



Evaluating Small Sphere Limit of the Wang–Yau Quasi-Local Energy

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Abstract: In this article, we study the small sphere limit of the Wang–Yau quasi-local energy defined in Wang and Yau (Phys Rev Lett 102(2):021101, 2009, Commun Math Phys 288(3):919–942, 2009). Given a point p in a spacetime N , we consider a canonical family of surfaces approaching p along its future null cone and evaluate the limit of the Wang–Yau quasi-local energy. The evaluation relies on solving an “optimal embedding equation” whose solutions represent critical points of the quasi-local energy. For a spacetime with matter fields, the scenario is similar to that of the large sphere limit found in Chen et al. (Commun Math Phys 308(3):845–863, 2011). Namely, there is a natural solution which is a local minimum, and the limit of its quasi-local energy recovers the stress-energy tensor at p . For a vacuum spacetime, the quasi-local energy vanishes to higher order and the solution of the optimal embedding equation is more complicated. Nevertheless, we are able to show that there exists a solution that is a local minimum and that the limit of its quasi-local energy is related to the Bel–Robinson tensor. Together with earlier work (Chen et al. 2011), this completes the consistency verification of the Wang–Yau quasi-local energy with all classical limits.

1. Introduction

In general relativity, a spacetime is a 4-manifold N with a Lorentzian metric $g_{\alpha\beta}$ satisfying the *Einstein equation*

$$R_{\alpha\beta} - \frac{R}{2}g_{\alpha\beta} = 8\pi T_{\alpha\beta},$$

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where $R_{\alpha\beta}$ and R are the Ricci curvature and the scalar curvature of the metric $g_{\alpha\beta}$, respectively. On the right hand side of the Einstein equation, $T_{\alpha\beta}$ is the stress-energy tensor of the matter field, a divergence free and symmetric 2-tensor. For most matter fields, $T_{\alpha\beta}$ satisfies the dominant energy condition. For a vacuum spacetime where $T_{\alpha\beta} = 0$ (which implies $R_{\alpha\beta} = 0$), one way of measuring the gravitational energy is to consider the *Bel–Robinson tensor* [2]

$$Q_{\mu\nu\alpha\beta} = W^\rho{}_\mu{}^\sigma{}_\alpha W_{\rho\nu\sigma\beta} + W^\rho{}_\mu{}^\sigma{}_\beta W_{\rho\nu\sigma\alpha} - \frac{1}{2}g_{\mu\nu}W_\alpha{}^{\rho\sigma\tau}W_{\beta\rho\sigma\tau},$$

where $W_{\alpha\beta\gamma\delta}$ is the Weyl curvature tensor of the spacetime N . For a vacuum spacetime, the Bel–Robinson tensor is a divergence free and totally symmetric 4-tensor which also satisfies a certain positivity condition [9]. The stress-energy tensor and the Bel–Robinson tensor are useful in studying the global structure of the maximal development of the initial value problem in general relativity, see for example [3, 9].

We recall that given a spacelike 2-surface Σ in a spacetime N , the Wang–Yau quasi-local energy $E(\Sigma, X, T_0)$ is defined in [18, 19] with respect to each pair (X, T_0) of an isometric embedding X of Σ into the Minkowski space $\mathbb{R}^{3,1}$ and a constant future time-like unit vector $T_0 \in \mathbb{R}^{3,1}$. If the spacetime satisfies the dominant energy condition and the pair (X, T_0) is admissible (see [19, Definition 5.1]), it is proved that $E(\Sigma, X, T_0) \geq 0$. The Wang–Yau quasi-local mass is defined to be the infimum of the quasi-local energy among all admissible pairs (X, T_0) . The Euler–Lagrange equation for the critical points of the quasi-local energy is derived in [19] and the solutions are referred to as the optimal embeddings. The definition of the Wang–Yau quasi-local mass and the optimal embedding equation are reviewed in more details in Sect. 2.

For a family of surfaces Σ_r and a family of isometric embeddings X_r of Σ_r into $\mathbb{R}^{3,1}$, the limit of $E(\Sigma_r, X_r, T_0)$ is evaluated in [20, Theorem 2.1] under the compatibility condition

$$\lim_{r \rightarrow \infty} \frac{|H_0|}{|H|} = 1, \tag{1.1}$$

where H and H_0 are the mean curvature vectors of Σ_r in N and the image of X_r in $\mathbb{R}^{3,1}$, respectively. Under the compatibility condition, the limit of $E(\Sigma_r, X_r, T_0)$ becomes a linear function of T_0 .

The compatibility condition (1.1) holds naturally in the following situations:

- A family of surfaces approaching the spatial infinity of an asymptotically flat spacetime. The limit of the Wang–Yau quasi-local energy is evaluated in [20]. It is proved that the limit of the quasi-local energy of the coordinate spheres of an asymptotically flat initial data is the linear function dual to the Arnowitt–Deser–Misner (ADM) energy-momentum vector [1].
- A family of surfaces approaching the null infinity of an asymptotically flat spacetime. The limit of the Wang–Yau quasi-local energy is evaluated in [6] where the null infinity is modeled using the Bondi coordinates. It is proved that the limit of the quasi-local energy of the coordinate spheres is the linear function dual to the Bondi–Trautman energy-momentum vector [4, 17].
- A family of surfaces approaching a point p in a spacetime along the null cone of p . This is the small sphere limit we study in this article. It is expected that the leading term of the quasi-local energy recovers the stress-energy tensor in spacetimes with matter fields and the Bel–Robinson tensor for vacuum spacetimes.

In this article, we confirm the last expectation and thus complete the consistency verification of the Wang–Yau energy with all classical limits. The setting for the small sphere limit is as follows: Let p be a point in a spacetime N . Let C_p be the future null hypersurface generated by future null geodesics starting at p . Pick any future directed timelike unit vector e_0 at p . Using e_0 , we normalize a null vector L at p by

$$\langle L, e_0 \rangle = -1.$$

We consider the null geodesics of the normalized L and let r be the affine parameter of these null geodesics. Let Σ_r be the family of surfaces on C_p defined by the level sets of the affine parameter r . The inward null normal \underline{L} of Σ_r is normalized so that

$$\langle L, \underline{L} \rangle = -1.$$

The Wang–Yau quasi-local mass is defined to be the infimum of the quasi-local energy among all admissible pairs (X, T_0) . To evaluate the small sphere limit of the quasi-local mass, we first need to understand the limit of the optimal embedding equation. For the large sphere limit, the optimal embedding equation at infinity of an asymptotically flat spacetime is solved in [6]. We computed the linearization of the optimal embedding equation and obtained a unique optimal embedding which locally minimizes the energy. It is observed that the invertibility of the linearized operator comes from the positivity of the total energy. For the small sphere limit, we apply a similar approach to analyze the optimal embedding equation. For a spacetime with matter fields, there is a unique choice of the leading term of T_0 such that the leading term of the optimal embedding equation is solvable. Moreover, the optimal embedding equation can be solved by iteration. However, for a vacuum spacetime, the quasi-local energy vanishes to higher order and the invertibility of the optimal embedding equation is more subtle. In fact, the leading order term of the optimal embedding equation is solvable for any choice of T_0 and the obstruction to solve the optimal embedding equation only occurs in the third order term of the optimal embedding equation.

