), which will be one of our data. Integration of (8) yields

\[
\frac{dv}{d\eta}(v) = \frac{dv}{d\eta}(v_0) \exp \int_{v_0}^{v} \frac{1}{8} \partial_i e^{pq} \partial_i e_{pq} dv.
\]  

(9)

Since \( d/d\eta \) is the parallel transport of a non-zero vector at \( S_0 \), it is non-zero everywhere on the generator, so (9) implies that

\[
dv|_v = dv|_{v_0} \exp \int_{v_0}^{v} \frac{1}{8} \partial_i e^{pq} \partial_i e_{pq} dv,
\]  

(10)

along the generators. Therefore, if \( v \) is a good parameter (\( dv \neq 0 \) on the generator) at some value \( v_0 \) and \( e_{pq} \) is a continuously differentiable function of \( v \), then \( v \) is a good parameter at all finite values of \( v \). A breakdown of \( v \) as a parameter requires a (sufficiently strong) singularity in \( \partial_i e_{pq} \). We shall admit only initial data that are smooth in the coordinates, so \( v \) is guaranteed to be good.

On a branch \( N_A \) the coordinate \( v^A \) thus ranges from 1 on \( S_0 \) to its value, \( \bar{v}^A \), on \( S_A \), with \( \bar{v}^A \) being a smooth function of the \( \theta \) which is \( > 0 \) and \( \neq 1 \).

2.2. The data

Two types of data will be used: geometrical data that reflect the spacetime geometry, that is, the diffeomorphism equivalence class of the metric, and diffeomorphism data which reflect the choice of metric within the diffeomorphism equivalence class.

The inclusion of the diffeomorphism data may seem odd in a diffeomorphism invariant theory. However, the geometrical data are not enough to express the symplectic 2-form on \( N' \) for all the variations we will consider. Because \( N' \) has a boundary, not all infinitesimal diffeomorphisms are degeneracy vectors of the symplectic 2-form, \( \omega_{N'} \), on \( N' \). That is, some degrees of freedom measuring diffeomorphisms of the spacetime metric are non-gauge in the sense that their variations contribute to the symplectic 2-form. In order to express the symplectic 2-form in terms of the variations of initial data on \( N' \), it is therefore necessary in general to include in the data variables parametrizing these degrees of freedom.

\(^3\) A smooth function on a domain with a boundary is defined to be one that possesses a smooth extension to an open domain. See [AMR03, chapter 7]. Consequently, a smooth manifold with boundary necessarily has an extension to a smooth manifold without boundary, and an embedding of a manifold with boundary is smooth iff there exists a smooth extension of the embedding to a manifold without boundary.
This does not necessarily mean that the diffeomorphism data are ‘physical’. Indeed, they seem to play no essential role in the phase space formulation of vacuum GR within the domain of dependence of $\mathcal{N}$. They seem rather to be auxiliary quantities used in the intermediate stages of the construction of this formulation. They may however be important for the definition of quasi-local linear and angular momenta associated with $\mathcal{N}$. Indeed, their role may well be analogous to that of the centre-of-mass coordinates in an isolated mechanical system, which are superfluous to a description of the internal dynamics of the system but central to the definition of its total linear momentum.

The diffeomorphism data will be discussed at the end of this section. The geometrical data we will use consist of $\epsilon_{pq}$, specified on the branches of $\mathcal{N}$ as a function of the $v$ and $\theta$ coordinates, and further data given only on $S_0$ as functions of the $\theta^p$, namely $\rho_0$, $\lambda = -\ln |n_L \cdot n_R|$ and the twist

$$\tau_p = \frac{n_L \cdot \nabla_p n_R - n_R \cdot \nabla_p n_L}{n_L \cdot n_R}. \quad (11)$$

Here, $n_A = \partial_v A$ is the tangent to the generators of $\mathcal{N}_A$ and inner products $(\cdot)$ are taken with respect to the spacetime metric. These data will be called $v$ data. They are regular if the data on $S_0$ are smooth functions of the $\theta$ chart, and $\epsilon_{pq}$ is smooth in the $v\theta$ chart on each branch of $\mathcal{N}$.

Smooth solutions induce regular $v$ data on any smooth double null sheet $\mathcal{N}$, provided that on each branch the generators are either everywhere converging or everywhere diverging and free of caustics, and the $\theta^p$ form a smooth chart on $\mathcal{N}$.

Sachs [Sac62] and Dautcourt [Dau63] argue that a similar set of data is free, and complete in the sense that it determines the solution geometry. More precisely, they demonstrate that their data determine uniquely the spacetime metric and all its derivatives on $\mathcal{N}$, but do not examine the convergence of the corresponding power series solution on spacetime.

Sachs’ data consist of $\epsilon_{pq}$ on $\mathcal{N}$, but given as a function of an affine parameter $\eta$ on the generators instead of $v$, and the following data on $S_0$: $\rho_0$, $\partial_\eta^p \rho$, $\partial_\eta^p \rho_x$, and $\tau_\eta$ (which is the twist (11), but calculated from the tangents $\partial_\eta^p$ instead of the $n_A = \partial_v A$). (Sachs actually takes as his final datum a pair of quantities he writes as $CA_1, 2$ with $A = 1, 2$. These are the components of $-\tau_\eta$, as can be seen most easily from his equation (19). When a forgotten factor of $1/2$ is restored and it is rewritten in our notation, this equation reads

$$\frac{1}{2} C_{p,1} = \partial_\eta^p \cdot \nabla_\eta \partial_\eta^x. \quad (12)$$

The normalization condition $\partial_\eta^p \cdot \partial_\eta^x = -1$, which Sachs imposes on the affine parameters, implies that the right side equals $-1/2\tau_\eta$.)

Regular $v$ data are equivalent to Sachs data. We will demonstrate that all regular $v$ data determine unique corresponding Sachs data such that any solution matching the $v$ data also matches the Sachs data, and conversely, any solution matching the Sachs data matches the original $v$ data. It follows that if the Sachs data are free and complete, then regular $v$ data are also. Suppose a solution matches a set of $v$ data; then, it also matches a uniquely determined set of Sachs data. If the Sachs data determine the solution uniquely (up to diffeomorphisms), then so does the $v$ data. That is, the $v$ data are complete. To establish that it is free it must be shown that any regular $v$ data matches a solution. But if Sachs data are free, then the Sachs data corresponding to the $v$ data necessarily match a solution, and according to our result, this solution also matches the $v$ data.

In fact, it has been proved by Rendall that any smooth Sachs data match a unique solution in some neighbourhood of $S_0$ [Ren90], and it is a reasonable conjecture that it matches a unique
solution on all of $\mathcal{N}$ provided $\mathcal{N}$ is free of caustics. (See discussion in the introduction.) The Sachs data corresponding to regular $v$ data are indeed free of caustics on $\mathcal{N}$. Thus, if the conjecture is valid, regular $v$ data are free and complete on $\mathcal{N}$.

(In his proof of existence and uniqueness, Rendall actually takes as a datum $\partial_i g_{0\mu}$ (where $g$ is the 4-metric and the components are referred to the basis $d\eta^\mu$, $d\eta^R$, $d\theta^\rho$) in place of $\tau_{0\mu} = \partial_i g_{0\mu}|p$. But in Rendall’s spacetime coordinates $\partial_i g_{0\mu}$ is determined by the remaining (Sachs) data, so his proof applies just as well if $\tau_\mu$ is used as the datum.)

We now turn to the proof of the equivalence of regular $v$ data and Sachs data. The proof consists in demonstrating that in solution spacetimes regular $v$ data on $\mathcal{N}$ determine the Sachs data on $\mathcal{N}$. Moreover, without assuming a priori that a solution matching the $v$ data exists, Sachs data corresponding to any regular $v$ data may be defined using the transformation that holds on solutions. Finally, it is shown that any solution matching Sachs data obtained in this way from regular $v$ data also matches the original $v$ data.

The Sachs data differ from the $v$ data essentially by a coordinate transformation. The Sachs data are functions of an affine parameter along the generators, while the $v$ data are functions of the area parameter $v$. As the first step in the equivalence proof let us demonstrate that in a solution an affine parameter $\eta$ along the generators can be calculated from the $v$ data and the area parameter $v$. The resulting function $\eta(v)$ then determines the map from the coordinates $v, \theta^1$ and $\theta^2$ to which the $v$ data are referred, to Sachs’ coordinates $\eta, \theta^1$ and $\theta^2$.

The field equation $R_{uv} = 0$ on $\mathcal{N}$ implies that any affine parameter $\eta$ along the generators satisfies the focusing equation (8). But from the integrated form (9) of the focusing equation it is clear that $e_{\mu\nu}$, which is a smooth function of $v$ on the compact interval $[1, \bar{v}]$, determines $\eta(v)$ up to an affine transformation, that is, up to a constant rescaling and a constant shift. The possible affine parameters are thus precisely the solutions to (9).

(When the field equation $R_{uv} = 0$ does not hold a solution $\eta(v)$ to (9) is not an affine parameter, but it is still determined up to affine transformations, and it is a good parameter, for it follows directly from (9) that $\eta(v)$ is smooth and monotonic with a non-zero derivative (provided $\partial_\mu$ is set to a non-zero vector at $S_0$). If the parameter $\eta$ that Sachs data are referred to is interpreted to be this parameter, then all spacetime geometries, solutions or not, that match regular $v$ data, also match the corresponding Sachs data. The only role of the field equations in the equivalence of regular $v$ data and Sachs data is that they ensure that $\eta(v)$ is an affine parameter in accordance with the standard spacetime interpretation of Sachs data.)

The shift and rescaling freedom in $\eta(v)$ can be parameterized by the values of $\eta$ and $\partial_v \eta$ at $S_0$. For the Sachs coordinates $\eta^A$ and $\eta^\mu$, this amounts to four functions $A_A = \eta^A|S_0$ and $B_A = \partial_A \eta^\mu|S_0$ on $S_0$, which are restricted by the Sachs condition $\partial_{\mu\nu} \cdot \partial_\rho - 1 = -1$ at $S_0$. Rewriting this condition in terms of the vectors $n_A = \partial_\mu \eta^\mu A_A$ one obtains

\[-B_{\mu} B_{\rho} = n_{\mu} \cdot n_{\rho} = -\sigma_L \sigma_R |n_L \cdot n_R| = -\sigma_L \sigma_R e^{-\lambda},\]  

(13)

where $\sigma_A = 1$ if $v^A$ increases towards the future (i.e. $\bar{v}_A > 1$) and $\sigma_A = -1$ if it decreases towards the future. (The signature of the 4-metric is taken to be $+++$, which implies that the inner product of future directed tangents to the $L$ and $R$ generators is negative.)

Since $e^{\nu\lambda}$ is smooth in $v$ and $v$ is non-stationary on the generators (9) implies that $\eta(v)$ is smooth, with a non-zero derivative, and thus has a smooth inverse $v(\eta)$. As claimed, the $v$ data (and the parameters $A_L, A_R$, and $B_R$ or $B_I$) determine a smooth and smoothly invertible transformation from the chart $(v^A, \theta^\rho)$ to Sachs’ chart $(\eta^A, \theta^\rho)$. The shift and rescaling degrees of freedom can be eliminated by fixing the parameters $A_L, A_R$ and $B_R$ once and for all. We will set $A_L = A_R = 0$, and $B_R = 1$.

The coordinate transformation allows us to obtain $e_{\mu\nu}$ as a function of the Sachs coordinates. Note that $e_{\mu\nu}$ transforms as a scalar under this particular change of chart. This is
because the line element on $\mathcal{N}_A$, $d\mathbf{s}^2 = h_{pq}d\theta^p d\theta^q$, is degenerate, with no contribution from displacements along the generators. Since the $\theta$ coordinates are the same in the two charts the components $h_{pq}$ at a given point on $\mathcal{N}_A$ are the same. That is, $h_{pq}$ transforms as a scalar under the change of charts. It follows that $e_{pq} = h_{pq}/\sqrt{h}$ does also. The result of the transformation, $e_{pq}(\eta, \theta^1, \theta^2)$, is smooth on the branches of $\mathcal{N}$.

It remains to calculate the Sachs data on $S_0$. Namely $\rho_0, \partial_{\eta}\rho, \partial_\theta \rho$, and $\tau_\theta$. The $v$ data of course already include $\rho_0$, and the derivatives of $\rho = \rho_0 \tilde{v}^2$ are easily obtained from the $v$ data:

$$\partial_\eta \rho |_{S_0} = \rho_0 2\tilde{v}^2 \partial_\eta \tilde{v}^k |_{S_0} = 2\rho_0 B^{-1}_R = 2\rho_0,$$

(14)

$$\partial_\theta \rho |_{S_0} = \rho_0 2\tilde{v}^k \partial_\eta \tilde{v}^k |_{S_0} = 2\rho_0 \sigma_L \sigma_R e^\lambda B_R = 2\rho_0 \sigma_L \sigma_R e^\lambda.$$

(15)

Finally, $\tau_\eta$ is given by the same expression as the $v$ datum $\tau_\eta = \left[n_L \cdot \nabla_{\rho} n_R - n_R \cdot \nabla_{\rho} n_L\right]/n_L \cdot n_R$, but with the vectors $n_A$ replaced by $\partial_\eta = B^{-1}_A n_A$. Thus,

$$\tau_\eta = \tau + d \ln B_L - d \ln B_R,$$

(16)

$$= \tau - d\lambda - 2d \ln B_R = \tau - d\lambda.$$

(17)

All the Sachs data are determined by the $v$ data. (They also depend on the diffeomorphism data $\tilde{v}^k$ because the signs $\sigma_A$ are the signs of $\tilde{v}^k - 1$, but the $\tilde{v}^k$ are implicit in the specification of the $v$ datum $e^{pq}$ which is given as a function of $v$ on the range from 1 to $\tilde{v}$ on each generator.) Note that even if it is not assumed that the $v$ data match a solution, the function $q(v)$, and thus the Sachs datum $e^{pq}(\eta)$, may be calculated from any regular $v$ data using (9). Similarly, the remaining Sachs data may be obtained from (14), (15) and (17).

The transformation from regular $v$ data to Sachs data we have found is invertible. Solving (14), (15) and (17) yields

$$\lambda = \ln |\partial_\eta \rho|_{S_0}| + \ln |\partial_\theta \rho|_{S_0} - 2 \ln(2\rho_0),$$

(18)

$$\tau = \tau_\eta + d \ln(\partial_\theta \rho|_{S_0}) - d \ln(\partial_\theta \rho|_{S_0}).$$

(19)

(For Sachs data corresponding to regular $v$ data, the derivatives of $\rho$ in the logarithms do not vanish, as can be seen from (14) and (15).) The focusing equation (8) can be rewritten in the form

$$\partial_\eta \partial_\tau v = \frac{v}{8} \partial_\tau e_{pq} \partial_\rho e^{pq}.$$

(20)

Since $v^k = 1$ on $S_0$, and the Sachs data determine $\partial_\tau v^k |_{S_0} = \frac{1}{8m} \partial_\rho \rho|_{S_0}$ and $e_{pq}(\eta^4)$, (20) has a unique solution $v^k(\eta^4)$ on each branch. $v^k(\eta^4)$ and $e_{pq}(\eta^4, \theta)$ then determine the $v$ datum $e_{pq}(v^k, \theta)$, showing that all $v$ data can be reconstructed from the Sachs data. In particular, if a solution matches the Sachs data, then the $v$ data induced by the solution must be the original $v$ data from which the Sachs data were obtained. In other words, the solution must match the $v$ data. This completes the demonstration of the equivalence of regular $v$ data and Sachs data.