The first main result of this article is the following theorem:

Theorem 1.1. *Let Σ_r be the above family of surfaces approaching p and with respect to e_0 .*

- (1) *For the isometric embeddings X_r of Σ_r into \mathbb{R}^3 , the limit of the quasi-local energy $E(\Sigma_r, X_r, T_0)$ as r goes to 0 satisfies*

$$\lim_{r \rightarrow 0} r^{-3} E(\Sigma_r, X_r, T_0) = \frac{4\pi}{3} T(e_0, T_0),$$

where $T(\cdot, \cdot)$ is the stress-energy tensor at p

- (2) *Suppose $T(e_0, \cdot)$ is dual to a timelike vector V at p . There is a family of $(X_r, T_0(r))$ which locally minimizes the energy of Σ_r . Moreover, for this family of pairs, we have*

$$\lim_{r \rightarrow 0} r^{-3} E(\Sigma_r, X_r, T_0(r)) = \frac{4\pi}{3} \sqrt{-\langle V, V \rangle}.$$

For a vacuum spacetime, the quasi-local energy vanishes to higher order. We proved that the leading order term of the Wang–Yau quasi-local energy is of $O(r^5)$. In order to describe the result in the vacuum case, we pick a local coordinate system (x^0, x^1, x^2, x^3) near p such that $e_0 = \frac{\partial}{\partial x^0}$ at p and denote by \bar{W}_{0kmn} the value of $W(e_0, \frac{\partial}{\partial x^k}, \frac{\partial}{\partial x^m}, \frac{\partial}{\partial x^n})$

at p and by \bar{W}_{0m0n} the value of $W(e_0, \frac{\partial}{\partial x^m}, e_0, \frac{\partial}{\partial x^n})$ at p , etc. From the definition of the Bel–Robinson tensor, for $T_0 = (a^0, a^1, a^2, a^3)$, we have

$$Q(e_0, e_0, e_0, T_0) = \left(\frac{1}{2} \sum_{k,m,n} \bar{W}_{0kmn}^2 + \sum_{m,n} \bar{W}_{0m0n}^2 \right) a^0 + 2 \sum_{m,n,i} \bar{W}_{0m0n} \bar{W}_{0min} a^i.$$

We prove the following theorem:

Theorem 1.2. *Let Σ_r be the above family of surfaces approaching p and with respect to e_0 . Suppose the stress-energy tensor vanishes in an open set in N containing p .*

- (1) *For each observer T_0 , there is a pair $(X_r(T_0), T_0)$ solving the leading order term of the optimal embedding equation of Σ_r (see Lemmas 6.1 and 6.3). For this pair $(X_r(T_0), T_0)$, we have*

$$\lim_{r \rightarrow 0} r^{-5} E(\Sigma_r, X_r(T_0), T_0) = \frac{1}{90} \left[Q(e_0, e_0, e_0, T_0) + \frac{\sum_{m,n} \bar{W}_{0m0n}^2}{2a^0} \right].$$

- (2) *Suppose $Q(e_0, e_0, e_0, \cdot)$ is dual to a timelike vector. Let \mathcal{P} denote the set of (X, T_0) admitting a power series expansion given in Eq. (4.1). We have*

$$\inf_{(X, T_0) \in \mathcal{P}} \lim_{r \rightarrow 0} r^{-5} E(\Sigma_r, X, T_0) = \inf_{(a^0, a^i) \in \mathbb{H}^3} \frac{1}{90} \left[Q(e_0, e_0, e_0, T_0) + \frac{\sum_{m,n} \bar{W}_{0m0n}^2}{2a^0} \right].$$

where \mathbb{H}^3 denotes the set of unit timelike future directed vector in $\mathbb{R}^{3,1}$. The infimum is achieved by a unique $(a^0, a^i) \in \mathbb{H}^3$.

There have been many previous works [5, 10, 11, 21] on evaluating the small sphere limit of different notions of quasi-local energy. In Brown et al. [5], evaluated the small sphere limit of the canonical QLE (a modified Brown–York energy). In Yu [21], evaluated the small sphere limit of a modified Liu–Yau mass (with light cone reference embedding instead of \mathbb{R}^3 reference). In both of the above papers, the family of physical surfaces considered is the same as the one we use in this article. In Fan et al. [10], evaluated the small sphere limit of the Brown–York mass and the Hawking mass, for surfaces approaching a point in a totally geodesic hypersurface in a spacetime. See [16] for a survey of different notions of quasi-local energy and their limiting behaviors.

When the stress-energy density $T_{\alpha\beta}$ is non-vanishing at the point p , all the above small sphere limits of different notions of quasi-local energy give the same result. Namely, the leading order term is $\frac{4\pi r^3}{3} T(e_0, e_0)$. However, if the stress energy density vanishes near p , then the above results give different answers, although all of them are of order $O(r^5)$ and are related to the Bel–Robinson tensor. We compare our calculation with others in the following:

1) In our case, the Lorentzian symmetry is recovered and our energy and momentum components of the limits are computed from the same quasi-local energy expression. By comparison, in the previous results, either there is only the energy component or the momentum components come from a separate definition.

2) In our limit in a vacuum spacetime, the isometric embedding equation into \mathbb{R}^3 is explicitly solved and used to evaluate the limit. While the existence of such isometric embedding is guaranteed by the solution of the Weyl problem by Nirenberg [14] and Pogorelov [15], computing the embedding in terms of the Weyl curvatures at p is needed

for the evaluation of the small sphere limit in a vacuum spacetime. This difficulty is circumvented in several previous works by using the light cone reference instead.

In Sect. 3, we compute the expansion of the induced metric, the second fundamental forms and the connection 1-form of the family of surfaces Σ_r . Using this information, we compute the non-vacuum small sphere limit of the Wang–Yau quasi-local energy in Sect. 4. The rest of the paper is devoted to the small sphere limit in vacuum spacetimes. In Sect. 5, we compute several functions, tensors, and integrals on S^2 that will be used repeatedly in later sections. In Sect. 6, for each observer T_0 , we compute the $O(r^3)$ term of the isometric embedding using the leading order term of the optimal embedding equation. The isometric embeddings, which depends on the choice of T_0 , is denoted by $X_r(T_0)$. In the next four sections, the quasi-local energy associated to the pair $(X_r(T_0), T_0)$ is computed. Sections 7, 8 and 9 are used to compute the three separate terms in the quasi-local energy and these results are combined in Sect. 10 to evaluate $E(\Sigma_r, X_r(T_0), T_0)$. In Sect. 11, we show that there is exactly one T_0 that minimizes $E(\Sigma_r, X_r(T_0), T_0)$ and study the optimal embedding equation in further details.

2. Review of the Wang–Yau Quasi-Local Mass

Let Σ be a closed embedded spacelike 2-surface in the spacetime N . We assume the mean curvature vector H of Σ is spacelike. Let J be the reflection of H through the future outgoing light cone in the normal bundle of Σ . The data used in the definition of the Wang–Yau quasi-local energy is the triple $(\sigma, |H|, \alpha_H)$ on Σ where σ is the induced metric, $|H|$ is the norm of the mean curvature vector, and α_H is the connection 1-form of the normal bundle with respect to the mean curvature vector

$$\alpha_H(\cdot) = \langle \nabla_{(\cdot)}^N \frac{J}{|H|}, \frac{H}{|H|} \rangle$$

where ∇^N is the covariant derivative in N .

Given an isometric embedding $X : \Sigma \rightarrow \mathbb{R}^{3,1}$ and a future timelike unit vector T_0 in $\mathbb{R}^{3,1}$, suppose the projection \tilde{X} of $X(\Sigma)$ onto the orthogonal complement of T_0 is embedded, and denote the induced metric, the second fundamental form, and the mean curvature of the image surface $\tilde{\Sigma}$ of \tilde{X} by $\hat{\sigma}_{ab}$, \hat{h}_{ab} , and \hat{H} , respectively. The Wang–Yau quasi-local energy $E(\Sigma, X, T_0)$ of Σ with respect to the pair (X, T_0) is

$$E(\Sigma, X, T_0) = \frac{1}{8\pi} \int_{\tilde{\Sigma}} \hat{H} d\hat{\Sigma} + \frac{1}{8\pi} \int_{\Sigma} \left[\sqrt{1 + |\nabla\tau|^2} \cosh \theta |H| + \nabla\tau \cdot \nabla\theta - \alpha_H(\nabla\tau) \right] d\Sigma,$$

where

$$\theta = \sinh^{-1} \left(\frac{-\Delta\tau}{|H| \sqrt{1 + |\nabla\tau|^2}} \right),$$

∇ and Δ are the gradient and Laplace operator of σ , respectively, and $\tau = -\langle X, T_0 \rangle$ is considered as the time function on Σ .

If the spacetime satisfies the dominant energy condition, Σ bounds a spacelike hypersurface in N , and the pair (X, T_0) is admissible, it is proved in [19] that $E(\Sigma, X, T_0) \geq 0$. The Wang–Yau quasi-local mass is defined to be the infimum of the quasi-local energy

$E(\Sigma, X, T_0)$ among all admissible pairs (X, T_0) . The Euler–Lagrange equation for a critical point (X, T_0) of the quasi-local energy is the elliptic equation

$$-(\widehat{H}\widehat{\sigma}^{ab} - \widehat{\sigma}^{ac}\widehat{\sigma}^{bd}\widehat{h}_{cd})\frac{\nabla_b\nabla_a\tau}{\sqrt{1+|\nabla\tau|^2}} + div_\sigma\left(\frac{\nabla\tau}{\sqrt{1+|\nabla\tau|^2}}\cosh\theta|H| - \nabla\theta - \alpha_H\right) = 0$$

coupled with the isometric embedding equation for X . This Euler–Lagrange equation is referred to as the optimal embedding equation and a solution is referred to as an optimal embedding.

The corresponding data for the image of the isometric embedding in the Minkowski space can be used to simplify the expression for the quasi-local energy and the optimal embedding equation. Denote the norm of the mean curvature vector and the connection 1-form with respect to the mean curvature vector of $X(\Sigma)$ in $\mathbb{R}^{3,1}$ by $|H_0|$ and α_{H_0} , respectively. We have the following identities relating the geometry of the image of the isometric embedding X and the image surface $\widehat{\Sigma}$ of \widehat{X} .

$$\begin{aligned} \sqrt{1+|\nabla\tau|^2}\widehat{H} &= \sqrt{1+|\nabla\tau|^2}\cosh\theta_0|H_0| - \nabla\tau \cdot \nabla\theta_0 - \alpha_{H_0}(\nabla\tau), \\ &\quad - (\widehat{H}\widehat{\sigma}^{ab} - \widehat{\sigma}^{ac}\widehat{\sigma}^{bd}\widehat{h}_{cd})\frac{\nabla_b\nabla_a\tau}{\sqrt{1+|\nabla\tau|^2}} \\ &\quad + div_\sigma\left(\frac{\nabla\tau}{\sqrt{1+|\nabla\tau|^2}}\cosh\theta_0|H_0| - \nabla\theta_0 - \alpha_{H_0}\right) = 0, \end{aligned}$$

where

$$\theta_0 = \sinh^{-1}\left(\frac{-\Delta\tau}{|H_0|\sqrt{1+|\nabla\tau|^2}}\right).$$

The first identity is derived in [19, Proposition 3.1]. The second identity simply states that a surface inside $\mathbb{R}^{3,1}$ is a critical point of the quasi-local energy with respect to isometric embeddings of the surface back to $\mathbb{R}^{3,1}$ with other time functions. This can be proved by either the positivity of the Wang–Yau quasi-local energy or by a direct computation [7].

We substitute these relations into the expression for $E(\Sigma, X, T_0)$ and the optimal embedding equation and rewrite them in term of the following function f (In [8], we denote this function by ρ):

$$f = \frac{\sqrt{|H_0|^2 + \frac{(\Delta\tau)^2}{1+|\nabla\tau|^2}} - \sqrt{|H|^2 + \frac{(\Delta\tau)^2}{1+|\nabla\tau|^2}}}{\sqrt{1+|\nabla\tau|^2}}. \tag{2.1}$$

The quasi-local energy becomes

$$\begin{aligned} &E(\Sigma, X, T_0) \\ &= \frac{1}{8\pi} \int_\Sigma \left[f(1+|\nabla\tau|^2) + \Delta\tau \sinh^{-1}\left(\frac{f\Delta\tau}{|H_0||H|}\right) - \alpha_{H_0}(\nabla\tau) + \alpha_H(\nabla\tau) \right] d\Sigma, \end{aligned} \tag{2.2}$$

and the optimal embedding equation becomes

$$div_\sigma\left(f\nabla\tau - \nabla[\sinh^{-1}\left(\frac{f\Delta\tau}{|H_0||H|}\right)] - \alpha_{H_0} + \alpha_H\right) = 0. \tag{2.3}$$

In [6], we studied the large sphere limit of the optimal embedding equation using the expression in Eq. (2.3) and derived an iteration scheme to find a solution which minimizes the energy. In later sections, we analyze the small limit of the optimal embedding equation using the same expression.

3. The Expansion of the Physical Data

Let Σ_r be the family of surfaces approaching a point p in the spacetime N constructed in the introduction. In this section, we compute the expansions of the induced metric, the second fundamental forms and the connection 1-form of Σ_r . The result here is essentially the same as the expansions computed in [5] using the Newman-Penrose formalism. However, the quantities are computed in a different frame to adapt to our situation. This simplifies the computation in the later sections.

3.1. Leading order expansion in non-vacuum spacetimes. In this subsection, we compute the expansion of the geometric quantities in terms of the affine parameter r . We compute enough terms in the expansion in order to evaluate the small sphere limit of the Wang–Yau quasi-local mass in spacetimes with matter fields. Expansions to higher order in vacuum spacetimes are given in the next subsection.

We parametrize Σ_r in the following way. Consider a smooth map

$$X : S^2 \times [0, \epsilon) \rightarrow N \tag{3.1}$$

such that for each fixed point in S^2 , $X(\cdot, r)$, $r \in [0, \epsilon)$ is a null geodesic parametrized by the affine parameter r , with $X(\cdot, 0) = p$ and $\frac{\partial X}{\partial r}(\cdot, 0) \in T_p N$ a null vector such that $\langle \frac{\partial X}{\partial r}(\cdot, 0), e_0 \rangle = -1$. Let $L = \frac{\partial X}{\partial r}$ be the null generator, $\nabla_L^N L = 0$. We also choose a local coordinate system $\{u^a\}_{a=1,2}$ on S^2 such that $\partial_a = \frac{\partial X}{\partial u^a}$, $a = 1, 2$ form a tangent basis to Σ_r . Let \underline{L} be the null normal vector field along Σ_r such that $\langle L, \underline{L} \rangle = -1$. Denote

$$\begin{aligned} l_{ab} &= \langle \nabla_{\partial_a}^N \partial_b, L \rangle \\ n_{ab} &= \langle \nabla_{\partial_a}^N \partial_b, \underline{L} \rangle \\ \eta_a &= \langle \nabla_L^N \partial_a, \underline{L} \rangle \end{aligned}$$

for the second fundamental forms in the direction of L and \underline{L} and the connection 1-form in the null normal frame, respectively. We consider these as tensors on S^2 that depend on r and use the induced metric on Σ_r , $\sigma_{ab} = \langle \partial_a, \partial_b \rangle$ to raise or lower indexes. Let ∇ and Δ be the covariant derivative and the Laplacian with respect to σ , respectively.