Let us turn to the diffeomorphism data. The diffeomorphism data that will be used are $\tilde{v}_A(\theta)$, the area parameter at the endpoint on $S_0$ of the generator specified by $\theta$, and $s_A = \tilde{v}_A^k(\theta)$, a map which gives the position of this endpoint in a fixed chart $y_A$ on $S_A$. A fixed chart is one that is, so to speak, ‘painted on the manifold’, unlike moving charts, such as Riemann normal coordinates or our $v\theta$ chart, which change at a given manifold point when the metric or other fields change. Recall that a manifold consists of a set of $a priori$ identifiable points and an atlas of charts on these. These charts are the fixed charts. They are important for the concept of the variation of a field, since they facilitate the comparison of different valuations of a field
at the same point, and of course they are essential to the definition of diffeomorphism degrees of freedom. See the appendix for a more detailed discussion of fixed and moving charts.

The status of \( v^A \) as a datum is curious. It is implicit in the specification of the \( v \) data on \( \mathcal{N}_A \), since it defines the range of \( v^A \) on which \( e^{\theta_{\nu\nu}} \) is given, but it is not a function of the \( v \) data. It is independent of the \( v \) data if \( e^{\theta_{\nu\nu}} \) is specified on a fixed, reference range of \( v \theta \) coordinates and \( \tilde{v}^A \) delimits the subset of this range that corresponds to points on \( \mathcal{N} \). The entire set of data, consisting of the diffeomorphism data \( \tilde{v}_A \) and \( s_A \) and the \( v \) data, is then free, since the diffeomorphism data can be varied independently of the \( v \) data by acting on the spacetime metric with suitable diffeomorphisms, which of course map solutions to solutions.

These data and their variations suffice to determine \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \), when the variations \( \delta_1 \) and \( \delta_2 \) are what we will call ‘admissible’. (This is explained in detail in subsection 4.1.) This is enough for our purposes because the evaluation of the Poisson brackets of the data carried out in [Rei07] and [Rei08] requires the symplectic 2-form only on admissible variations.

The diffeomorphism data play a role in the calculation of the Poisson bracket in [Rei08], but are they essential? Should they be regarded as ‘physical’? It seems to depend on what one wants to do. The diffeomorphism data do not seem to be necessary for the description of the gravitational field in the interior of the domain of dependence \( \mathcal{D}[\mathcal{N}] \) of \( \mathcal{N} \). They do not affect the diffeomorphism equivalence class of the metric on \( \mathcal{D}[\mathcal{N}] \), and even though not all diffeomorphisms are gauge they do not affect the gauge equivalence class of the metric on any compact domain in the interior of \( \mathcal{D}[\mathcal{N}] \). Since such a domain always excludes some open neighbourhood of \( \partial \mathcal{N} \) any (identity connected), diffeomorphism of the compact domain can be extended to a diffeomorphism that leaves invariant an open neighbourhood of \( \partial \mathcal{N} \), and such diffeomorphisms are gauge according to subsection 3.1. Similarly, the diffeomorphism invariant observables defined in the introduction are also independent of the diffeomorphism data. The requirement that the Poisson bracket of the data reproduces the brackets between observables, which (1) ensures, can thus at most determine the brackets between the \( v \) data. In subsection 4.2, it will be shown directly that (1) does not determine the brackets of the diffeomorphism data, indeed it does not involve them at all.

It seems therefore that in the canonical theory of the gravitational field in the domain of dependence of \( \mathcal{N} \) the diffeomorphism data have only an auxiliary role. Indeed, the \( v \) data are found to form a closed Poisson subalgebra, that is, their brackets are functions only of \( v \) data [Rei08], so the diffeomorphism data could be eliminated altogether from the canonical formalism.

On the other hand, the diffeomorphism data may be relevant to quasi-local energy or other quantities associated with the boundary \( \partial \mathcal{N} \). Note the diffeomorphism data, unlike the remaining data, ‘know’ about the boundary \( \partial \mathcal{N} \). In the present work, the diffeomorphism data are included in the initial data because the expression for the symplectic 2-form used in the calculation of the Poisson brackets in [Rei08] does depend on them, and it is the main aim of this work to present a derivation of this expression.

Before closing this subsection let us state precisely the complete set of data to be used: It consists of

- 10 real \( C^\infty \) functions, \( \rho_0, \lambda, \tau_p, \tilde{v}_A \) and \( s'_A \), on a domain \( D \in \mathbb{R}^2 \) having the topology of a closed disc, with \( \tilde{v}_A > 0 \) and \( \neq 1 \), and \( ds^2_A \wedge ds^2_A \neq 0 \) on all of \( D \),
- two \( C^\infty \), real, symmetric, unimodular \( 2 \times 2 \) matrix valued functions \( (e_{pq} \mid \mathcal{N}_L \text{ and } \mathcal{N}_R) \) on the domains \( [\theta \in D, \min(1, \tilde{v}_A(\theta)) \leq v^A \leq \max(1, \tilde{v}_A(\theta))] \), \( A = L, R \) which match at \( v^L = v^R = 1 \) (i.e. on \( S_0 \)).

Our phase space is the space of valuations of these data.
3. The symplectic 2-form of the Einstein–Hilbert action

In the present section, we will define the symplectic 2-form $\omega_{/\Sigma_1}$ of an arbitrary, fixed, oriented hypersurface $\Sigma_1$ embedded in spacetime, and calculate it in terms of the spacetime metric and its variations. In subsequent sections, this expression is reduced to one in terms of our free initial data in the special case that the hypersurface is a double null sheet.

The symplectic 2-form $\omega_{/\Sigma_1}$ will be defined for metrics $g$ that satisfy the vacuum field equations and variations that lie in the space $L_g$ of solutions to the field equations linearized about $g$. Although $\omega_{/\Sigma_1}$ is an on shell quantity it depends on the off shell action (on solutions the Einstein–Hilbert action is zero!), and it is most naturally defined as a pullback to the space of solutions of a symplectic 2-form $\Omega_{/\Sigma_1}$ defined by the action functional on all smooth metrics and variations. More precisely, $\omega_{/\Sigma_1}$ is the restriction of $\Omega_{/\Sigma_1}$ to metrics that satisfy the field equations and to variations in $L_g$. (See [LW90] for the uses of $\Omega_{/\Sigma_1}$.)

(At linearization stable solutions $\omega_{/\Sigma_1}$ is the pullback of $\Omega_{/\Sigma_1}$ to the space of solutions since at such solutions $L_g$ coincides with the tangent space to the solution manifold. At non-linearization stable solutions $L_g$ is larger than the tangent space. In fact, whether or not $L_g$ coincides with the tangent space to the manifold of solutions will not affect our considerations.)

The symplectic 2-form will be calculated from the Einstein–Hilbert action,

$$ I = \frac{1}{16\pi G} \int_Q R \varepsilon, $$

(21)

where $\varepsilon$ is the metric 4-volume form and the domain of integration $Q$ is a compact 4-manifold with boundary, which may be chosen freely. The sign conventions for the curvature tensor and scalar are those of [Wald84], that is, $R = R_{ab}{}^{cd}$ with

$$ [\nabla_a, \nabla_b] \beta_c = R_{abc} \beta_d $$

(22)

for any 1-form $\beta$.

The variation of the action due to a variation $\delta$ of the metric consists of a bulk term, which vanishes on solutions, and a boundary term which determines the symplectic 2-form.

The variation of $(16\pi G)$ times the Einstein–Hilbert Lagrangian is

$$ \delta[R \varepsilon] = [R_{ab} - \frac{1}{2} R g_{ab}] \delta g^{ab} \varepsilon + \delta R_{ab} g^{ab} \varepsilon, $$

(23)

where $R_{ab} = R_{ac}{}^{bc}$ is the Ricci tensor. Clearly, the first term vanishes on solutions. The second term is a divergence: From the definition (22), it follows that $\delta R_{abc} \delta \Gamma_{d}{}^{e}{}_{f} = -2 \nabla_a \delta \Gamma_{d}{}^{e}{}_{f} \varepsilon$.

$$ \delta R_{ab} g^{ab} \varepsilon = -2 \nabla_a \delta \Gamma_{d}{}^{e}{}_{f} \varepsilon. $$

(24)

The integral of this divergence is the boundary term in the variation of the action. For any vector field $v$

$$ \nabla_a v^a \varepsilon = d \wedge (v \varepsilon), $$

(25)

so $\delta R_{ab} g^{ab} \varepsilon = d \wedge \alpha$ with

$$ \alpha = -2 \delta \Gamma_{e}{}^{d}{}_{c} \varepsilon_{a} \varepsilon_{b} \varepsilon_{d}. $$

(26)

(The symbol $\wedge$ between a vector and tensor indicates that the vector preceding is contracted with the first covariant index of the tensor. Abstract index notation has also been used. We will occasionally mix abstract index notation with index free notation. To avoid confusion when some indices of a tensor are written and other, uncontracted, indices are not, the unwritten indices are indicated by dots.)

The boundary term in the variation of the action is thus

$$ B[\delta] = -\frac{1}{8\pi G} \int_{\partial Q} \delta \Gamma_{e}{}^{d}{}_{c} g^{ab} \varepsilon_{a} \varepsilon_{b}. $$

(27)
The symplectic potential associated with a portion $\Sigma$ of $\partial Q$ is obtained by restricting the boundary integral (27) to $\Sigma$:

$$\Theta_\Sigma[\delta] = -\frac{1}{8\pi G} \int_{\Sigma} \delta \Gamma_{\alpha\beta}^\mu \rho^\mu \epsilon_\alpha \ldots$$

The symplectic 2-form on a pair of variations $\delta_1$ and $\delta_2$ is

$$\Omega_\Sigma[\delta_1, \delta_2] = \delta_1 \Theta_\Sigma[\delta_2] - \delta_2 \Theta_\Sigma[\delta_1] - \Theta_\Sigma[[\delta_1, \delta_2]]$$

$$= -\frac{1}{8\pi G} \int_{\Sigma} \delta_2 \Gamma_{\alpha\beta}^\mu \delta_1 (g^\mu \rho \epsilon_\alpha \ldots) - (1 \leftrightarrow 2).$$

See [CW87] and [LW90]. $\Omega_\Sigma[\delta_1, \delta_2]$ may be interpreted as the curl of $\Theta_\Sigma$ in the space of metric fields, evaluated on two tangent vectors, $\delta_1$ and $\delta_2$, to this space.

The definition of $\Theta_\Sigma$ given is in fact ambiguous. The boundary integral $B$ in the variation is quite unambiguously defined, but the integrand of $\Theta_\Sigma$ is not. Adding an exact form to it would not affect $B$, but would alter $\Theta_\Sigma$ by an integral over $\partial \Sigma$. There is also the freedom to add a boundary term to the action. At first sight it would seem that such a boundary term only adds a total variation to $\Theta_\Sigma$, which would not affect $\Omega_\Sigma$. However, whether this is so actually depends on the precise prescription used to determine the integrand of $\Theta_\Sigma$ from the Lagrangian. Lee and Wald [LW90] give such a prescription (in which boundary terms added to the action can produce boundary terms in $\omega_\Sigma$ if they depend on derivatives of the fields). Our expression (28) for $\Theta_\Sigma$ corresponds to the Einstein–Hilbert action without a boundary term according to this prescription. But is there a physical reason to prefer the Lee–Wald prescription? Are boundary terms in $\omega_\Sigma$ important?

The Poisson bracket should not depend on boundary terms. The Peierls bracket is expressed directly in terms of the advanced and retarded Green’s functions, which are not affected by boundary terms in the action. Thus, if all that is required of the Poisson bracket $\{\cdot, \cdot\}_*\Sigma$ on initial data is that it reproduces the Peierls bracket on observables, then this Poisson bracket need not depend on boundary terms either. This can be seen directly from condition (1) which ensures the matching to the Peierls bracket. It is manifestly unaffected by the addition of boundary terms to the symplectic 2-form. In [Rei08], (1) actually had to be supplemented by additional conditions to yield a unique bracket, and these could be sensitive to boundary terms. But as long as no compelling motivation is found for the particular auxiliary conditions used, one has to conclude that only the physically less well-motivated features of the brackets between the initial data can depend on the boundary terms chosen, and that the choice made here and in [Rei08] of adding no boundary terms to the Einstein–Hilbert action is as justified as any other. Note that brackets obtained in [Rei08] do not ‘know’ where the boundary $\partial \Sigma$ is, that is, they are unchanged by a displacement of the boundary, except in the case of the brackets of the diffeomorphism data which themselves encode features of the boundary.

On the other hand, the canonical generators of diffeomorphisms that move the boundary $\partial \Sigma$ do seem to depend on boundary terms in $\omega_\Sigma$. Such generators define quasi-local notions of energy, angular momentum, etc and the correct boundary terms would presumably be defined by the properties one wants these quasi-local quantities to have. This interesting direction will not be explored here. Rather we shall simply adopt the symplectic potential (28) corresponding to the Einstein–Hilbert action without the boundary term.

4 The Green functions depend only on the field equations derived from the action with a suitable source term. The boundary terms we are considering are ones such as the York–Gibbons–Hawking term, which are matched to boundary conditions on the variations of the fields so that the presence of the boundary does not affect the field equations that result from extremizing the action. We are not considering boundary terms which represent a physical feature at the boundary, and of course would affect Green’s functions.
3.1. Diffeomorphisms

The degeneracy vectors of the symplectic 2-form are variations $\Delta$ such that $\omega_\Sigma[\Delta, \delta] = 0$ for all smooth solutions to the linearized field equations $\delta$. These are called gauge variations, although it is not clear that this is the most appropriate definition of ‘gauge’ when $\Sigma$ has boundaries. In GR, Lie derivatives of the metric along vector fields, satisfying certain conditions at $\partial \Sigma$, are degeneracy variations of $\omega_\Sigma$. This is the familiar diffeomorphism gauge invariance of GR. If $\psi_t$ is a family of diffeomorphisms parameterized by $t \in \mathbb{R}$, then the $t$ derivative of the image metric $\psi_t^* (g)$ is $\frac{d}{dt} \psi_t^* (g) = -\mathcal{L}_v g$, where $v$ is the field of tangents to the orbits of the manifold points under $\psi_t$, so Lie derivatives generate diffeomorphisms.