In particular, we have

$$\begin{aligned} \nabla_{\partial_a}^N L &= -l_a^c \partial_c - \eta_a L \\ \nabla_{\partial_a}^N \partial_b &= \gamma_{ab}^c \partial_c - l_{ab} \underline{L} - n_{ab} L \\ \nabla_{\partial_a}^N \underline{L} &= -n_a^c \partial_c + \eta_a \underline{L}, \end{aligned} \tag{3.2}$$

where γ_{ab}^c are the Christoffel symbols of σ_{ab} . Let

$$\begin{aligned} \hat{l}_{ab} &= l_{ab} - \frac{1}{2}(\sigma^{cd} l_{cd})\sigma_{ab} \\ \hat{n}_{ab} &= n_{ab} - \frac{1}{2}(\sigma^{cd} l_{cd})\sigma_{ab} \end{aligned}$$

be the traceless part of l_{ab} and n_{ab} .

The following identities for covariant derivatives are useful.

$$\begin{aligned} \nabla_L^N \partial_a &= -l_a^c \partial_c - \eta_a L \\ \nabla_L^N \underline{L} &= -\eta^b \partial_b. \end{aligned}$$

We first derive the following:

Lemma 3.1. *The induced metric, the second fundamental forms and the connection 1-form satisfy the following differential equations:*

$$\partial_r \sigma_{ab} = -2l_{ab} \tag{3.3}$$

$$\partial_r l_{ab} = R_{LabL} - l_{ac} l_b^c \tag{3.4}$$

$$\partial_r n_{ab} = R_{Lab\underline{L}} - l_b^c n_{ac} + \nabla_a \eta_b - \eta_a \eta_b \tag{3.5}$$

$$\partial_r \eta_a = R_{LaL\underline{L}} + l_a^b \eta_b \tag{3.6}$$

$$\partial_r (\sigma^{ab} l_{ab}) = \frac{1}{2} (\sigma^{ab} l_{ab})^2 + \hat{l}_a^b \hat{l}_b^a + Ric(L, L) \tag{3.7}$$

$$\partial_r (\sigma^{ab} n_{ab}) = Ric(L, \underline{L}) + R_{L\underline{L}L\underline{L}} + l^{ab} n_{ab} + div_\sigma \eta - \eta_a \eta^a. \tag{3.8}$$

Ric and $R_{\alpha\beta\gamma\delta}$ are the Ricci curvature and the full Riemannian curvature tensor of the spacetime N , respectively.

Proof. Equation (3.3) follows from the definition of second fundamental form. For l_{ab} ,

$$\begin{aligned} \partial_r l_{ab} &= \partial_r \langle \nabla_{\partial_a}^N \partial_b, L \rangle \\ &= R_{LabL} + \langle \nabla_{\partial_a}^N \nabla_L^N \partial_b, L \rangle \\ &= R_{LabL} - l_{ac} l_b^c. \end{aligned}$$

We derive

$$\partial_r (\sigma^{ab} l_{ab}) = l^{ab} l_{ab} + Ric(L, L).$$

Equation (3.7) follows from the decomposition $l^{ab} l_{ab} = \hat{l}^{ab} \hat{l}_{ab} + \frac{1}{2} (\sigma^{ab} l_{ab})^2$. Indeed, this is the Raychaudhuri equation.

For the connection 1-form, we have

$$\begin{aligned} \partial_r \eta_a &= \partial_r \langle \nabla_{\partial_a}^N L, \underline{L} \rangle \\ &= R_{LaL\underline{L}} + l_a^b \eta_b. \end{aligned}$$

For n_{ab} , we have

$$\begin{aligned} \partial_r n_{ab} &= \partial_r \langle \nabla_{\partial_a}^N \partial_b, \underline{L} \rangle \\ &= R_{Lab\underline{L}} + \langle \nabla_{\partial_a}^N (\nabla_L^N \partial_b), \underline{L} \rangle + \langle \nabla_{\partial_a}^N \partial_b, \nabla_L^N \underline{L} \rangle \\ &= R_{Lab\underline{L}} - \langle \nabla_{\partial_a}^N (l_b^c \partial_c + \eta_b L), \underline{L} \rangle - \langle \nabla_{\partial_a}^N \partial_b, \eta^c \partial_c \rangle \\ &= R_{Lab\underline{L}} - l_b^c n_{ac} + \nabla_a \eta_b - \eta_a \eta_b \end{aligned} \tag{3.9}$$

and

$$\begin{aligned} \partial_r (\sigma^{ab} n_{ab}) &= \sigma^{ab} \partial_r n_{ab} + (\partial_r \sigma^{ab}) n_{ab} \\ &= \sigma^{ab} R_{Lab\underline{L}} - l^{ab} n_{ab} + div_\sigma \eta - \eta^a \eta_a + 2l^{ab} n_{ab} \\ &= Ric(L, \underline{L}) + R_{L\underline{L}L\underline{L}} + l^{ab} n_{ab} + div_\sigma \eta - \eta^a \eta_a. \end{aligned} \tag{3.10}$$

□

In the rest of this subsection, we consider the expansions of geometric data as $r \rightarrow 0$. As we remarked, we consider $\sigma_{ab}, l_{ab}, n_{ab}, \eta_a$ as tensors on $S^2 \times [0, \epsilon)$, or tensors on S^2 that depend on the parameter r . We shall see below that they have the following expansions.

$$\begin{aligned} \sigma_{ab} &= \tilde{\sigma}_{ab}r^2 + O(r^3) \\ l_{ab} &= -\tilde{\sigma}_{ab}r + O(r^2) \\ n_{ab} &= \frac{1}{2}\tilde{\sigma}_{ab}r + O(r^2) \\ \eta_a &= \frac{1}{3}\beta_a r^2 + O(r^3) \end{aligned}$$

where $\beta_a = \lim_{r \rightarrow 0} R_{LaL\underline{L}}$ is considered as a $(0, 1)$ tensor on S^2 , $\tilde{\sigma}_{ab}$ denotes the standard metric on unit S^2 . Let $\tilde{\nabla}$ and $\tilde{\Delta}$ be the covariant derivative and the Laplacian with respect to $\tilde{\sigma}_{ab}$, respectively.