Let us evaluate $\omega_\Sigma[\mathcal{L}_v, \delta]$ for any $C^\infty$ vector field $v$ on spacetime and $\delta \in L_v$.

$$\omega_\Sigma[\mathcal{L}_v, \delta] = \mathcal{L}_v \Theta_\Sigma [\delta] - \delta \Theta_\Sigma [\mathcal{L}_v] - \Theta_\Sigma[[\mathcal{L}_v, \delta]].$$

(31)

Now

$$\Theta_\Sigma [\delta] = \frac{1}{16 \pi G} \int_\Sigma \alpha,$$

(32)

with $\alpha$ being the 3-form defined in (26). Thus,

$$\mathcal{L}_v \Theta_\Sigma [\delta] = \frac{1}{16 \pi G} \int_\Sigma \mathcal{L}_v \alpha$$

(33)

$$= \frac{1}{16 \pi G} \int_\Sigma v[ \partial \wedge \alpha ] + d \wedge [ v \alpha ].$$

(34)

But $d \wedge \alpha = \delta R_{ab} g^{ab} \epsilon$ is the divergence term in the variation of the Einstein–Hilbert Lagrangean density, which vanishes because $\delta$ satisfies the linearized vacuum field equation $\delta R_{ab} = 0$. Therefore,

$$\mathcal{L}_v \Theta_\Sigma [\delta]$$

(35)

$$= \frac{1}{16 \pi G} \int_{\partial \Sigma} v \partial \alpha$$

(36)

$$= - \frac{1}{8 \pi G} \int_{\partial \Sigma} \tilde{v}^b \delta \Gamma^c_{ebg} \epsilon_{ab}.$$  

(37)

$$= \frac{1}{8 \pi G} \int_{\partial \Sigma} v^a \left( \nabla^b \delta \epsilon_{ab} + \frac{1}{2} \nabla^b \delta g^{cb} \epsilon_{ab} \right) .$$

(38)

In the last line, the identity

$$\delta \Gamma^a_{eb} = \frac{1}{2} \delta_e \{ \nabla_b \delta g_{da} + \nabla_d \delta g_{eb} - \nabla_d \delta g_{ab} \}$$

(39)

has been used.

The second term in (31) is the $\delta$ variation of

$$\Theta_\Sigma [\mathcal{L}_v] = - \frac{1}{8 \pi G} \int_\Sigma \mathcal{L}_v \Gamma^c_{ebg} \epsilon_{ab}.$$  

(40)

But (39) and Einstein’s field equation, which $g$ satisfies, imply that

$$\mathcal{L}_v \Gamma^c_{ebg} \epsilon_{ab} = \left( \nabla^a v^b - \frac{1}{2} \nabla_v v^b - \frac{1}{2} \nabla^b v^a \right) \epsilon_{ab} .$$

(41)

$$= \nabla_v v^a \epsilon_{ab} .$$

(42)

$$= \frac{1}{2} d \wedge (v^a \epsilon_{ab} ).$$

(43)
Thus,
\[ \Theta_{\Sigma}[\mathcal{L}_v] = -\frac{1}{16\pi G} \int_{\partial\Sigma} \nabla^a v^b \varepsilon_{ab}. \] (44)

Since
\[ [\mathcal{L}_v, \delta g] = -\mathcal{L}_{\delta v} g, \] (45)
it follows that
\[ \Theta_{\Sigma}[[\mathcal{L}_v, \delta]] = \frac{1}{16\pi G} \int_{\partial\Sigma} \nabla^a \delta v^b \varepsilon_{ab}. \] (46)

Subtracting (46) and the variation of (44) from (38), one obtains
\[ \omega_{\Sigma}[\mathcal{L}_v, \delta] = \frac{1}{16\pi G} \int_{\partial\Sigma} v^a (2 \nabla^b \delta \varepsilon_{ab} + \nabla_c \delta g^{bc} \varepsilon_{ab} \cdot \cdot) + \delta (\nabla^a v^b \varepsilon_{ab}) - \nabla^a \delta v^b \varepsilon_{ab}. \] (47)

\[ = \frac{1}{16\pi G} \int_{\partial\Sigma} 3 v^b \delta \Gamma^c_{\cdot db} g^{bd} \varepsilon_{ab} \cdot \cdot + \delta [g^{ca} \varepsilon_{ab}] \nabla_c v^b. \] (48)

This integral obviously vanishes when \( v \) and \( \nabla v \) vanish on \( \partial \Sigma \). The corresponding variation \( \mathcal{L}_v \) is therefore a degeneracy vector of the symplectic 2-form.

4. The symplectic 2-form on \( \mathcal{N} \) in terms of the free null data

In this section, the symplectic 2-form \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \) defined in section 3 will be expressed in terms of the free null initial data defined in subsection 2.2, for variations \( \delta_1 \) and \( \delta_2 \) that satisfy the linearized field equations and a series of further conditions that define what we will call ‘admissible variations’.

Admissible variations are fairly special, but our expression for \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \) will in fact be applicable to a much larger class of variations. We will show that any pair of variations, \( \delta_1 \in L_g \) and \( \delta_2 \in L^0_g \), may be replaced in \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \) by corresponding admissible variations without changing the value of the symplectic 2-form. (Recall that \( L^0_g \) is the space of solutions to the linearized field equations that vanish in a spacetime neighbourhood of \( \partial \mathcal{N} \).) Our expression for the symplectic 2-form in terms of the free null data therefore suffices to convert (1) into an explicit condition on the Poisson brackets of these data.

In [Rei08], the Poisson brackets of the initial data are obtained from a somewhat strengthened version of (1), which can also be expressed in terms of the initial data using the expression for \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \) on admissible variations.

The first subsection treats conceptual issues involved in expressing \( \omega_{\mathcal{N}}[\delta_1, \delta_2] \) in terms of the null data of subsection 2.2 and it is demonstrated that attention may be restricted to the class of admissible variations. In the following subsection, the limited role of the diffeomorphism data defined in section 2.2 is demonstrated. The third subsection presents some charts used in the calculations. In the fourth subsection the symplectic potential is evaluated in terms of the free null data. Finally, in the last subsection, this expression for the symplectic potential is used to calculate the symplectic 2-form in terms of the free null data.

4.1. Variations in terms of null initial data and admissible variations

According to (30) the symplectic 2-form on \( \mathcal{N} \), at a given spacetime metric \( g \), is
\[ \omega_{\mathcal{N}}[\delta_1, \delta_2] = -\frac{1}{8\pi G} \int_{\mathcal{N}} \delta_1 \epsilon_{\gamma}^{[\alpha} \delta_{\beta]} (g^\gamma_{\cdot b} \varepsilon_{ab \cdot}) - (1 \leftrightarrow 2), \] (49)
where $\delta_1 g$ and $\delta_2 g$ are solutions to the field equations linearized about $g$. Our task is to express $\omega_N[\delta_1, \delta_2]$ in terms of the free null initial data and their variations in the case that $N^\prime$ is a double null sheet of $g$, $\delta_1 \in L_g$, and $\delta_2 \in L_g^0$.

It is not a priori obvious that this can be done. By definition the spacetime metrics matching the null data make the hypersurfaces $N^\prime_1$ and $N^\prime_2$ null, so the variations of these data only parametrize variations $\delta \in L_g$ that preserve the nullness of $N^\prime_1$ and $N^\prime_2$. Arbitrary variations will not in general do this. Recall that $\Sigma$ in (30), and thus $N^\prime$ here, is a fixed hypersurface in the spacetime manifold. It does not adjust when the metric is changed.

The fact that the symplectic 2-form $\omega_N[\delta_1, \delta_2]$ can nevertheless be expressed in terms of the variations of null data for all $\delta_1 \in L_g$ and $\delta_2 \in L_g^0$ is a consequence of the diffeomorphism gauge invariance of GR.

Although the branches of the fixed hypersurface $N^\prime$ may cease to be null when the spacetime metric is changed slightly, it is always possible, by a small deformation of $N^\prime$, to obtain a new hypersurface $N^\prime$ which is a double null sheet of the new metric. (The double null sheet $N^\prime_0$, swept out by the future null normal geodesics from $S_0$ in the new metric is an example.) Thus, if the given change in the metric is followed by the action on the metric of a suitable diffeomorphism, which moves $N^\prime_2$ to $N^\prime$, then the resulting total alteration of the metric preserves the double null sheet character of $N^\prime$. Any variation $\delta$ may therefore be split into the sum of a null sheet preserving variation $\delta'$, that is, one that preserves the null sheet character of $N^\prime$, and a diffeomorphism generator $\epsilon_u$.

Applying this decomposition to the two arguments $\delta_1, \delta_2 \in L_g$ of the symplectic 2-form, one obtains

$$\omega_N[\delta_1, \delta_2] = \omega_N[\delta'_1, \delta'_2] + \omega_N[\delta'_1, \epsilon_u] + \omega_N[\epsilon_u, \delta'_2] + \omega_N[\epsilon_u, \epsilon_u].$$

(50)

If the diffeomorphism generators are degeneracy vectors of $\omega_N$, that is, if they are gauge, then all terms but the first vanish, and in this first term only the null sheet preserving variations $\delta'$ appear. In this case, the fact that the variations of null data can only parametrize nullness preserving variations would not be an impediment to expressing the symplectic 2-form in terms of these data. Indeed, the $v$ data of subsection 2.2 determine corresponding Sachs data, and thus the metric and its first derivatives on $N^\prime$ up to diffeomorphisms that map $N^\prime$ to itself.

If the generators of all such diffeomorphisms were degeneracy vectors, then the $v$ data and their variations would suffice by themselves to determine $\omega_N[\delta'_1, \delta'_2]$. The $v$ data and their variations would determine the metric and its derivatives, and the gauge equivalence class of their variations under $\delta'_1$ and $\delta'_2$, up to a diffeomorphism mapping $N^\prime$ to itself, and the integral (49) is invariant under such diffeomorphisms.

However, not all diffeomorphism generators are degeneracy vectors of the symplectic 2-form. Equation (48) shows that the diffeomorphism terms in (50) are integrals over the boundary of $N^\prime$ that might not vanish. Indeed, some $\delta \in L_g$ might not be gauge equivalent to any null sheet preserving variation. There might not exist any null sheet preserving variation $\delta'$ such that $\delta' - \delta$ is a degeneracy vector. (In fact, it seems plausible that this is the case for some $\delta$, but it has not been demonstrated.) If this is so then $\omega_N[\delta_1, \delta_2]$ cannot be expressed in terms of null initial data for all $\delta_1, \delta_2 \in L_g$.

Fortunately, we do not need to do this for completely general $\delta_1$ and $\delta_2$ in $L_g$. We are interested in the case in which $\delta_1$ is arbitrary, but $\delta_2 g_{ab}$ vanishes in a spacetime neighbourhood of $\partial N^\prime$, that is, $\delta_1 \in L_g$, $\delta_2 \in L_g^0$. This is the case relevant for the calculation of the Poisson bracket via (1) in [Rei08].

---

5 It is possible to define variations of null data under general variations of the metric, if the null data live not on $N^\prime$ but on a metric-dependent double null sheet associated with $N^\prime$. Working along these lines one arrives ultimately at the same theory as presented here.
Let us suppose then that $\delta_2 \in L_0^0$. This restriction suffices to ensure that the diffeomorphism terms in \((50)\) vanish. If $\delta_2$ vanishes in a neighbourhood of $\partial \mathcal{N}$, then $\omega_N[\xi_{01}, \delta_2]$ is zero because it is an integral over $\partial \mathcal{N}$ of an integrand proportional to $\omega_{\mathcal{N}} g_{ab}$ and its derivatives there. Furthermore, when $\delta_2$ vanishes in a neighbourhood of $\partial \mathcal{N}$, the field $u_2$ may be chosen so that it also vanishes in a (generally different) neighbourhood of $\partial \mathcal{N}$ (see below). This implies that $\omega_N[\delta_1, \xi_{01}]$ is also zero. Thus, when $\delta_2 \in L_0^0$,

$$\omega_N[\delta_1, \delta_2] = \omega_N[\delta_1', \delta_2']$$

\((51)\)

This means that $\omega_N[\delta_1, \delta_2]$ can be expressed in terms of null initial data, that is, in terms of data sufficient to determine the metric and its derivatives up to gauge on $\mathcal{N}$ assuming $\mathcal{N}$ is a double null sheet. In section 4.5, such an expression is given explicitly, in terms of the free null data defined in subsection 2.2.

Before continuing let us return to the diffeomorphism generator $\xi_{02} = \delta_2 - \delta_1'$ and show that $u_2$ may indeed be chosen so that it vanishes in a neighbourhood of $\partial \mathcal{N}$. To this end, we define a new metric-dependent double null sheet $\tilde{\mathcal{N}}_{\partial \mathcal{N}}$ swept out by past normal null geodesics from $S_L$ and $S_R$ rather than future normal null geodesics from $S_0$. The generators of $\mathcal{N}$ may be regarded as normal null geodesics emerging to the past from $S_L$ or $S_R$ and truncated where they meet at $S_0$. When the metric is changed these past normal null geodesics from $S_L$ and $S_R$ are also changed, and sweep out new null hypersurfaces $\tilde{N}_{S_L}$ and $\tilde{N}_{S_R}$. If $\delta$ is a variation that vanishes in a neighbourhood $\mathcal{W}$ of $\partial \mathcal{N}$, then it will not disturb the geodesics that make up the portion $\partial \mathcal{N} - S_L - S_R$ of the boundary of $\mathcal{N}$, and these will still meet at $\partial S_0$. Furthermore, if the change in the metric is small enough, $\tilde{N}_{S_L}$ and $\tilde{N}_{S_R}$ will intersect on a disc, $S_0$, where they may be truncated, and thus truncated will contain no caustics. Thus, $\tilde{N}_{\partial \mathcal{N}} = \tilde{N}_{S_L} \cup \tilde{N}_{S_R}$ is a double null sheet of the perturbed metric. It is clear that the perturbed and unperturbed generators from $S_L$ coincide until they leave $\mathcal{W}$. Thus, $\tilde{N}_{\partial \mathcal{N}}$ coincides with $\mathcal{N}$ in a neighbourhood of $S_A$, and also in a neighbourhood of $\partial \mathcal{N} - S_L - S_R$, since generators sufficiently near $\partial \mathcal{N} - S_L - S_R$ never leave $\mathcal{W}$.

\(\text{(This follows from the compactness of the generator segments that sweep out} \partial \mathcal{N} - S_L - S_R)\)

As a consequence, $\tilde{N}_{\partial \mathcal{N}}$ can be mapped to $\mathcal{N}$ by a diffeomorphism that reduces to the identity in a neighbourhood of $\partial \mathcal{N}$. That is, $\delta_2 \in L_0^0$ implies that $u_2$ may be chosen to vanish in a neighbourhood of $\partial \mathcal{N}$.

Condition (1) defining the Poisson bracket, $\delta A = \omega_N\{[A, \cdot]_\#, \delta\} \forall \delta \in L_0^0$, may also be expressed in terms of the null initial data. The variation $[A, \cdot]_\#$ is null sheet preserving by virtue of its definition. The bracket $\{\cdot, \cdot\}_\#$ is a Poisson bracket on the null initial data, so $\{A, \cdot\}_\#$ is a variation of these initial data, which of course defines a null sheet preserving variation of the spacetime metric (up to diffeomorphisms, which do not affect the value of $\omega_N\{[A, \cdot]_\#, \delta\}$ when $\delta \in L_0^0$). (See [Rei07, appendix C].) The variations $\delta$ may be restricted to null sheet preserving variations without weakening the condition on $[A, \cdot]_\#$ that (1) implies. The variation $\delta$ may be replaced by $\delta'$ on both sides of the equation without altering the value of either, on the left because the observable $A$ is diffeomorphism invariant, and on the right because of \((51)\). Finally, any variation of $A$ may be written as a sum of the corresponding variations of the initial data integrated against suitable smearing functions. The smearing functions are the

\(\text{6 The branch $N_A$ of $\mathcal{N}$ is the image under the exponential map of a compact solid cylinder $N_A$ in the normal bundle of $S_A$, the generators being the images of parallel straight null lines in $N_A$ which will also be called generators. The preimage $Z \subset N_A$ of the subset $\mathcal{W} \cap N_A$ of $N_A$ is open in $N_A$, since $\mathcal{W} \cap N_A$ is open in $N_A$ and the exponential map is continuous. (Here the open sets in a subset $S$ of an ambient space $X$ are the intersections of open sets of $X$ space with the subset $S$.) Thus, $Z$ can be expressed as a union of open solid cylinders of the form $c = l \times x$, with $l$ being an open line segment parallel to the generators and $x$ is an open subset of $S_A$. Since any generator from $\partial S_A$ lies in $Z$ it is covered by these cylinders. But since it is compact it has a finite subcover $\{\psi_i\}$. The intersection $y = \cap \gamma_i$ is a neighbourhood of the base point of the generator in $\partial S_A$, open in $S_A$, such that generators from $y$ lie entirely in $Z$. Taking the union of such $y$s one obtains an open neighbourhood $Y$ of $\partial S_A$ in $S_A$ such that all generators from $Y$ remain in $Z$ until they leave $N_A$. See [Rei07] proposition B.8. for a different proof.)}
functional derivatives of $A$ by the initial data, which are well defined because $A$ is functionally
differentiable in the spacetime metric, and variations of the metric satisfying the linearized
field equations are determined, up to diffeomorphisms, by the variations of the initial data. 
(See [Rei07, appendix C].) $A$ may thus be replaced in (1) by a sum of smeared null initial
data, yielding an equation entirely in terms of the variation $\delta'$ of the null initial data, and the
Poisson brackets of these data.

The requirement that $\delta'_1 = \delta_1 - \xi_u$, preserves the double null sheet character of $\mathcal{N}$
leaves considerable freedom in the choice of $u_1$. This freedom will be exploited to restrict the variations we have to consider still further. We will require

1. that the variations map the generators that lie in the boundary $\partial \mathcal{N}$ to themselves,
2. that they leave invariant the area density $\tilde{\rho}$ in the fixed chart $\gamma_A$ on the truncation surface
$S_A$ of each branch,

and finally,

3. that they leave invariant a special chart constructed from the metric field in a spacetime
neighbourhood of each truncation surface $S_A$.

These special charts, the $a_L$ and $a_R$ charts defined in subsection 4.3, will play an important
role in the evaluation of the symplectic 2-form in terms of null data.

All these conditions already hold for $\delta'_1$ because this variation leaves the entire metric field
invariant in a spacetime neighbourhood of $\partial \mathcal{N}$. They can be made to hold for $\delta'_1$ by adding a
suitable diffeomorphism generator, that is, by adjusting $u_1$. If $\delta'_1$ perturbs the generators in
$\partial \mathcal{N}$, then clearly a suitable diffeomorphism returns them to their unperturbed courses. If $\delta'_1$
alters the $y$ chart area density $\rho_y = \det(\partial \theta/\partial y)\rho$ at the endpoint of a generator on $S_A$, then
the generator can always be extended or shortened so that $\rho_y$ at the new endpoint equals the
unperturbed value of $\rho_y$ at the old endpoint on $S_A$, because $\rho_y \propto v^a$ is nowhere stationary along
the generator. The generators thus lengthened or shortened can then be mapped to the original
generators of $\mathcal{N}_A$ by a diffeomorphism. It remains only to ensure that the $a_A$ chart is preserved by
$\delta'_1$ in a neighbourhood of $S_A$. Clearly, this can be done by adding a diffeomorphism generator
to $\delta'_1$. What has to be shown is that it can be done without violating the other conditions on $\delta'_1$.

Let us suppose that $\delta'_1$ preserves the double null sheet character of $\mathcal{N}$, and that it satisfies
conditions 1 and 2. As will be explained in subsection 4.3 the $a_A$ chart consists of an extension
to a spacetime region of a chart on $\mathcal{N}_A$, formed from the coordinates $\gamma'_a$, $r = v/\bar{r}$, and a
fourth coordinate $u$. The $y'$ label the generators, with each generator taking the values of $y'$ of
its endpoint on $S_A$, while $r$ labels the points within each generator. Finally, $u$ is a coordinate
transverse to the hypersurface $\mathcal{N}_A$ swept out by the generators. It vanishes on $\mathcal{N}_A$ itself.

On $S_A$ the coordinates $\gamma'_a$ are fixed by definition, and $\delta'_1$ preserves them on $\partial \mathcal{N}_A - S_A - S_0$
because of condition 1. It also preserves $u = 0$ on $\mathcal{N}_A$ because it is null sheet preserving, implying that the generators remain in $\mathcal{N}_A$. Thus, condition 3, the fact that the variation leaves
invariant all the $a$ coordinates in a spacetime neighbourhood of $S_A$ can be realized by adding a
diffeomorphism generator which leaves $\partial \mathcal{N}_A$ invariant and maps $\mathcal{N}_A$ to itself (that is, one that
corresponds to a vector field that vanishes on $\partial \mathcal{N}_A$ and is tangent to $\mathcal{N}_A$ on the interior of $\mathcal{N}_A$).
But such a diffeomorphism generator clearly preserves conditions 1 and 2, and the null sheet character of $\mathcal{N}_A$. It is therefore possible to find a $u_1$ so that $\delta'_1$ meets all our requirements. The
null sheet preserving variations satisfying conditions 1–3 will be called admissible variations. (In [Rei08], a somewhat smaller set of variations was termed ‘admissible’.)

Our results can be seen from an alternative point of view, in which the variations are not
restricted to be null sheet preserving, but rather the definitions of the null data are extended to
geometries in which the fixed hypersurface $\mathcal{N}$ is not null. We will not adopt this point of view,
but let us sketch it here. Suppose $\delta$ is a, not necessarily null sheet preserving, variation. Recall that the action $\delta^*\varphi(\theta, v)$ of a null sheet preserving component $\delta^* = \delta - \xi_a$ of $\delta$ on a null datum $\varphi(\theta, v)$ on $N$ is equal to the action of $\delta$ on the same datum on a double null sheet $N'$ that varies with the metric. A choice of this double null sheet suitable for $\delta_1$ is $N' = N_{S_0}$, since it is defined for all variations in $L^\theta_g$. For $\delta_2$, a suitable choice is $N' = N_{A_{N'}}$, since it is defined for all variations in $L^\theta_g$ and corresponds to $\mu_2 = 0$ in a neighbourhood of $\partial N$. With this interpretation of the null data in the variations, the explicit expression for the symplectic 2-form in terms of these data we obtain (in section 4.5) applies directly to any pair of variations $\delta_1 \in L^\theta_g$, $\delta_2 \in L^\theta_g$, whether they are null sheet preserving or not.

Condition (1) reduces to an equation on the Poisson brackets of the null data on $N_{S_0}$ as follows. As we have seen, $\omega_N[A, ]_\ast, \delta]$ may be expressed in terms of the $\delta$ variations of data on $N_{A_{N'}}$ and the variations under $[A, ]_\ast$ of data on $N_{S_0}$. Furthermore, $\delta A$ may be expressed as a sum of the $\delta$ variations of the data on $N_{A_{N'}}$, smeared with the functional derivatives of $A$ by these data. Now note that the functional derivatives of $A$ by the data on $N_{A_{N'}}$ and on $N_{S_0}$ are in fact the same, because the variation of the metric produced by a variation of the data on $N_{A_{N'}}$ and that produced by the same variation of the data on $N_{S_0}$ differ by a diffeomorphism, and $A$ is diffeomorphism invariant. Thus, $[A, ]_\ast$ can be expanded into a sum of the Poisson actions of the initial data on $N_{S_0}$, smeared with the same functions (of $\theta$ and $v$) as those that appear in the expansion of $\delta A$ in terms of variations of the data on $N_{A_{N'}}$.

4.2. The limited role of the diffeomorphism data

What is the role of the diffeomorphism data introduced in subsection 2.2? Recall that the free data defined in subsection 2.2 consists of the so-called $v$ data, which are equivalent to Sachs’ free null initial data and the diffeomorphism data $s_A$ and $\tilde{v}_A$. These latter data constitute partial information about how the $v\theta$ charts, to which the $v$ data are referred, are placed on $N$.

The diffeomorphism data appear in the expression for the symplectic 2-form found in [Rei07] and used in [Rei08]. Indeed, Poisson brackets are calculated for them. However, it was also argued in subsection 2.2 that the diffeomorphism data are not essential to the canonical formulation of GR in the domain of dependence of $N$. They neither affect the spacetime geometry in the domain of dependence, nor the so-called observables, which are functionals of the geometry, nor the Poisson brackets between these observables. Thus, condition (1), which ensures that the Poisson bracket on the data reproduces the Peierls brackets of the observables, ought not define brackets for the diffeomorphism data.

Here this expectation will be confirmed. It will be shown that the symplectic 2-form $\omega_N[\delta_1, \delta_2]$ does not depend on the variations of the diffeomorphism data if $\delta_2$ vanishes in a neighbourhood of $\partial N$, and that (1) provides no information about the Poisson brackets of the diffeomorphism data.

The diffeomorphism data will nevertheless be retained in this work. This is done mainly for consistency with [Rei08], which the present work underpins. In [Rei08], a strengthened version of (1), in which the test variation $\delta$ need not vanish in a neighbourhood of $\partial N$, is used to define a Poisson bracket on all the free data of subsection 2.2, including the diffeomorphism data. This strengthened condition requires an expression for $\omega_N[\delta_1, \delta_2]$ in terms of the null initial data valid for all admissible variations. It is this expression, which depends on the variations of the diffeomorphism data $s_A$, that is obtained in subsection 4.5.

Let us turn to the demonstration of the claims made above. Recall that when $\delta_2 \in L^\theta_g$ one may replace $\delta_1$ and $\delta_2$ in $\omega_N[\delta_1, \delta_2]$ by corresponding admissible variations without changing the value of $\omega_N[\delta_1, \delta_2]$, and that the admissible variation corresponding to $\delta_2$ still lies in $L^\theta_g$. Thus, we may restrict our attention to admissible $\delta_1$ and $\delta_2$ without loss of generality.
The variations of the $v$ data determine $\delta g_{ab}$ and $\nabla_c \delta g_{ab}$ on $\mathcal{N}$ up to diffeomorphism generators. So they characterize $\delta_1$ sufficiently for the calculation of the symplectic 2-form $\omega_\mathcal{N}[^{\delta_1}\mathcal{N}, ^{\delta_2}\mathcal{N}]$ when $\delta_1$ and $\delta_2$ are admissible variations in $L_s^\mathcal{N}$ and $L_2^\mathcal{N}$, respectively. The situation is a little more subtle for $\delta_2$. Since $\omega_\mathcal{N}[^{\delta_1}\mathcal{N}, ^{\delta_2}\mathcal{N}]$ is not invariant under the addition of non-gauge diffeomorphism generators to $^{\delta_2}\mathcal{N}$, the variation under $^{\delta_2}\mathcal{N}$ of non-gauge diffeomorphism degrees of freedom must be specified. The diffeomorphism data, $\bar{s}_A$ and $\bar{v}_A$, measure such degrees of freedom. However, because $\delta_2 g_{ab}$ is required to vanish in a spacetime neighbourhood of $\partial \mathcal{N}$ the variations of the $v$ data under $^{\delta_2}\mathcal{N}$ in fact determine those of the diffeomorphism data modulo gauge. Thus, ultimately $\omega_\mathcal{N}[^{\delta_1}\mathcal{N}, ^{\delta_2}\mathcal{N}]$ depends only on the variations under $^{\delta_1}\mathcal{N}$ and $^{\delta_2}\mathcal{N}$ of the $v$ data, and of course the unperturbed values of the $v$ data and of $\bar{v}_A$. (It does not depend on the unperturbed values of $\bar{s}_A$ because $\bar{s}_A$ can be set to any desired value by a diffeomorphism that maps $\mathcal{N}$ to itself, and $\omega_\mathcal{N}[^{\delta_1}\mathcal{N}, ^{\delta_2}\mathcal{N}]$ is invariant under such diffeomorphisms.)

How does this come about? Because $^{\delta_2}\mathcal{N}$ vanishes in a neighbourhood of $\partial \mathcal{N}$ the $y$ chart area density on $\mathcal{S}_A$, $\bar{\rho}_A(y)$, is invariant under $^{\delta_2}\mathcal{N}$. Thus, the variation of

$$
\bar{v}_A(\theta) = \sqrt{\bar{\rho}_A(s_A(\theta)) \det[\partial s_A/\partial \theta]} \rho_0
$$

is determined by those of $\rho_0$ and $s_A$. (In fact, by definition all admissible variations leave $\bar{\rho}_A(y)$ invariant, so the variations of $\bar{v}_A$ can be eliminated from $\omega_\mathcal{N}[^{\delta_1}\mathcal{N}, ^{\delta_2}\mathcal{N}]$ in favour of variations of $\rho_0$ and $s_A$ whenever $^{\delta_1}\mathcal{N}$ and $^{\delta_2}\mathcal{N}$ are admissible, even if neither lies in $L_1^\mathcal{N}$. Precisely, this will be done in our calculation of the symplectic 2-form on admissible variations.)

It remains to show that the variations of $s_A$ under $^{\delta_2}\mathcal{N}$ in $L_2^\mathcal{N}$ are determined by those of the $v$ data. In fact, there is a trivial sense in which $s_A$ can vary independently of the $v$ data when there is enough symmetry. The field $s_A$ depends on the choice of $\theta$ coordinates on $\mathcal{S}_0$, which is a gauge choice in our formalism. If the spacetime geometry near $\mathcal{N}$ admits an isometry, a rotation, that maps $\mathcal{N}$ to itself, then it is possible to change $s_A$ without changing the $v$ data, by rotating the $\theta$ chart. But of course such a variation is pure gauge. It does not contribute to the symplectic 2-form because it does not change the spacetime metric components or their derivatives at any point of $\mathcal{N}$, and the symplectic 2-form depends only on the variations of the spacetime metric. Such gauge variations will be eliminated by holding the $\theta$ chart fixed in the variations we consider. As we will now see, once this restriction is imposed $^{\delta_2}s_A$ is indeed determined by the corresponding variations of the $v$ data.

Suppose $\delta$ and $\bar{\delta}$ are two admissible variations in $L_2^\mathcal{N}$, that induce the same variations of $v$ data. If the $v\theta$ charts on the branches of $\mathcal{N}$ are given, then the $v$ data determine the metric and its derivatives on each branch $\mathcal{N}_A$ up to diffeomorphisms that fix the points of $\mathcal{N}$. If the $v$ data are given but the placement of the $v\theta$ charts is not specified, then there is of course an additional freedom in the metric corresponding to movements of this chart. It follows that

$$
\delta g_{ab} - \bar{\delta} g_{ab} = \xi^a g_{ab},
$$

where the vector field $\xi$ generates a diffeomorphism that maps $\mathcal{N}$ to itself, and furthermore that on $\mathcal{N}$ the field $\xi$ reduces to the difference in the $\delta$ and $\bar{\delta}$ variations of the $v$ and $\theta$ coordinates: $\delta \theta^p - \bar{\delta} \theta^p = \xi^p$, $\delta v - \bar{\delta} v = \xi^i$.