We shall also consider the pull-back of tensors from the null hypersurface. For example, we consider $R(L, \cdot, L, \underline{L})$ as a tensor defined on C_p and take its pull-back through (3.1), which is then consider as a $(0, 1)$ tensors on S^2 that depends on r (or on $S^2 \times [0, \epsilon)$). We shall abuse the notations and still denote the pull-back tensor by $R_{LaL\underline{L}}$. In particular, $R_{LabL}, R_{LaL\underline{L}}, R_{L\underline{L}L\underline{L}}$ are considered as r dependent $(0, 2)$ tensor, $(0, 1)$ tensor, and a scalar function on S^2 , respectively, of the following orders

$$R_{LabL} = O(r^2), \quad R_{LaL\underline{L}} = O(r) \text{ and } R_{L\underline{L}L\underline{L}} = O(1).$$

To describe their expansions, we first write down the expansions of L and ∂_a . Let $x^0, x^i, i = 1, 2, 3$ be a normal coordinates system at p such that the original future timelike vector $e_0 \in T_pN$ is $\frac{\partial}{\partial x^0}$. The parametrization (3.1) is given by

$$X(u^a, r) = X^0(u^a, r)\frac{\partial}{\partial x^0} + X^i(u^a, r)\frac{\partial}{\partial x^i}$$

with the following expansions:

$$\begin{aligned} X^0(u^a, r) &= r + O(r^2) \\ X^i(u^a, r) &= r\tilde{X}^i(u^a) + O(r^2), \end{aligned}$$

where $\tilde{X}^i(u^a)$ are the three first eigenfunctions of the standard metric $\tilde{\sigma}_{ab}$ on S^2 . For example, if we take the coordinates $u_a, a = 1, 2$ to be the standard spherical coordinate system θ, ϕ with $\tilde{\sigma} = d\theta^2 + \sin^2\theta d\phi^2$, then $\tilde{X}^1 = \sin\theta \sin\phi, \tilde{X}^2 = \sin\theta \cos\phi$, and $\tilde{X}^3 = \cos\theta$. In particular,

$$\begin{aligned} L &= \frac{\partial X}{\partial r} = \frac{\partial}{\partial x^0} + \tilde{X}^i(u^a)\frac{\partial}{\partial x^i} + O(r) \\ \partial_a &= \frac{\partial X}{\partial u^a} = r\frac{\partial \tilde{X}^i}{\partial u^a}\frac{\partial}{\partial x^i} + O(r^2), \quad a = 1, 2. \end{aligned} \tag{3.11}$$

We have the following expansions for the curvature tensor:

$$\begin{aligned} R_{LabL} &= r^2\bar{R}_{LabL} + O(r^3) \\ R_{LaL\underline{L}} &= r\bar{R}_{LaL\underline{L}} + O(r^2) \\ R_{L\underline{L}L\underline{L}} &= \bar{R}_{L\underline{L}L\underline{L}} + O(r), \end{aligned} \tag{3.12}$$

where \bar{R}_{LabL} , \bar{R}_{LaLL} and \bar{R}_{LLLL} correspond to the appropriate rescaled limit of the respective tensors as $r \rightarrow 0$. For example,

$$\bar{R}_{LabL} = \lim_{r \rightarrow 0} \frac{1}{r^2} R_{LabL} = R\left(\frac{\partial}{\partial x^0} + \tilde{X}^i \frac{\partial}{\partial x^i}, \frac{\partial \tilde{X}^j}{\partial u^a}, \frac{\partial \tilde{X}^k}{\partial u^b}, \frac{\partial}{\partial x^0} + \tilde{X}^l \frac{\partial}{\partial x^l}\right)(p)$$

is considered as a $(0, 2)$ tensor on the standard S^2 .

Lemma 3.2. *We have the following expansions:*

$$l_{ab} = -r\tilde{\sigma}_{ab} + \frac{2}{3}r^3\bar{R}_{LabL} + O(r^4) \tag{3.13}$$

$$\sigma_{ab} = r^2\tilde{\sigma}_{ab} - \frac{1}{3}r^4\bar{R}_{LabL} + O(r^5) \tag{3.14}$$

$$l_a^c = -r^{-1}\delta_a^c + \frac{1}{3}r\bar{R}_{LabL}\tilde{\sigma}^{bc} + O(r^2) \tag{3.15}$$

$$\eta_a = \frac{1}{3}r^2\bar{R}_{LaLL} + O(r^3). \tag{3.16}$$

Proof. Suppose we have the expansions

$$\begin{aligned} \sigma_{ab} &= r^2\tilde{\sigma}_{ab} + r^3\sigma_{ab}^{(3)} + r^4\sigma_{ab}^{(4)} + O(r^5) \\ \eta_a &= r^2\eta_a^{(2)} + O(r^3). \end{aligned}$$

Using $R_{LabL} = r^2\bar{R}_{LabL} + O(r^3)$ and Eq. (3.4), we conclude

$$l_{ab} = -r\tilde{\sigma}_{ab} + \frac{2}{3}r^3\bar{R}_{LabL} + O(r^4). \tag{3.17}$$

From Eq. (3.3), this implies

$$\sigma_{ab} = r^2\tilde{\sigma}_{ab} - \frac{r^4}{3}\bar{R}_{LabL} + O(r^5). \tag{3.18}$$

From Eq. (3.6) for η and expansion for l_{ab} , we derive

$$\eta_a = \frac{1}{3}r^2\bar{R}_{LaLL} + O(r^3).$$

□

Next, we derive the expansion for the mean curvature in the direction of L and \underline{L} .

Lemma 3.3. *We have the following expansions for $\sigma^{ab}l_{ab}$ and $\sigma^{ab}n_{ab}$*

$$\sigma^{ab}l_{ab} = -\frac{2}{r} + \frac{1}{3}r\bar{R}ic(L, L) + O(r^2), \tag{3.19}$$

$$\sigma^{ab}n_{ab} = \frac{1}{r} + r(\sigma^{ab}n_{ab})^{(1)} + O(r^2), \tag{3.20}$$

where

$$(\sigma^{ab}n_{ab})^{(1)} = \frac{1}{2}\bar{R}_{LLLL} + \frac{1}{2}\bar{R}ic(L, \underline{L}) + \frac{1}{12}\bar{R}ic(L, L) + \frac{1}{6}\tilde{\nabla}^a\bar{R}_{LaLL}.$$

Proof. The expansion for $\sigma^{ab}l_{ab}$ follows from the expansions for l_{ab} and σ_{ab} . Equation (3.5) for n_{ab} is equivalent to

$$r\partial_r(r^{-1}n_{ab}) = R_{Lab\underline{L}} - (l_b^c + r^{-1}\delta_b^c)n_{ac} + \nabla_a\eta_b - \eta_a\eta_b.$$

Since $n_{ab} = \frac{1}{2}r\tilde{\sigma}_{ab} + O(r^2)$, it follows that

$$r\partial_r(r^{-1}n_{ab}) = r^2(\bar{R}_{Lab\underline{L}} - \frac{1}{6}\bar{R}_{LabL} + \tilde{\nabla}_a\eta_b^{(2)}) + O(r^3).$$

Integrating with respect to r , we obtain

$$n_{ab} = \frac{1}{2}r\tilde{\sigma}_{ab} + \frac{1}{2}r^3(\tilde{\nabla}_a\eta_b^{(2)} + \bar{R}_{Lab\underline{L}} - \frac{1}{6}\bar{R}_{LabL}) + O(r^4).$$

Using the expansion for σ_{ab} again, we finish the proof of the lemma. \square

The term $(\sigma^{ab}n_{ab})^{(1)}$ can be further simplified by the following lemma.