This has two immediate consequences. First, since the $\theta$ chart (and of course also $v = 1$) is fixed on $\mathcal{S}_0$, $\xi = 0$ there. Second, since $\delta - \bar{\delta} \in L_2^\mathcal{N}$, the diffeomorphism generated by $\xi$ must reduce to an isometry in a neighbourhood $U$ of $\partial \mathcal{N}$. But since $\xi$ vanishes on $\mathcal{S}_0$, $\mathcal{S}_0 \cap U$ is fixed under the isometry, as are its two future null normal directions. Because the area density $\rho = \rho_0 v^2$ is not constant along the generators, these future null directions cannot be rescaled isometrically. The isometry must preserve not only the directions but also the vectors $\partial_\theta$. In sum, the isometry preserves $\mathcal{S}_0 \cap U$ and a complete basis of spacetime vectors at $\mathcal{S}_0 \cap U$. The isometry is therefore trivial, that is, $\xi = 0$, throughout $U$. This implies in particular that $\delta \theta^p - \bar{\delta} \theta^p = 0$ at $\mathcal{S}_A$, so $\delta s_A = \bar{\delta} s_A$. (Isometries are rigid in any connected spacetime with a
smooth non-degenerate metric: they are completely determined by their actions on one point of the spacetime and on the tangent space at that point. See [Wald84] p 442 for a proof.)

Extending the preceding argument one can conclude that condition (1), \( \delta A = \omega N([A, \cdot]_\bullet, \delta) \forall \delta \in L^0_g \), does not define, nor impose any restriction on, the brackets of the diffeomorphism data, because brackets involving these data do not enter the condition. The observable \( A \) is diffeomorphism invariant by definition, so \([A, \cdot]_\bullet\) does not depend on \([s, \cdot]_\bullet\) or \([\tilde{v}, \cdot]_\bullet\). Furthermore, because \( \delta g_{ab} \) vanishes in a neighbourhood of \( \partial N \), \( \omega_N([A, \cdot]_\bullet, \delta) \) does not depend on \([A, s]_\bullet\) or \([A, \tilde{v}]_\bullet\). Thus, no bracket involving \( s \) or \( \tilde{v} \) enters (1). In addition, the fact that the variations of the diffeomorphism data are determined by those of the \( v \) data under \( \delta \in L^0_g \) implies that \( \delta s \) and \( \delta \tilde{v} \) do not enter (1) either.

How was it then possible to obtain the brackets of the diffeomorphism data in [Rei08]? In [Rei08], brackets were obtained for all the data, including the diffeomorphism data, by imposing a strengthened version of (1). The bracket was required to satisfy the conditions

\[
\delta A = \omega_N([A, \cdot]_\bullet, \delta) \forall \delta \in C \quad (53)
\]

\[
[A, \cdot]_\bullet \in C \quad (54)
\]

with \( C \) being a subset of the admissible variations\(^7\) containing the null sheet preserving variations in \( L^0_g \) as a proper subset. These conditions define an essentially unique bracket on all of the data.

(In [Rei08], one natural condition on the bracket is relaxed, namely the requirement that the changes in the metric on \( N \) be real. But the complex variations of the metric that are generated via the resulting bracket are special modes that represent shock waves that propagate along \( N \) and do not affect the metric on the interior of the domain of dependence of \( N \). A similar relaxation of the reality conditions on the data probably has to be made also to obtain a Poisson bracket satisfying (1). This ultimately seems to be a consequence of insisting on defining the Poisson bracket on initial data smeared with any smooth compactly supported test function on \( N \), which may not be necessary for a complete canonical formulation of GR.)

Recall that \( \delta \) in condition (1) may be restricted to null sheet preserving variations in \( L^0_g \) without weakening this condition, so the fact that \( C \) contains all these variations implies that (53) is at least as strong as (1). Of course, any bracket satisfying the stronger condition (53) also satisfies the weaker condition (1), so the brackets of the \( v \) data given in [Rei08] are a solution to (1).

### 4.3. The \( a \) and \( b \) charts

Two types of special spacetime charts, called ‘\( a \)’ charts and ‘\( b \)’ charts, will be used. The charts \( b_L \) and \( b_R \) extend the \( \psi \theta \) charts on \( N_L \) and \( N_R \) to charts on an open spacetime neighbourhood of the interior, \( S_0 - \partial S_0 \), of \( S_0 \). Both are formed from the same coordinates \( v^L, v^R, \theta^1 \) and \( \theta^2 \), but they differ in the ordering of these coordinates: \( b^L_R = (v^L, v^R, \theta^1, \theta^2) \) and \( b^R_L = (v^R, v^L, \theta^2, \theta^1) \). That is, the roles of \( v^L \) and \( v^R \) are interchanged in the two charts, as are those of \( \theta^1 \) and \( \theta^2 \), so that the charts have the same orientation. The coordinates \( v^L, v^R, \theta^1 \) and \( \theta^2 \) are obtained from the \( \psi \theta \) charts by setting \( v^R = 1 \) on \( N_L \) and \( v^L = 1 \) on \( N_R \), and then extending the functions \( u^L, v^R, \theta^1 \) and \( \theta^2 \) arbitrarily, but smoothly, off \( N \). Lowercase indices \( \mu, \nu, \ldots \) from the latter part of the Greek alphabet will represent \( b \) coordinate indices.

The \( a_A \) chart, associated with the branch \( N_A \), is defined in much the same way as the \( b_A \) chart, but with the truncating 2-surface \( S_0 \) playing the role of \( S_0 \). It consists of the ordered

\(^7\) In [Rei08], the term ‘admissible variation’ is defined more narrowly than here and refers only to the variations in \( C \).
coordinates $\alpha_i^\alpha = (u_\alpha, r_\alpha, y_\alpha^1, y_\alpha^2)$. $y^1$ and $y^2$ are constant on the generators of $\mathcal{N}_\alpha$, and coincide on $S_\alpha$ with the fixed $y$ chart already introduced to define the diffeomorphism datum $\mathcal{N}$. The coordinate $r$ is an area parameter along the generators like $v$, but normalized to 1 on $S_\alpha$, so $r = \sqrt{\rho}/\bar{\rho} = v/\bar{v}$, where $\rho$ is the area density on cross sections of $\mathcal{N}_\alpha$ in the $y$ chart and $\bar{\rho}$ is the area density on $S_\alpha$ in this chart. The coordinates $r$, $y^1$ and $y^2$ are extended off $\mathcal{N}_\alpha$ by holding them constant on the null geodesics normal to the equal $r$ cross sections of $\mathcal{N}_\alpha$ and transverse to $\mathcal{N}_\alpha$. Finally, $u$ is a parameter along these geodesics set to 0 on $\mathcal{N}_\alpha$ and chosen such that $\partial_u \cdot \partial_v = -1$. Greek lowercase indices $\alpha$, $\beta$, $\ldots$ from the beginning of the alphabet will represent a coordinate indices. To lighten notation, the branch index, $\alpha$, is usually be suppressed when there is little risk of confusion.

On $\mathcal{N}_\alpha$ the transformation between the $a$ and $b$ charts is quite simple:

$$r = v/\bar{v}(\theta) \quad y^i = s^i(\theta) \quad u = 0. \quad (55)$$

In the $a$ chart, the spacetime line element at $\mathcal{N}_\alpha$ takes the form

$$\mathrm{d}x^2 = -2 \, \mathrm{d}u \, \mathrm{d}r + h_{ij} \, \mathrm{d}y^i \, \mathrm{d}y^j = -2 \, \mathrm{d}u \, \mathrm{d}r + r^2 \bar{\rho} e_{ij} \, \mathrm{d}y^i \, \mathrm{d}y^j, \quad (56)$$

where the $e_{ij}$ are the $y$ chart components of the conformal 2-metric, a (two-dimensional) weight $-1$ tensor density. The spacetime line element at $S_\alpha$ is also simple in the $b$ chart. It is

$$\mathrm{d}x^2 = 2\chi \, \mathrm{d}v^l \, \mathrm{d}v^R + h_{pq} \, \mathrm{d}\theta^p \, \mathrm{d}\theta^q, \quad (57)$$

with $\chi = \partial_v \cdot \partial_s \cdot \partial_y$.

It will be necessary to have control over the orientations of the charts we have defined. The sign of the integral of a form over a manifold depends on the orientation of the manifold. Given this orientation the integral of the form can be reduced to an iterated definite integral by choosing a chart $x$ oriented coherently with the manifold, and expressing the integrand as a multiple of the coordinate volume form: $\int f \, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \cdots \wedge \mathrm{d}x^n$, where $f$ is a suitable function. The integral is then $\int f \, \mathrm{d}x^1 \, \mathrm{d}x^2 \cdots \mathrm{d}x^n$, with the integration over each coordinate $x^i$ running from lesser to greater values of $x^i$. (See [CDD82].)

An orientation will be chosen, once and for all, for spacetime (or at least a neighbourhood of $\mathcal{N}$). Which orientation is chosen does not matter, because whichever choice is made, the sign of the 4-volume form $\varepsilon$ will be chosen so that its integral over a spacetime region is positive. The value of the action (21) is thus independent of the orientation of spacetime chosen.

The $a$ charts will be positively oriented, that is, their orientations will be chosen to match that of spacetime. This can be achieved by choosing a suitable orientation for the $y_\alpha$ chart on $S_\alpha$.

We shall take $\mathcal{N}$ to be future oriented. A chart $(x^1, x^2, x^3)$ on a non-timelike hypersurface is future oriented if a spacetime chart $(t, x^1, x^2, x^3)$ formed from the $x$ coordinates and a time coordinate $t$ which is constant on the hypersurface and increasing towards the future is positively oriented. It is with this convention that equation (1) ensures that the Poisson bracket on initial data reproduces the Peierls bracket [Rei07].

If $r$ increases towards the future on $\mathcal{N}_\alpha$, then $u$ must also, because $g_{\alpha\beta} = -1$ and the metric is assumed to have signature $-+++$. In this case, $u$ may be taken as the time coordinate in the preceding definition. With a suitably chosen $y$, chart $(u, r, y^1, y^2)$ will be a positively oriented chart on spacetime, and thus $(r, y^1, y^2)$ a future oriented chart on $\mathcal{N}_\alpha$, matching the orientation of this manifold. By a similar argument, if $r$ decreases towards the future, then $u$ decreases towards the past.

---

8 Two overlapping charts are said to be coherently oriented if the transformation between them has positive Jacobian determinant. The orientation of a manifold is defined by the choice of a coherently oriented atlas on the manifold. (A manifold may or may not admit a coherently oriented atlas. If it does it is orientable, and if it does not it is non-orientable.) See [CDD82]. The orientation of a chart on an oriented manifold is said to be positive, or to match that of the manifold, if the chart is coherently oriented with the atlas that defines the orientation of the manifold.
is \(-u\) a time coordinate increasing towards the future and the \(y\) chart may be chosen so that \((-u, -r, y^1, y^2)\) is a positively oriented chart. Then, \((-r, y^1, y^2)\) is a future oriented chart on \(\mathcal{N}_A\). In either case, the coordinate along the generators of the future oriented chart increases from \(S_0\) to \(S_A\). Thus,

\[
\int_{\mathcal{N}_A} f \, dr \wedge dy^1 \wedge dy^2 = \int_{S_A} d^2y \int_{r_0}^1 dr f,
\]

where the \(y\) integrals run from lesser to greater values of these coordinates, or, equivalently, \(d^2y\) is interpreted as the positive Euclidean coordinate measure on \(S_A\) defined by the \(y\) chart. On each generator, \(r_0 = 1/\bar{v}\) is the value of \(r\) at \(S_0\).

A future orientation can be defined on the two-dimensional cross sections of \(\mathcal{N}_A\) in an entirely analogous manner, with \(\mathcal{N}_A\) now playing the role of spacetime in the preceding definition. The \(y\) charts chosen above give precisely this future orientation to \(S_A\) when \(\mathcal{N}_A\) is future oriented in spacetime. This is also the orientation that \(S_A\) has as part of \(\partial \mathcal{N}_A\) (see [Wald84, appendix B]).

The \(\theta_\alpha\) chart will be oriented coherently with the \(y_A\) chart. Therefore, if \(S_0^{(A)}\) is \(S_0\) oriented coherently with \(\partial \mathcal{N}_A\), and thus past oriented with respect to \(\mathcal{N}_A\), then

\[
\int_{S_0^{(A)}} d\theta_\alpha^1 \wedge d\theta_\alpha^2 = -\int_{S_0} d^2\theta.
\]

Since \(S_0^{(L)}\) and \(S_0^{(R)}\) have opposite orientations, it follows at once that the charts \(\theta_R\) and \(\theta_L\) must be oppositely oriented. If \((\theta^1, \theta^2)\) is coherently oriented with \(y_R\), then \(\theta_R^\mu = (\theta^1, \theta^2)\) and \(\theta_L^\mu = (\theta^2, \theta^1)\) satisfy our requirements. These correspond to the \(b\) charts \(b_R^\mu = (v^L, v^R, \theta^1, \theta^2)\) and \(b_L^\mu = (v^R, v^L, \theta^2, \theta^1)\) defined earlier. The use of these two \(b\) charts, instead of just one, \(\theta_R\) say, makes possible a completely symmetrical treatment of the two branches.

### 4.4. The symplectic potential in terms of the free null data

According to (28) the contribution to the symplectic potential of a branch \(\mathcal{N}_A\) of \(\mathcal{N}\) is

\[
\Theta_A[\delta] = -\frac{1}{8\pi G} \int_{\mathcal{N}_A} \delta \Gamma^{\nu}_{\alpha \beta} \partial_{\mu} e_{\nu}.,
\]

with the whole symplectic potential given by \(\Theta_\mathcal{N} = \Theta_L + \Theta_R\). Our task is to rewrite \(\Theta_\mathcal{N}[\delta]\) in terms of our free initial data for admissible variations \(\delta\). Taking the curl of this potential then yields the symplectic 2-form in terms of these data and variations. Note that knowledge of the potential on admissible variations suffices to determine the symplectic 2-form on such variations because the commutator of two admissible variations is itself an admissible variation. (This follows immediately from the definition, which characterizes admissible variations as variations that leave certain structures invariant.)

In the following, only \(\Theta_R\) will be computed explicitly. \(\Theta_L\) is entirely analogous, except that \(\tau\) is replaced by \(-\tau\) because exchanging \(L\) and \(R\) in the definition (11) of \(\tau\) produces an expression equal to \(-\tau\).