Lemma 3.4.

$$\tilde{\nabla}^b(\bar{R}_{LbLL}) = 3\bar{R}_{LLLL} + \bar{R}ic(L, \underline{L}) + \frac{1}{2}\bar{R}ic(L, L).$$

Proof. For this, we go back to general Σ_r and compute

$$\sigma^{ab}(\partial_a(R_{LbLL}) - \gamma_{ab}^c R_{LcLL})$$

on Σ_r . This term is of order $\frac{1}{r}$ and the leading coefficient is $\tilde{\sigma}^{ab}\tilde{\nabla}_a(\bar{R}_{LbLL})$. On the other hand, we use the Leibniz rule and derive

$$\begin{aligned} & \sigma^{ab}(\partial_a(R_{LbLL}) - \gamma_{ab}^c R_{LcLL}) \\ &= \sigma^{ab}(\nabla_a^N R)_{LbLL} - (\sigma^{ab}l_{ab})R_{LLLL} - l^{bc}R_{Lbc\underline{L}} - \sigma^{ab}\eta_a R_{LbLL} + n^{bc}R_{LbcL}. \end{aligned}$$

Leading terms of the $O(\frac{1}{r})$ are the second, the third, and the fifth terms and the coefficient is $3\bar{R}_{LLLL} + \bar{R}ic(L, \underline{L})$. \square

In summary, we have the following expansions on the surfaces Σ_r :

Lemma 3.5. *We have the following expansions for the data $(\sigma, |H|, \text{div}\alpha_H)$ on S^2 :*

$$\begin{aligned} \sigma_{ab} &= r^2\tilde{\sigma}_{ab} - \frac{1}{3}r^4\bar{R}_{LabL} + O(r^5) \\ |H|^2 &= \frac{4}{r^2} + [4\bar{R}_{LLLL} + \frac{8}{3}\bar{R}ic(L, \underline{L})] + O(r) \\ \text{div}\alpha_H &= \tilde{\Delta} \left[\frac{1}{2}\bar{R}_{LLLL} + \frac{1}{6}\bar{R}ic(L, L) + \frac{1}{3}\bar{R}ic(L, \underline{L}) \right] \\ &\quad - \bar{R}_{LLLL} - \frac{1}{3}\bar{R}ic(L, \underline{L}) - \frac{1}{6}\bar{R}ic(L, L) + O(r). \end{aligned} \tag{3.21}$$

Proof. This follows from

$$\begin{aligned} |H|^2 &= -2(\sigma^{ab}l_{ab}) \cdot (\sigma^{cd}n_{cd}) \\ \text{div}\alpha_H &= -\frac{1}{2}\Delta \ln(-\sigma^{ab}l_{ab}) + \frac{1}{2}\Delta \ln(\sigma^{ab}n_{ab}) - \text{div}\sigma\eta, \end{aligned} \tag{3.22}$$

the expansions of σ and η in Lemma 3.2 and the expansions of $\sigma^{ab}l_{ab}$ and $\sigma^{ab}n_{ab}$ in Lemma 3.3. We also apply Lemma 3.4 to compute the divergence. \square

3.2. *Further expansions in vacuum spacetimes.* In this subsection, we assume the spacetime is vacuum and compute the higher order terms in the expansions for the physical data. Again, enough expansions are obtained to evaluate the leading term of the small sphere limit of the Wang–Yau quasi-local mass in vacuum. In a vacuum spacetime, the only non-vanishing components of the curvature tensor are the Weyl curvature tensor. We decompose the Weyl curvature tensor at the point p using the null frame $\{e_a, L, \underline{L}\}$ following the notation of Christodoulou and Klainerman in [9] (our convention is $\langle L, \underline{L} \rangle = -1$ though):

$$\begin{aligned}
 \alpha_{ab} &= \bar{W}_{aLbL} \\
 \underline{\alpha}_{ab} &= \bar{W}_{a\underline{L}b\underline{L}} \\
 \beta_a &= \bar{W}_{aL\underline{L}\underline{L}} \\
 \underline{\beta}_a &= \bar{W}_{a\underline{L}\underline{L}\underline{L}} \\
 \rho &= \bar{W}_{\underline{L}\underline{L}\underline{L}\underline{L}} \\
 \sigma &= \epsilon^{ab} \bar{W}_{ab\underline{L}\underline{L}}.
 \end{aligned} \tag{3.23}$$

From the vacuum condition and the Bianchi equations, we obtain the following relations:

$$\begin{aligned}
 \bar{W}_{Lab\underline{L}} &= \frac{1}{2} \tilde{\sigma}_{ab} \rho + \frac{1}{4} \epsilon_{ab} \sigma \\
 \bar{W}_{abcL} &= -\epsilon_{ab} \epsilon_{cd} \beta^d \\
 \bar{W}_{abc\underline{L}} &= \epsilon_{ab} \epsilon_{cd} \underline{\beta}^d \\
 \bar{W}_{ab\underline{L}\underline{L}} &= \frac{1}{2} \epsilon_{ab} \sigma.
 \end{aligned} \tag{3.24}$$

All α , $\underline{\alpha}$, β , $\underline{\beta}$, ρ and σ are considered as tensors on S^2 through the limiting process described above and we compute the covariant derivatives of them with respect to the standard metric $\tilde{\sigma}_{ab}$.

Lemma 3.6.

$$\begin{aligned}
 \tilde{\nabla}_c \alpha_{ab} &= (\tilde{\sigma}_{ca} \tilde{\sigma}_{bd} + \tilde{\sigma}_{cb} \tilde{\sigma}_{ad} + \epsilon_{ca} \epsilon_{bd} + \epsilon_{cb} \epsilon_{ad}) \beta^d \\
 \tilde{\nabla}_c \underline{\alpha}_{ab} &= \frac{1}{2} (\tilde{\sigma}_{ca} \tilde{\sigma}_{bd} + \tilde{\sigma}_{cb} \tilde{\sigma}_{ad} + \epsilon_{ca} \epsilon_{bd} + \epsilon_{cb} \epsilon_{ad}) \underline{\beta}^d \\
 \tilde{\nabla}_a \beta_b &= -\frac{3}{4} \sigma \epsilon_{ab} + \frac{3}{2} \rho \tilde{\sigma}_{ab} - \frac{1}{2} \alpha_{ab} \\
 \tilde{\nabla}_a \underline{\beta}_b &= \frac{3}{8} \sigma \epsilon_{ab} + \frac{3}{4} \rho \tilde{\sigma}_{ab} - \underline{\alpha}_{ab} \\
 \tilde{\nabla}_a \rho &= -\beta_a - 2 \underline{\beta}_a \\
 \tilde{\nabla}_a \sigma &= 2 \epsilon_{ab} (\beta^b - 2 \underline{\beta}^b).
 \end{aligned} \tag{3.25}$$

Proof. All of them are defined as limiting quantities as $r \rightarrow 0$ and we can represent them in terms of the limiting frame as $r \rightarrow 0$:

$$\begin{aligned}
 L &= \frac{\partial}{\partial x^0} + \tilde{X}^i \frac{\partial}{\partial x^i} \\
 \underline{L} &= \frac{1}{2} \left(\frac{\partial}{\partial x^0} - \tilde{X}^i \frac{\partial}{\partial x^i} \right) \\
 e_a &= (\tilde{\nabla}_a \tilde{X}^i) \frac{\partial}{\partial x^i}.
 \end{aligned}
 \tag{3.26}$$

To compute the covariant derivative of α_{ab} , we expand

$$\alpha_{ab} = \tilde{\nabla}_a \tilde{X}^i \tilde{\nabla}_b \tilde{X}^k [\bar{W}_{i0k0} + \tilde{X}^l \bar{W}_{i0kl} + \tilde{X}^j \bar{W}_{ijk0} + \tilde{X}^j \tilde{X}^l \bar{W}_{ijkl}]$$

and differentiate using the relations:

$$\begin{aligned}
 \tilde{\nabla}_a \tilde{\nabla}_a \tilde{X}^i &= -\tilde{\sigma}_{ab} \tilde{X}^i, \quad \sum_{i=1}^3 \tilde{X}^i \tilde{\nabla}_a \tilde{X}^i = 0, \\
 \sum_{i=1}^3 \tilde{\nabla}_a \tilde{X}^i \tilde{\nabla}_b \tilde{X}^i &= \tilde{\sigma}_{ab}, \quad \tilde{\nabla}^a \tilde{X}^i \tilde{\nabla}_a \tilde{X}^j = \delta_{ij} - \tilde{X}^i \tilde{X}^j
 \end{aligned}$$

where $\tilde{\sigma}_{ab}$ is used to raise or lower indexes. Note that all the Weyl curvature coefficients are constants valued at p .