It will be convenient to decompose the variation \(\delta\) into the sum of a diffeomorphism generator \(\xi_\tau\) that accounts for the displacement of the \(a_R\) chart under \(\delta\), and a variation \(\delta^\alpha = \delta - \xi_\tau\), that leaves this \(a\) chart fixed. As is explained in detail in the appendix, \(\delta^\alpha g\) is the part of the variation of the metric arising from changes of the \(a\) chart components of the metric, that is, \(\delta^\alpha g_{\nu \mu}(\alpha) = \delta[g_{\nu \mu}(\alpha)]\) in this chart. The corresponding decomposition of \(\Theta_R\),

\[
\Theta_R[\delta] = \Theta_R[\delta^\alpha] + \Theta_R[\xi_\tau],
\]

neatly separates the contribution from the variations of the bulk datum, the conformal 2-metric \(\epsilon\) and the variations of the surface data on \(S_0\).
\[ \Theta_R[\delta^\eta] \] depends only on the variation of \( \eta \). Indeed, in the \( a \) chart the metric at \( \mathcal{N}_R \) is restricted to the form
\[
\begin{bmatrix}
0 & -1 \\
-1 & 0
\end{bmatrix}, \quad \bar{g}^{\alpha\beta} = \begin{bmatrix}
0 & -1 \\
-1 & 0
\end{bmatrix},
\]
with \( h^i \) being the inverse of \( h_{ij} \). (See (56).) Furthermore \( h_{ij} = r^2 \bar{\rho} e_{ij} \). Since \( \bar{\rho} \) the \( y \) chart area density on \( S_R \) is invariant under admissible variations, \( e_{ij} \) is the only degree of freedom that can vary in \( g_{ab} \).

\[ \Theta_R[\xi_0], \text{ on the other hand, is a surface integral. By (44),} \]
\[ \Theta_R[\xi_0] = -\frac{1}{16\pi G} \int_{\partial \mathcal{N}_R} \nabla^a \xi_b \, e_{ab}. \]  

In fact, the integral reduces to one over \( S_0 \), because the integrand vanishes elsewhere. Since \( \delta^\eta \) preserves the \( a \) chart, \( \xi \) is determined by
\[ \delta a^a = \delta^\eta a^a + \xi_0 a^a = 0 + \xi \, du^a = \xi^a. \]

On \( S_R \) both the coordinates \( a^a \) and their gradients are invariant under admissible variations, so \( \xi \) and \( \nabla \xi \) vanish there. There is thus no contribution to (63) from \( S_R \). The fact that the contribution from \( \partial \mathcal{N}_R - S_R - S_0 \) also vanishes is most easily understood by expressing the integrand of (63) on this surface in terms of \( a \) chart components. The pullback of \( du \) to \( \partial \mathcal{N}_R - S_R - S_0 \) vanishes, and those of \( dy^1 \) and \( dy^2 \) are linearly dependent, so the pullback of \( \nabla^a \xi_b \, e_{ab} \) is equal to the pullback of \( 2\nabla^i (u^i \xi_i) \, e_{ai} \, dr \wedge dy^j \). But
\[ \nabla^i (u^i \xi_i) = g^{\alpha\beta} \nabla^i (u^i \xi_i) = -h_{ik} \partial_k \xi_i. \]

Since admissible variations are null sheet preserving, \( \delta u = 0 \) on \( \mathcal{N}_R \). Thus, \( \xi_i = -\xi^a = 0 \), and it follows that \( \partial_k \xi_i = 0 \). Since admissible variations preserve the generators on \( \partial \mathcal{N}_R - S_R - S_0 \), \( \delta y^j = 0 \) there. Thus, \( \xi_k = h_{ik} \xi^i = 0 \), and \( \partial_k \xi_k = 0 \), which establishes the claim. The diffeomorphism term is therefore
\[ \Theta_R[\xi_0] = -\frac{1}{16\pi G} \int_{\partial \mathcal{N}_R} \nabla^a \xi_b \, e_{ab}. \]

where \( S_0^{\mathcal{N}_R} \) is \( S_0 \) oriented coherently with \( \partial \mathcal{N}_R \).

The form of the vector field \( \xi \) can be restricted quite a bit by gauge fixing the variations further. In particular, one can ensure that the variations leave the \( b \) chart fixed in a spacetime neighbourhood of \( S_0 - \partial S_0 \). First, one adds a diffeomorphism generator \( \xi_0 \) to each variation so that the generators, and the \( v \) parameter on these, are invariant under the total variation within some neighbourhood of \( S_0 \). This can be achieved with a diffeomorphism \( \xi_0 \) which is pure gauge, that is, without affecting the value of the symplectic 2-form, and without affecting the admissibility of the variation. Recall that admissible variations already preserve the double null sheet character of the fixed manifold \( \mathcal{N} \), and map the generators in \( \partial \mathcal{N} \) to themselves. Thus, \( u \) must be tangent to \( \mathcal{N} \) and to the generators on \( \partial \mathcal{N} \) within a neighbourhood of \( S_0 \). We will set \( u \) to zero in neighbourhoods of \( S_L \) and \( S_R \) and tangent to \( \mathcal{N} \) and to the generators on \( \partial \mathcal{N} \) wherever it is non-zero. Then, the modified variation is still admissible. Moreover, the change in the symplectic potential due to the addition of \( \xi_0 \), \( \Theta_N[\xi_0] \), vanishes on \( S_L \) and \( S_R \) because \( u \) vanishes in a neighbourhood of these surfaces, and on \( \partial \mathcal{N} - S_L - S_R \) by the argument of the preceding paragraph. Alternatively, one may note that the addition of \( \xi_0 \) to \( \delta \) does not affect \( \delta^\eta \) but does transform \( \xi \to \xi + \xi_0 \). Since the new variation \( \delta + \xi_0 \) is still
admissible, the contribution to $\Theta_g[E_\xi]$ from $\partial \mathcal{N}_R - S_R - S_0$ remains zero. The contribution from $S_0$, (66), is affected by the addition of $u$ to $\xi$, but the sum,

$$\Theta_g[E_\xi] + \Theta_L[E_\xi] = \frac{1}{16\pi G} \int_{S_0^0} \nabla^a [\xi_L - \xi_R] a_{ab},$$

(67)
is not because $u$ cancels out in the difference $\xi_L - \xi_R$. (The minus sign is due to the fact that the orientation of $S_0^{(L)}$ is opposite to that of $S_0^{(R)}$.)

To ensure that the $b$ chart is fixed under the gauge fixed variations, the $\theta^1$ and $\theta^2$ must be set equal to fixed coordinates on $S_0$. (Recall that the choice of the $\theta$ chart is a gauge degree of freedom in our formalism, additional to the spacetime diffeomorphism gauge freedom.) This fixes the $b$ coordinates on $\mathcal{N}$ in a neighbourhood of $S_0$. They may then be smoothly extended to a fixed chart on a spacetime neighbourhood of the interior of $S_0$.

Once this gauge fixing has been carried out, $\xi$ simply measures the variation of the transformation from the $b$ chart to the $a$ chart, within the neighborhood of $S_0$ in which the $b$ chart is fixed. On $\mathcal{N}_R$, the transformation between these charts is (55),

$$r = v/\bar{v}(\theta), \quad y^i = s^i(\theta), \quad u = 0.$$  

(68)

Thus,

$$\xi = \delta r \partial_r + \delta y^i \partial_{y^i} = -r\delta \ln \bar{v} \partial_r + \delta s^i \partial_{y^i},$$

(69)

which is completely determined by the variations of the $S_0$ data $s^i$ and $\bar{v}$.

Let us evaluate the bulk term,

$$\Theta_R[\delta \alpha] = -\frac{1}{8\pi G} \int_{\mathcal{N}_R} \delta^a \Gamma^a_{\beta\gamma}(a) \delta \alpha^\beta \cdot \delta \alpha\gamma,$$

(70)
in the symplectic potential in terms of the initial data. It is convenient to use the $a$ chart, since the $a$ coordinates are fixed under $\delta \alpha$, and the $a$ components of the variation under $\delta \alpha$ of a field is simply the variation under $\delta$ of the $a$ components of the field. In particular,

$$\left[ \delta^a \Gamma^a_{\beta\gamma}(a) \right] = \delta \left[ \Gamma^a_{\beta\gamma}(a) \right],$$

(71)

where the variation $\delta$ on the right-hand side is of the connection coefficients $\Gamma^a_{\beta\gamma}$ evaluated at a fixed $a$ coordinate point $a$.

The form (62) of the metric in the $a$ chart implies that $\sqrt{-g} = \sqrt{\text{det}[h_{ij}]} \equiv \rho_y$, and therefore, since the $a$ chart is positively oriented, that $\varepsilon = \rho_y \, du \wedge dr \wedge dy^i \wedge dy^j$. Pulling the last three indices of this 4-volume form back to $\mathcal{N}_R$, one obtains

$$\varepsilon_{\beta\gamma} = \rho_y \delta^a_{\beta\gamma} \, dr \wedge dy^i \wedge dy^j.$$  

(72)

The integrand in (70) thus reduces to $dr \wedge dy^i \wedge dy^j$ times the function

$$\delta^a \Gamma^a_{\beta\gamma} \delta \rho_y = \frac{1}{2} \left[ \delta a \delta a + g^{\alpha\beta} \delta \Gamma^a_{\alpha\gamma} \right] \rho_y$$

(73)

$$= -\frac{1}{2} \left[ \delta a \delta a \ln \sqrt{-g} + 2 \delta \Gamma^a_{\alpha\gamma} \right] \rho_y$$

(74)

$$= -\frac{1}{2} \left[ \delta a \delta a \ln \rho_y + \delta a \delta a \rho_y + \rho_y h^{ij} \delta a h_{ij} \right] \rho_y.$$

(75)

Now $\rho_y(y, r) = r^2 \bar{\rho}(y)$ and $\delta \bar{\rho} = 0$ for admissible variations. It follows that

$$\delta a \ln \rho_y = \delta a/2r = 0.$$  

(76)

and

$$\frac{1}{2} h^{ij} \delta \rho_y \delta a h_{ij} = \delta a \ln \rho_y - \frac{1}{2} \partial_i \left[ \rho_y e_{ij} \right] \delta a e_{ij} \rho_y = -\frac{1}{2} \partial_i \left[ e_{ij} \right] \delta a e_{ij}.$$  

(77)
Here use has been made of the fact that, for any variation $\Delta$, $e_{ij}\Delta e^{ij} = -\Delta \ln \det[e_{ij}] = -\Delta 0 = 0$. Recall that $e^{ij}$ is the inverse of $e_{ij}$, not $e_{ij}$ with indices raised by $h$.

The remaining, middle, term in (75) is proportional to $\delta\Gamma^r_{rr}$, since on $N_R$

$$\partial_ug_{rr} = 2\Gamma^r_{rr}. \quad (78)$$

Because $N_R$ is oriented towards the future, the form integral (70) reduces to an iterated definite integral according to formula (58). Substituting in our results on the integrand one obtains

$$\Theta_R[\delta\nu] = -\frac{1}{16\pi G} \int_{\Sigma_0} d^2y \int_{t_0}^{t_1} \frac{1}{2} \left[ \partial_r e_{ij} \delta^a e^{ij} - 2\delta^a \Gamma^r_{rr} \right] dr, \quad (79)$$

where $d^2y$ is the positive euclidean coordinate measure associated with the $y$ chart. The first term in the integrand is expressed in terms of the bulk datum $\nu$. The second term combines with a term in the surface contribution to the symplectic potential to form a total variation, which may be dropped from the potential without affecting the symplectic 2-form.

Let us now turn to the surface term, $\Theta_R[\xi_i]$, in the symplectic potential. Here, it is convenient to work with the $b_R$ chart, since the $S_0$ data are defined in terms of the $b$ coordinates.

Our first task will be to calculate the 4-volume form in this $b$ chart. Because $n_L = \partial_\nu$, and $n_R = \partial_{\nu^C}$ are null and normal to $S_0$, the spacetime line element at $S_0$ takes the form (57)

$$d^2s = 2\chi \, dv^L \, dv^R + h_{pq} \, d\theta^p \, d\theta^q, \quad (80)$$

with $\chi = n_L \cdot n_R$. But the sign of $\chi$ depends on the direction in which $v^L$ and $v^R$ increase. Recall the definition $\sigma_\lambda = 1$ if $v^\lambda$ increases to the future, and $-1$ if it decreases. Then, $\sigma_L n_L$ is future directed and $\sigma_R n_R$ is negative. Indeed $\chi = -\sigma_L \sigma_R e^{-\lambda}$.

The chart $(\sigma_1 v^L, \sigma_R v^R, \theta^1, \theta^2)$ has the same, positive, orientation as the $a_R$ chart, so the 4-volume form is

$$\varepsilon = |\chi| \rho_0 \sigma_R \sigma_L \, dv^L \wedge dv^R \wedge d\theta^1 \wedge d\theta^2 \quad (81)$$

$$= -\chi \rho_0 \, dv^L \wedge dv^R \wedge d\theta^1 \wedge d\theta^2 \quad (82)$$

$$= -\rho_0 n_R \wedge n_L \wedge d\theta^1 \wedge d\theta^2. \quad (83)$$

In the last line, the $n_\lambda$ denote the 1-forms $n_{L,\lambda} = \chi \partial_\lambda v^R$ and $n_{R,\lambda} = \chi \partial_\lambda v^L$, obtained by lowering the indices of the tangent vectors $n^\lambda$ with the metric.

In (66), the first two indices of $\varepsilon_{abcd}$ are contracted and the last two indices are pulled back to $S_0$. When thus pulled back, $\varepsilon_{ab}$ becomes

$$\varepsilon_{ab} = -2\frac{\rho_0}{\chi} n_R a_n \xi \, d\theta^1 \wedge d\theta^2. \quad (84)$$

Substituting this expression into (66) yields

$$\Theta_R[\xi_i] = \frac{1}{16\pi G} \int_{\Sigma_0} \frac{1}{\chi} \left[ n_{L, a} \nabla_n \xi - n_{R, a} \nabla_{n^a} \xi \right] \rho_0 \, d^2\theta, \quad (85)$$

with $d^2\theta$ being the positive Euclidean measure defined by the $\theta$ chart on $S_0$. Formula (59), which takes into account the orientation of $S_0$ employed in (66), has been used to turn (66) into a definite integral.

The derivative along $n_L$ may be eliminated in favour of a variation of $\chi$:

$$\delta \chi = n_{L,\lambda}^\beta n_{R,\mu}^\delta \varepsilon_{\lambda \mu \rho \beta} = n_{L,\lambda}^\beta n_{R,\mu}^\delta \left[ \delta \varepsilon_{\lambda \mu \rho \beta} + \xi_{\lambda, \mu} \varepsilon_{\rho \beta} \right]$$

$$= n_{L,\lambda}^\beta n_{R,\mu}^\delta \delta \varepsilon_{\lambda \mu \rho \beta} + 2n_{L,\lambda}^\beta n_{R,\mu}^\delta \nabla_{(\alpha} \xi_{\beta)}.$$
But \( n_R^0 = \partial_v \delta^\beta_\gamma = 1/\bar{v} \delta^\beta_\gamma \), and (by (62)) \( g_{\alpha\beta} = -\delta^\alpha_\beta \), which is of course invariant, so
\[
\delta \chi = n_R \cdot \nabla n_x \xi + n_L \cdot \nabla n_v \xi.
\] (88)

The integrand of (85) is thus equal to
\[
\frac{1}{\chi} [\delta \chi - 2n_L \cdot \nabla n_x \xi] \rho_0 = -\rho_0 \delta \lambda - 2 \frac{\delta \lambda}{\chi} n_L \cdot \nabla n_v \xi,
\] (89)
since \( \lambda = -\ln |\chi| \).

Note that the \( \theta \) components of \( \xi \), \( \xi^\theta = \xi j d\theta^p = \delta \theta^p \partial_j \theta^p \), are independent of \( v \). This means that \( \xi^\perp = \xi^\beta \partial_\beta \) is Lie dragged along \( n_R = \partial_v \cdot \xi \)
\[
= \xi^\beta \nabla n_v \xi - \nabla n_\xi n_R,
\] (90)
for in the \( b \) chart the Lie derivative along \( n_R \) reduces to simply the \( v \) partial derivative of the \( b \) components of \( \xi^\perp \).

The second term in (89) may therefore be expanded according to
\[
2n_L \cdot \nabla n_v \xi = 2n_L \cdot \nabla n_x [\xi^\perp + \xi^v n_R] = 2n_L \cdot \nabla n_v n_R + 2 \xi^v n_L \cdot \nabla n_v n_R + 2 \chi \partial_v n_v \xi^v.
\] (91)

The first term in this expansion is linear in the twist \( \tau \). By the definition (11) of \( e \)
\[
2n_L \cdot \nabla n_v n_R = \partial_v \chi + \chi \partial_\perp \rho e n \tau = -\chi \partial_\perp \rho e n \tau \cdot d\lambda - \tau \cdot [\delta \lambda].
\] (92)

The second and third terms in (91) are proportional to the values on \( S_0 \) of \( \xi^v \) and \( d_{n_\lambda}e = \partial_\perp \xi^v \), respectively. In a neighbourhood of \( S_0 \), \( \delta \tau = 0 \), so \( \delta \tau^v = -\xi^v \), there. It follows that
\[
\xi^v = -\delta \tau^v = -\delta \tau^v [r/r_0] = v \delta \tau^v [r_0],
\] (93)
and therefore on \( S_0 \)
\[
\xi^v = \partial_v \xi^v = \delta \tau^v [r/r_0].
\] (94)

The second term in (91) also contains a factor \( n_L \cdot \nabla n_v n_R \). Since \( n_R = \partial_v \rho_0 \partial_\perp \)
\[
n_L \cdot \nabla n_v n_R = n_L \cdot \rho_0 \partial_\perp \nabla n_\perp \partial_\perp = n_L \cdot \rho_0 \Gamma_{rr} n_R = \chi \rho_0 \Gamma_{rr}.
\] (95)

The second and third terms are the ones that will combine with a term from the bulk contribution to the symplectic potential to form a total variation.

Substituting our results into (85) and adding the bulk contribution \( \Theta_N [\delta^n] \) we obtain the complete symplectic potential of \( N_R \):
\[
\Theta_N [\delta] = -\frac{1}{16 \pi G} \int_{S_0} \left[ \delta \lambda - \xi^\perp \cdot (d\lambda - \tau) + 2 \delta \tau^v [r_0 + \rho_0 \Gamma_{rr}] \right] d^2 \theta
\]
\[+ \int_{S_0} d^2 y \tilde{\rho} \int_{r_0}^1 \frac{1}{2} r^2 \partial_\rho e_i \delta \tau^v e^j - 2 r^2 \delta \tau^v \Gamma_{rr} \right] d\theta.
\] (96)

The dependence on \( \Gamma_{rr} \) can be eliminated. As has already been pointed out, adding the variation of a functional of the data to the symplectic potential does not affect its curl, the symplectic 2-form. Thus, we are free to subtract from \( \Theta_N [\delta] \) the variation
\[
\delta \left[ \frac{1}{8 \pi G} \int_{S_0} d^2 y \tilde{\rho} \int_{r_0}^1 \left[ r + 2 \Gamma_{rr} \right] d\theta \right]
\]
\[= \frac{1}{8 \pi G} \int_{S_0} d^2 y \tilde{\rho} \int_{r_0}^1 r^2 \delta \tau^v \Gamma_{rr} d\theta - \int_{S_0} d^2 \theta \rho_0 \delta \tau^v \ln \rho_0 (1 + \rho_0 \Gamma_{rr}).
\] (97)

Recall that the variation \( \delta [F] \) of the \( a \) chart components of a field \( F \), at a fixed \( a \) coordinate point, is given by the \( a \) chart components of \( \delta^n F \). This is the reason for the appearance of \( \delta^n \)
in (97). (See (A.11) of the appendix.) Use has also been made of the fact that \( r_0^2 \hat{\rho} \) is the \( y \) chart area density on \( S_0 \), so \( r_0^2 \hat{\rho} \, d^2 y = \rho_0 \, d^2 \theta \).

We will therefore take as the symplectic potential of \( \mathcal{N} \)

\[
\Theta'[\delta] = -\frac{1}{16\pi G} \int_{S_0} \left[ \delta \chi \left( \frac{\partial}{\partial \chi} + \mathfrak{a} \frac{\partial}{\partial \mathfrak{a}} \right) \right] \rho_0 \, d^2 \chi + \frac{1}{2} \int_{S_0} \frac{d^2 y}{r_0} \int_{\tau_0}^\tau \partial_r \delta \theta e_{ij} \delta \sigma^i e^j \, dr .
\]  

(98)

Proceeding in exactly the same way an analogous expression is obtained for \( \Theta'_r \), the symplectic potential of \( \mathcal{N}_r \), with the one difference that \( \tau \) is replaced with \( -\tau \), since interchanging \( L \) and \( R \) maps \( \tau \) to \( -\tau \).

Equation (98) and its \( L \) branch analogue provide an expression for the symplectic potential entirely in terms of our free null initial data. It depends on the \( v \) data \( \rho_0, \lambda, \) and \( \tau \) on \( S_0 \), and on \( \xi_{\perp A} = \delta \xi_{\perp} \, \partial_{\perp A} \) there. It further depends on the \( \alpha_A \) chart conformal 2-metric \( e_{ij} \) on \( \mathcal{N}_A \), the (invariant) \( \gamma_A \) chart area density \( \rho_A = \left| \det \frac{\partial \alpha_A}{\partial \gamma_A} \right|^{-1} \rho_0 \tilde{v}_{\perp A}^2 \) on \( S_A \), and on \( r_{\lambda 0} = 1/\tilde{v}_A \). Note that the transformation from the \( b \) chart conformal metric \( e_{\mu \nu}(v, \theta) \), which is one of our data, to \( e_{ij}(r, \theta) \) is determined by the transformation (55) from the \( b \) chart to the \( \alpha_A \) chart on \( \mathcal{N}_A \), which in turn is determined by the diffeomorphism data \( s_A \) and \( \tilde{v}_A \).

We have achieved our goal of expressing the symplectic potential in terms of the null initial data of subsection 2.2. It turns out however that a symplectic potential that is in some ways more useful can be obtained by replacing the datum \( \tau \) by two new data

\[
\tilde{\tau}_R \equiv \rho_0 (d\lambda - \tau) \, j \, \partial_{jR} \quad \text{and} \quad \tilde{\tau}_L \equiv \rho_0 (d\lambda + \tau) \, j \, \partial_{jL} .
\]

(99)

These are the coefficients of \( \delta \xi_{\perp} \) and \( \delta \xi_{\|} \) respectively in the surface term of the symplectic potential. In terms of these new data,

\[
\Theta'[\delta] = -\frac{1}{16\pi G} \int_{S_0} \rho_0 \delta \lambda - \tilde{\tau}_R \delta \xi_{\perp} \, d^2 \theta + \frac{1}{2} \int_{S_0} \frac{d^2 y}{r_0} \int_{\tau_0}^\tau \partial_r \delta \theta e_{ij} \delta \sigma^i e^j \, dr ,
\]

(100)

and \( \Theta'_r \) is given by a completely analogous expression. (In particular, \( \tilde{\tau}_L \) enters \( \Theta'_L \) in precisely the same way as \( \tilde{\tau}_R \) enters \( \Theta'_R \), since the difference in the sign with which \( \tau \) enters \( \Theta'_R \) and \( \Theta'_L \) has been absorbed into the definitions of \( \tilde{\tau}_R \) and \( \tilde{\tau}_L \).) In principle, \( \tilde{\tau}_R \) and \( \tilde{\tau}_L \) are related by the equation

\[
\tilde{\tau}_R \, d\xi_{\perp}^L + \tilde{\tau}_L \, d\xi_{\perp}^R = 2\rho_0 \, d\lambda .
\]

(101)

However, we shall extend the phase space by taking \( \tilde{\tau}_R \) and \( \tilde{\tau}_L \) to be independent, and then treat (101) as a constraint which defines our original phase space. This constraint generates the gauge transformations of the \( \theta \) chart [Rei07]. Thus, in the extended phase space, without the constraint, these transformations are not gauge, and the symplectic 2-form is in fact non-degenerate.

The introduction of constrained variables seems a step backward with respect to our aim of a canonical description in terms of free data, but the constraint introduced brings no real complications. Indeed, (101) may be solved easily for \( \tilde{\tau}_R \). If the \( \theta \) chart is then fixed via the gauge condition \( \xi_{\perp} = \text{id} \) (i.e. \( \theta = \gamma_{\perp} \)), then the physical phase space is parametrized by the remaining data, and the Dirac brackets of these remaining data are equal to their brackets in the extended phase space [Rei07].

A non-degenerate symplectic form can only be achieved by either extending the phase space as we do or by gauge fixing the \( \theta \) chart. The use of an unfixed, arbitrary, \( \theta \) chart has made it possible to treat the two branches of \( \mathcal{N} \) autonomously and symmetrically. This is also possible for some gauge fixed \( \theta \) charts. For instance, one could take the \( \theta^p \) to be isothermal coordinates of the metric on \( S_0 \). This gauge choice has the drawback that isothermal coordinates depend non-locally on the metric. As a result the Dirac bracket, unlike the extended phase
space Poisson bracket, does not always vanish between data on distinct generators. Other gauge fixings which avoid this complication can be defined, but all the same, leaving θ unfixed and working with the extended phase space seems the simplest choice.

4.5. The symplectic 2-form in terms of the free null data

The contribution of the hypersurface \( N_R \) to the symplectic form is

\[
\omega_R[\delta_1, \delta_2] = \delta_1 \Theta'_R[\delta_2] - \delta_2 \Theta'_R[\delta_1] - \Theta'_R[\delta_1, \delta_2].
\]  

(102)

Here, this expression will be evaluated in terms of the free null initial data for admissible variations \( \delta_1 \) and \( \delta_2 \). Since \( [\delta_1, \delta_2] \) is also admissible the symplectic potential is needed only on admissible variations. Equation (100) for \( \Theta'_R \) therefore provides a sufficient basis for the calculation.

The first term of \( \Theta'_R \) in (100) is a surface term, an integral over \( S_0 \), while the second term is a bulk term, an integral over \( N_R \). As a result \( \omega_R \) also consists of bulk and surface terms. The bulk term in \( \omega_R \) is obtained by varying the bulk term in \( \Theta'_R \) with \( r_0 \) held fixed. It is

\[
\frac{1}{32\pi G} \int_{S_0} d^2 y \rho_0 \int_{S_R} r^2 \delta_1^a \delta_2^b e^{ij} \partial_i \delta_2^b e_{ij} dr - (1 \leftrightarrow 2).
\]  

(103)

Since \( r_0 \) is held fixed, the domain of integration does not vary in the \( a \) chart. The variation of the integral is therefore just the integral of the variation of the integrand in this chart, that is, of \( \delta \) of the integrand. (See (A.11) of the appendix.)

In terms of the \( \psi \theta \) chart, the bulk term in \( \omega_R \) may be written as

\[
\frac{1}{32\pi G} \int_{S_0} d^2 \theta \rho_0 \int_{S_R} v^2 \delta_1^a \delta_2^b e^{ij} \partial_i \delta_2^b e_{ij} dv - (1 \leftrightarrow 2).
\]  

(104)

(46)

(Note that the transformation between \( y \) and \( \theta \) components is independent of \( r \), so it may be freely moved through the derivative, \( \partial_v \), in (103).)

The surface contribution to \( \omega_R \) comes both from the surface term in \( \Theta'_R \) and the variation of \( r_0 \) in the bulk term of \( \Theta'_R \). The surface term in \( \Theta'_R \) yields

\[
\frac{1}{16\pi G} \int_{S_0} \delta_1 \delta_2 \rho_0 - (1 \leftrightarrow 2).
\]  

(105)

The variation of \( r_0 \) in the bulk term in \( \Theta'_R \) produces

\[
\frac{1}{32\pi G} \int_{S_0} \delta_1^a \int_{S_R} [r^2 \partial_j e_{ij} \delta_2^j e^{ij}] v = \frac{1}{32\pi G} \int_{S_0} \delta_1^a \ln r_0 \partial_\psi e^{ij} \delta_2^j e_{ij} d\theta - (1 \leftrightarrow 2),
\]  

(106)

where \( \delta^a[r_0] = \delta^a r_0 \) is the variation of the scalar \( r_0(y) \) at constant \( y \). (See (A.11).)

In (106), \( \delta^a \) may be replaced by the variation \( \delta^a \equiv \delta - \xi\nu = \delta^\nu + \xi\nu, \partial^\nu, \partial, \) associated with the hybrid chart \( (v^0, v^\xi, \nu, \partial^\nu) \). Clearly, \( \delta^a \ln r_0 = \delta^\nu \ln r_0 \) since \( r_0 \) only depends on \( y \).

Furthermore, as will soon be demonstrated,

\[
\xi\nu = \xi^\nu \partial^\nu.
\]  

(107)

Substituting these two relations into the integrand of (106), and taking into account that by (94) \( \xi^\nu = \delta^\nu \ln r_0 = \delta^\nu \ln r_0 / S_0 \), one obtains

\[
\delta_1^a \ln r_0 \delta_2^b e^{ij} - (1 \leftrightarrow 2)
\]  

(108)

\[
= \{ \delta_1^a \ln r_0 \delta_2^b e^{ij} - \delta_1^a \ln r_0 \delta_2^b \ln r_0 \partial_\psi e^{ij} \} - (1 \leftrightarrow 2)
\]  

(109)

\[
= \delta_1^a \ln r_0 \delta_2^b e^{ij} - (1 \leftrightarrow 2).
\]  

(110)
Equation (107) can be demonstrated as follows. Any variation $\Delta h$ of the 2-metric on $\mathcal{N}_R$ gives rise to a variation
\[
\Delta g^{\mu \nu} = \Delta [\sqrt{\det h h^{\rho \sigma}}] = -h^{\rho \sigma} h^{\mu \nu} \sqrt{\det h} \left[ \Delta h_{\rho \sigma} - \frac{1}{2} h_{\rho \sigma} h^{\mu \nu} \Delta h_{\mu \nu} \right]
\]
(111) of the inverse conformal 2-metric. (Here $p, q, r, s, t,$ and $\nu$ are $\theta$ chart indices.) But because the $\nu$ components of the induced metric on $\mathcal{N}_R$ vanish
\[
\mathcal{L}_{\xi^\nu} h_{\rho \sigma} = \mathcal{L}_{\xi^\nu} g_{\rho \sigma}
\]
(112)
\[
= \xi^\rho \partial_{\nu} g_{\rho \sigma} + \partial_{\rho} \xi^\nu g_{\rho \sigma} + \partial_{\sigma} \xi^\nu g_{\rho \nu} = \xi^\rho \partial_{\nu} h_{\rho \sigma}.
\]
(113)
The result (107) follows directly from this relation and (111). (See (A.6) for a general definition of the Lie derivative.)