In effect, this is equivalent to differentiating \bar{W}_{aLbL} using the following relations:

$$\begin{aligned}
 \tilde{\nabla}_a L &= e_a \\
 \tilde{\nabla}_a \underline{L} &= -\frac{1}{2} e_a \\
 \tilde{\nabla}_a e_b &= (\underline{L} - \frac{1}{2} L) \tilde{\sigma}_{ab}.
 \end{aligned}
 \tag{3.27}$$

Therefore,

$$\begin{aligned}
 \tilde{\nabla}_c \alpha_{ab} &= \tilde{\nabla}_c \bar{W}_{aLbL} \\
 &= \bar{W}(\tilde{\sigma}_{ca} \underline{L}, L, e_b, L) + \bar{W}(e_a, e_c, e_b, L) + \bar{W}(e_a, L, \tilde{\sigma}_{cb} \underline{L}, L) + \bar{W}(e_a, L, e_b, e_c) \\
 &= \tilde{\sigma}_{ca} \beta_b + \tilde{\sigma}_{cb} \beta_a + \bar{W}_{acbL} + \bar{W}_{bcaL}.
 \end{aligned}$$

Substituting (3.24) gives the desired formula. Other formulae can be derived similarly, for example

$$\begin{aligned}
 \tilde{\nabla}_a \beta_b &= \tilde{\nabla}_a \bar{W}_{LbLL} \\
 &= \bar{W}_{abLL} + \bar{W}_{LbLL} \tilde{\sigma}_{ab} + \bar{W}_{LbaL} - \frac{1}{2} \bar{W}_{LbLa} \\
 &= -\frac{3}{4} \sigma \epsilon_{ab} + \frac{3}{2} \rho \tilde{\sigma}_{ab} - \frac{1}{2} \alpha_{ab}.
 \end{aligned}$$

□

Contracting with respect to $\tilde{\sigma}_{ab}$ and ϵ_{ab} , we obtain the following formulae:

Lemma 3.7.

$$\begin{aligned}
 \tilde{\nabla}^a \alpha_{ab} &= 4\beta_b, \epsilon^{ca} \nabla_c \alpha_{ab} = 4\epsilon_{bd} \beta^d \\
 \tilde{\nabla}^a \underline{\alpha}_{ab} &= 2\underline{\beta}_b, \epsilon^{ca} \nabla_c \underline{\alpha}_{ab} = 2\epsilon_{bd} \underline{\beta}^d \\
 \tilde{\nabla}^a \beta_a &= 3\rho, \epsilon^{ab} \tilde{\nabla}_a \beta_b = -\frac{3}{2}\sigma \\
 \tilde{\nabla}^a \underline{\beta}_a &= \frac{3}{2}\rho, \epsilon^{ab} \tilde{\nabla}_a \underline{\beta}_b = \frac{3}{4}\sigma.
 \end{aligned}
 \tag{3.28}$$

Proof. We apply the following two identities:

$$\begin{aligned}
 \tilde{\sigma}^{ca} (\tilde{\sigma}_{ca} \tilde{\sigma}_{bd} + \tilde{\sigma}_{cb} \tilde{\sigma}_{ad} + \epsilon_{ca} \epsilon_{bd} + \epsilon_{cb} \epsilon_{ad}) &= 4\sigma_{bd} \\
 \epsilon^{ca} (\tilde{\sigma}_{ca} \tilde{\sigma}_{bd} + \tilde{\sigma}_{cb} \tilde{\sigma}_{ad} + \epsilon_{ca} \epsilon_{bd} + \epsilon_{cb} \epsilon_{ad}) &= 4\epsilon_{bd}.
 \end{aligned}$$

□

In particular, it follows that $\tilde{\Delta}\rho = -6\rho$ and $\tilde{\Delta}\sigma = -6\sigma$. Moreover, we obtain the following lemma from equations (3.25) and (3.28).

Lemma 3.8.

$$\tilde{\nabla}_c |\alpha|^2 = 8\alpha_{cb} \beta^b \tag{3.29}$$

$$\tilde{\Delta} |\alpha|^2 = 32|\beta|^2 - 4|\alpha|^2 \tag{3.30}$$

Proof. We compute

$$\begin{aligned}
 \tilde{\nabla}_c |\alpha|^2 &= 2(\tilde{\nabla}_c \alpha_{ab}) \alpha^{ab} \\
 &= 2(\tilde{\sigma}_{ca} \tilde{\sigma}_{bd} + \tilde{\sigma}_{cb} \tilde{\sigma}_{ad} + \epsilon_{ca} \epsilon_{bd} + \epsilon_{cb} \epsilon_{ad}) \beta^d \alpha^{ab} \\
 &= 8\alpha_{cb} \beta^b.
 \end{aligned}$$

Equation (3.30) follows from computing the divergences of the two sides of Eq. (3.29) with the help of equations (3.25) and (3.28). □

We obtain the following two identities.

Corollary 1.

$$\int_{S^2} |\alpha|^2 dS^2 = 8 \int_{S^2} |\beta|^2 dS^2 \tag{3.31}$$

$$\int_{S^2} \tilde{X}^i |\alpha|^2 dS^2 = 16 \int_{S^2} \tilde{X}^i |\beta|^2 dS^2 \tag{3.32}$$

Proof. Equation (3.31) follows from integrating Eq. (3.30) on S^2 with the standard metric. Similarly, Eq. (3.32) follows from multiplying Eq. (3.30) with \tilde{X}^i and then integrating on S^2 . □

Furthermore, the covariant derivative in the spacetime N at p in the direction of L is denoted by the symbol D . For example,

$$D\alpha_{ab} = \nabla_L^N W(e_a, L, e_b, L)(p).$$

$D\alpha_{ab}$ is also considered as a tensor on S^2 through the limiting process and its covariant derivatives with respect to the standard metric $\tilde{\sigma}_{ab}$ can be computed in the same manner. Relations similar to Eq. (3.28) hold among D of the Weyl curvature components.

Lemma 3.9.

$$\begin{aligned}
\tilde{\nabla}^a D\beta_a &= 4D\rho \\
\tilde{\nabla}^a D^2\beta_a &= 5D^2\rho \\
\tilde{\nabla}^a (D\alpha_{ab}) &= 5D\beta_b \\
\tilde{\nabla}^a (D^2\alpha_{ab}) &= 6D^2\beta_b
\end{aligned} \tag{3.33}$$

Proof. We compute

$$\begin{aligned}
\tilde{\nabla}^a D\beta_a &= \tilde{\sigma}^{ab} \tilde{\nabla}_a (\nabla_L^N \bar{W}_{LbLL}) \\
&= \tilde{\sigma}^{ab} \nabla_a \bar{W}_{LbLL} + \nabla_L^N \tilde{\nabla}^a \bar{W}_{LaLL} \\
&= 4\nabla_L^N \bar{W}_{LLLL}.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\tilde{\nabla}^a D^2\beta_a &= \tilde{\sigma}^{ab} \tilde{\nabla}_a (\nabla_L^N \nabla_L^N \bar{W}_{LbLL}) \\
&= \tilde{\sigma}^{ab} (\nabla_a^N \nabla_L^N \bar{W}_{LbLL} + \nabla_L^N \nabla_a^N \bar{W}_{LbLL} + \nabla_L^N \nabla_L^N \tilde{\nabla}_a \bar{W}_{LbLL}) \\
&= \tilde{\sigma}^{ab} (\nabla_a^N \nabla_L^N - \nabla_L^N \nabla_a^N) \bar{W}_{LbLL} + 5\nabla_L^N \nabla_L^N \bar{W}_{LLLL}.
\end{aligned}$$