Using the invariance of $\bar{\rho}$, the variation $\delta^\nu \ln r_0$ may be expressed in terms of $\delta^\nu \rho_0$, $r_0^2 = \rho_0 \bar{\rho}$, where $\rho_0$ is the area density on $S_0$ in the $\gamma$ chart, so, since $\delta^\nu \bar{\rho} = \delta^\nu \rho = 0$,
\[
\delta^\nu \ln r_0 = \frac{1}{2} \frac{\delta^\nu \rho_0}{\rho_0}.
\]
(114)
But $\delta^\nu \rho_0$ is just $\delta^\nu \rho_0$ transformed, as a density, from the $\gamma$ chart to the $\chi$ chart, so
\[
\delta^\nu \rho_0 \big/ \rho_0 = \delta^\nu \rho_0 \big/ \rho_0.
\]
(See the discussion of the transformation under change of coordinates of comoving variations, such as $\delta^\nu \rho_0$, in the appendix.) Thus,
\[
\delta^\nu \ln r_0 = \frac{1}{2} \frac{\delta^\nu \rho_0}{\rho_0}.
\]
(115)
The contribution (106) to $\omega_{\theta}$ can therefore be written as
\[
\frac{1}{64 \pi G} \int_{S_0} \delta^\nu \rho_0 \partial_e g_{pq} \delta^\nu e^{pq} d^2 \theta - (1 \leftrightarrow 2).
\]
(116)
Summing (104), (116) and (105), one obtains
\[
\omega_{\theta} [\delta_1, \delta_2] = \frac{1}{16 \pi G} \int_{S_0} d^2 \theta \left\{ \delta_1 \lambda \delta_2 \rho_0 + \delta_1 \bar{\tau}_{\bar{R}} \delta_2 \rho' + \frac{1}{4} \delta_1 \rho_0 \partial_e g_{pq} \delta_2 e^{pq} \right\}
\]
\[
+ \frac{1}{2} \frac{\rho_0}{\rho_0} \int_1^\bar{\rho} v^2 \delta_1^\nu e^{pq} \partial_{\nu} \delta_2^\nu e_{pq} dv \right\} - (1 \leftrightarrow 2).
\]
(117)
The sum of (117) and its $L$ branch analogue is the desired expression for the symplectic 2-form $\omega_{\gamma} = \omega_{\theta} + \omega_{\pi}$, in terms of the free initial data, valid for admissible variations. It coincides with the expression given in [Rei08] (although there $\delta^e e$ was called $\delta^e e$).

The variations appearing in (117) are not simply the variations of the components of the initial data fields. For instance, $\delta^e \rho_0(\theta)$ is not the variation of $\rho_0(\theta)$ but rather this variation minus $\delta^e e_{pq}(\theta)$. Expressed directly in terms of the variations of the components of the initial data fields, each in a chart ‘natural’ to it, the symplectic form is
\[
\omega_{\theta} [\delta_1, \delta_2] = \frac{1}{16 \pi G} \left\{ \frac{1}{2} \int_{S_0} d^2 y \rho_0 \int_{r_0}^{\bar{R}} r^2 \delta_1 e_{ij} \partial_i \delta_2 e_{ij} r \right. + \frac{1}{4} \int_{S_0} \delta_1 \rho_0 \partial_e e_{ij} \delta_2 \bar{\tau}_{\bar{R}} [e^{ij}(\gamma)] d^2 y
\]
\[
+ \int_{S_0} \left[ \delta_1 \lambda \delta_2 \rho_0 + \delta_1 \bar{\tau}_{\bar{R}} \delta_2 \rho' \right] d^2 \theta - (1 \leftrightarrow 2) \right\}.
\]
(118)
This is the expression given in [Rei07]. In the first, bulk, term the components of $e$ are referred to the $\alpha$ chart; in the second term, a surface term, $e$ and $\rho_0$ are referred to the $\gamma$ chart on $S_0$; and in the last term $\lambda$, $\rho_0$, $\bar{\tau}_{\bar{R}}$, and $\delta_2 \rho'$ are referred to the $\theta$ chart. Of course, the components $\delta_2 \rho'$ of $S_0$ are also determined by the $\gamma$ chart. What is meant in this case is that the variation of these components is evaluated at constant $\theta$. 

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Appendix. Variations of fields and integrals

In the main text, extensive use is made of charts that are adapted to the metric, in particular the $a$ and $b$ charts. We call such charts moving charts because they can change under variations of the fields. In this appendix, some basic facts about the variations of fields and their components in such charts are derived.

In our formalism, fields will be defined by their components in charts. The components of a field $F$ in a chart $x$, denoted $[F]_x$, are a collection of numbers, or more precisely, $C$ valued functions of the coordinates $x^\mu$ of the chart $x$. Of the chart dependence of the components, we will require only that within the domain of $x$ the components of $F$ in any other chart $y$ are determined entirely by its $x$ components and the transition function from the $x$ to the $y$ chart. The advantage of this coordinate-dependent representation of fields is that it allows us to treat all the fields that we encounter, tensors, densities, connection coefficients and others, in a uniform manner.

Recall that by virtue of its definition a manifold comes equipped with an atlas of charts (see for example [Wald84]). We will call these the fixed charts. A fixed chart assigns definite values to the coordinates at each manifold point in its domain. Moving charts are families of fixed charts depending on the values of fields or parameters. The coordinate values they assign to points can depend on these fields or parameters. For instance, the $a_A$ chart defined in subsection 4.3 depends on the metric and moves when the metric is varied.

The variation of a function $f$ of a parameter $\lambda$ when $\lambda$ varies is simply another word for the derivative of $f$: $\delta f \equiv df/d\lambda$. We will be interested chiefly in the variations induced by variations of the metric field. Thus, we have a family of metric fields parameterized by $\lambda$ and we wish to find the derivative in $\lambda$ of quantities calculated from the metric.

The variation of a function of $\lambda$ only is thus unambiguously defined. But a field depends also on position in the manifold, and its components depend on the chart used. Thus, to define the variation of a field $F$ one must define what it means to hold the position and the chart constant while $\lambda$ is varied. Here, we define $\delta F$ in the usual way, as the $\lambda$ derivative of $F$ in a fixed chart. That is, we set the components $[\delta F]_x$ of $\delta F$ in a fixed chart equal to the variation of the $x$ components of $F$ at fixed values of the coordinates $x$:

$$[\delta F]_x = \delta [F]_x. \quad (A.1)$$

Variations may also be defined in an entirely analogous manner using moving charts. Let $C$ be an atlas of comoving charts, that is, an atlas of charts which are $\lambda$-dependent functions of the fixed charts, but have $\lambda$-independent transition functions among themselves. Then, the components of the comoving variation $\delta^C F$ in any chart $c \in C$ are

$$[\delta^C F]_c = \delta [F]_c, \quad (A.2)$$

where $\delta [F]_c$ denotes the variation of the $c$ components at fixed values of the $c$ coordinates. For any given value of $\lambda$, the moving chart $c$ coincides with a fixed chart $c_0$, and the components
of a field with respect to \( c \) are identified with the \( c_j \) components of the field. (But \( \delta[F] \), is the derivative \( d/d\lambda \) of \( [F]_\lambda = [F]_{c_\lambda} \) holding constant the values of the \( c \) coordinates, not those of the \( c_j \) coordinates at fixed \( \lambda \).) Note that within its domain a moving chart \( c \) defines its comoving atlas uniquely, and thus also the corresponding comoving variation, which may as well be written \( \delta' \). Thus, for instance the variation \( \delta'^{\alpha} \) used in the main text is defined by the \( a_\lambda \) chart.

**Proposition.**

\[
\delta^c = \delta + \xi_v. \tag{A.3}
\]

Here, \( \xi_v \) is the Lie derivative along the `velocity' \( v \) of the moving charts in \( C \) with respect to the fixed charts. \( v^\alpha \) is the \( \lambda \) rate of change of the fixed chart coordinate \( x^\alpha \) corresponding to constant values of the coordinates of the moving charts in \( C \). Equivalently, let \( \Phi^c_\lambda \) be the diffeomorphism such that \( \Phi^c_\lambda (\Phi^c_\lambda(p)) = \Phi^c_\lambda(p) \) for each chart \( c \in C \) and each point \( p \) in the domain of \( c_0 \). Then, \( v \) is the velocity of the flow \( \Phi^c_\lambda \), i.e. the tangent of the curve \( \lambda \mapsto \Phi^c_\lambda(p) \) at \( \lambda = 0 \). (Without loss of generality we may suppose that the variation is being evaluated at \( \lambda = 0 \).)

**Proof of the proposition.** The proposition simply expresses the fact that the variation of \([F]_\lambda\), the moving chart components of a field \( F \), can be resolved into the sum of a variation, \( \delta \), holding the chart fixed, and a variation, \( \xi_v \), holding the fixed chart components of \( F \) fixed. Thus,

\[
[\delta^c F]_{c_0} = [\delta F]_{c_0} = d/d\lambda([F]_{c_0}) + d/d\lambda([F_0]_{c_0}). \tag{A.4}
\]

where \( F_0 \) is the field \( F \) at \( \lambda = 0 \) in the sense that \([F_0]_\lambda = [F]_\lambda \) at \( \lambda = 0 \) in any fixed chart \( x \). The first term is \([\delta F]_{c_0}\). The second term turns out to be the Lie derivative of \( F \).

The Lie derivative is defined in terms of the action of diffeomorphisms on the field (see [Wald84]). The action \( \Phi^* \) of a diffeomorphism \( \Phi \) on a field \( F \) satisfies the requirement that for any chart \( x \)

\[
[\Phi^*(F)]_{\Phi^*(x)} = [F]_x, \tag{A.5}
\]

where \( \Phi^*(x) \circ \Phi = x \). That is, one requires that if one acts on both the chart and the field with the same diffeomorphism, then the components of the new field in the new chart are the same as those of the old field in the old chart. As a consequence \([F]_{c_\lambda} = [\Phi^c_\lambda^{-1}(F)]_{c_0} \) and thus at \( \lambda = 0 \)

\[
[\xi_v]_{c_0} = -d/d\lambda([\Phi^c_\lambda(F_0)]_{c_0}) = d/d\lambda([\Phi^c_\lambda^{-1}(F_0)]_{c_0}) = d/d\lambda([\Phi^c_\lambda(F_0)]_{c_0}), \tag{A.6}
\]

which completes the proof of the proposition.

Instead of viewing \( \delta^c F \) as the variation under \( \delta \) of the components of \( F \) in the moving atlas \( C \), one may view it as the variation under \( \delta + \xi_v \) of the components of \( F \) in fixed charts. Since the moveable atlas \( C \) is in fact fixed under the variation \( \delta + \xi_v \), the two interpretations are consistent. \( \delta^c \) may be regarded as a projection of \( \delta \) to variations that fix \( C \). (It is important to remember that \( v \) depends on \( \delta \). Thus for instance, if \( \delta \) already fixes \( C \), then \( v = 0 \).)

How do the components of \( \delta F \) and \( \delta^c F \) transform from one chart to another? Suppose \( x \) and \( y \) are two fixed charts. Recall that within the intersection of the domains of these charts the \( y \) components of a field \( F \) are determined by its \( x \) components via a transformation \( T \) depending only on the transition map \( \varphi = y \circ x^{-1} \) between the charts themselves. If we assume that \( T \) is functionally differentiable in \([F]_\lambda\), then

\[
[\delta F]_y = [\delta F]_x = \delta T ([F]_x) = DT_\lambda \delta[F]_x, \tag{A.7}
\]

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where $DT$ is the derivative of $T$ and $\partial$ denotes contraction. That is, $\delta F$ transforms according to the linearization of the transformation of $F$. In the cases of interest to us, $[F]_x$ is a function only of $[F]_y$ at the same manifold point. That is, $[F]_y(y) = \tau([F]_{\lambda}(\varphi^{-1}(y)))$ with $\varphi^{-1}(y)$ the $x$ coordinates of the point defined by the values $y$ of the $y$ coordinates, and $\tau$ an ordinary function of the space of components to itself. Then, the transformation law for $\delta F$ reduces to

$$[\delta F]_y = D\tau \partial [F]_x \circ \varphi^{-1},$$

(A.8)

with $D$ now the derivative in the space of components (which is finite dimensional for the fields we encounter) and the contraction also taken in this space.

The variations $\delta^i F$ transform in precisely the same way. Let $x'$ and $y'$ be the moving charts in $C$ formed by carrying $x$ and $y$ along the flow of $C$: $x'_x \circ \Phi_{C\lambda} = x$ and $y'_y \circ \Phi_{C\lambda} = y$. Then, by (A.2), $[\delta^i F]_{y'} = [\delta^i F]_{y'} = \delta [F]_{y'}$ and $[\delta^i F]_{y'} = \delta [F]_{y'}$ at $\lambda = 0$. But the transition map from the $x'$ to the $y'$ chart is unaffected by the flow. It is just the transition map $\varphi$ from $x$ to $y$ coordinates. The transformation from $x'$ to $y'$ components is thus also the same as that from $x$ to $y$ components: $[F]_{y'} = T([F]_{y'}).$ It follows that $\delta^i F$ transforms according to

$$[\delta^i F]_{y'} = \delta [F]_{y'} = \delta T([F]_{y'}) = DT \partial [F]_{y'} = DT \partial [\delta^i F]_{y'},$$

(A.9)

just like $\delta F$.

The variations of several integrals are evaluated in this work. In particular, part of the symplectic 2-form on $N_R$ is obtained by varying the bulk term in the symplectic potential on $N_R$. The latter is an integral of the form $\int_{N_R} F$ with $F$ a 3-form. Using the $\alpha_R$ chart this integral may be expressed as $\int_{S_0} \int_{r_0} F_{r12} d\tau d^2 y$, an integral over a domain in $\mathbb{R}^3$. Its variation is therefore

$$\delta \int_{N_R} F = \int_{S_0} \int_{r_0} \delta F_{r12} d\tau d^2 y - \int_{S_0} \delta [r_0]_y [F]_{r12} |_{r=0} d^2 y.$$  

(A.10)

Here, $\delta [r_0]_y$ is the variation of the scalar $r_0$ at constant $y$. This variation may be expressed in a coordinate-independent way in terms of the comoving variation $\delta^a$ associated with the $\alpha_R$ chart:

$$\delta \int_{N_R} F = \int_{S_0} \delta^a F - \int_{S_0} \delta [r_0]_y \partial_y J F,$$

(A.11)

with $S_0$ oriented so that $\int_{S_0} dy^1 \wedge dy^2 = \int_{S_0} d^2 y$, that is, opposite to $\partial N_R$.

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