It suffices to show that

$$\tilde{\sigma}^{ab} (\nabla_a^N \nabla_L^N - \nabla_L^N \nabla_a^N) \bar{W}_{LbLL} = 0.$$

We compute

$$\begin{aligned}
&\tilde{\sigma}^{ab} (\nabla_a^N \nabla_L^N - \nabla_L^N \nabla_a^N) \bar{W}_{LbLL} \\
&= \tilde{\sigma}^{ab} (\bar{W}_{aLL\alpha} \bar{W}_{\alpha bLL} + \bar{W}_{aLb\alpha} \bar{W}_{L\alpha LL} + \bar{W}_{aLL\alpha} \bar{W}_{Lb\alpha L} + \bar{W}_{aLL\alpha} \bar{W}_{LbL\alpha}) \\
&= \tilde{\sigma}^{ab} (\bar{W}_{aLL\alpha} \bar{W}_{\alpha bLL} + \bar{W}_{aLb\alpha} \bar{W}_{L\alpha LL}) \\
&= -\tilde{\sigma}^{ab} (\bar{W}_{aLLL} \bar{W}_{LbLL}) + \bar{W}_{LLLa} \bar{W}_{L\alpha LL} \\
&= \tilde{\sigma}^{ab} (-\bar{W}_{aLLL} \bar{W}_{LbLL} + \bar{W}_{LLLa} \bar{W}_{LbLL}) \\
&= 0.
\end{aligned}$$

The other two relations can be derived similarly. \square

Remark 1. It is also useful to evaluate the Weyl curvature tensor at the point p on

$$e_r = \tilde{X}^i \frac{\partial}{\partial x^i}.$$

For example,

$$\bar{W}_{rabr} = \bar{W}(\tilde{X}^i \frac{\partial}{\partial x^i}, \frac{\partial \tilde{X}^j}{\partial u^a}, \frac{\partial \tilde{X}^k}{\partial u^b}, \tilde{X}^l \frac{\partial}{\partial x^l}).$$

Lemma 3.10. *We have the following expansions for the Weyl curvature tensor:*

$$\begin{aligned}
W_{LaLL} &= r\beta_a + r^2 D\beta_a + \frac{1}{2}r^3 D^2\beta_a + O(r^4) \\
W_{LLLL} &= \rho + rD\rho + r^2[\frac{1}{2}D^2\rho - \frac{1}{3}|\beta|^2] + O(r^3).
\end{aligned} \tag{3.34}$$

Proof. We compute the expansion for W_{LaLL} .

$$\partial_r W_{LaLL} = \nabla_L^N W_{LaLL} - l_a^c W_{LcLL} - \eta^b W_{LaLb}. \tag{3.35}$$

This is equivalent to

$$r \partial_r (r^{-1} W_{LaLL}) = \nabla_L^N W_{LaLL} - (l_a^c + r^{-1} \delta_a^c) W_{LcLL} - \eta^b W_{LaLb}. \tag{3.36}$$

Using the expansion of l_a^c in Eq. (3.15) and the expansion of the curvature tensor in Eq. (3.12), we have

$$-(l_a^c + r^{-1} \delta_a^c) W_{LcLN} - \eta^b W_{LaLb} = O(r^3). \tag{3.37}$$

We differentiate $\nabla_L^N W_{LaLL}$ again and get

$$\partial_r (\nabla_L^N W_{LaLL}) = \nabla_L^N \nabla_L^N W_{LaLL} - l_a^c \nabla_L^N W_{LcLL} - \eta^b \nabla_L^N W_{LaLb}.$$

This is equivalent to

$$r \partial_r (r^{-1} (\nabla_L^N W)_{LaLL}) = r D^2 \beta_a + O(r^2).$$

Thus

$$\nabla_L^N W_{LaLL} = r D \beta_a + r^2 D^2 \beta_a + O(r^3). \tag{3.38}$$

Using equations (3.37) and (3.38) in Eq. (3.36), we rewrite

$$r \partial_r (r^{-1} W_{LaLL}) = r D \beta_a + r^2 D^2 \beta_a + O(r^3).$$

Integrating this equation, we obtain

$$W_{LaLL} = r \beta_a + r^2 D \beta_a + \frac{1}{2} r^3 D^2 \beta_a + O(r^4).$$

For W_{LLLL} , we have

$$\partial_r W_{LLLL} = \nabla_L^N W_{LLLL} - 2 W_{LaLL} \eta^a. \tag{3.39}$$

We compute

$$-2 W_{LaLL} \eta^a = -\frac{2}{3} r |\beta|^2 + O(r^2)$$

and

$$\nabla_L^N W_{LLLL} = D \rho + r D^2 \rho + O(r^2).$$

It follows that

$$W_{LLLL} = \rho + r D \rho + \frac{1}{2} r^2 \left(D^2 \rho - \frac{2}{3} |\beta|^2 \right) + O(r^3).$$

□

Lemma 3.11. *We have the following expansions for $\sigma^{ab}l_{ab}$, $\sigma^{ab}n_{ab}$ and η_a .*

$$\sigma^{ab}l_{ab} = -\frac{2}{r} + \frac{1}{45}r^3|\alpha|^2 + O(r^4) \tag{3.40}$$

$$\sigma^{ab}n_{ab} = \frac{1}{r} + r(\sigma^{ab}n_{ab})^{(1)} + r^2(\sigma^{ab}n_{ab})^{(2)} + r^3(\sigma^{ab}n_{ab})^{(3)} + O(r^4) \tag{3.41}$$

and

$$\eta_a = \frac{r^2}{3}\beta_a + \frac{r^3}{4}D\beta_a + r^4\left[\frac{1}{10}D^2\beta_a - \frac{1}{45}\alpha_{ab}\beta^b\right] + O(r^5), \tag{3.42}$$

where

$$\begin{aligned} (\sigma^{ab}n_{ab})^{(1)} &= \rho \\ (\sigma^{ab}n_{ab})^{(2)} &= \frac{2}{3}D\rho \\ (\sigma^{ab}n_{ab})^{(3)} &= \frac{3}{8}D^2\rho + \frac{1}{30}|\alpha|^2 - \frac{11}{45}|\beta|^2. \end{aligned} \tag{3.43}$$

Proof. We rewrite l_{ab} as

$$\begin{aligned} l_{ab} &= -r\tilde{\sigma}_{ab} - \frac{2}{3}r^3\alpha_{ab} + O(r^4) \\ &= (-r\tilde{\sigma}_{ab} - \frac{1}{3}r^3\alpha_{ab}) - \frac{1}{3}r^3\alpha_{ab} + O(r^4). \end{aligned}$$

Hence, \hat{l}_{ab} , the traceless part of l_{ab} , is given by

$$\hat{l}_{ab} = -\frac{1}{3}r^3\alpha_{ab} + O(r^4). \tag{3.44}$$

It follows that

$$\sigma^{ab}l_{ab} = -\frac{2}{r} + \frac{r^3}{45}|\alpha|^2 + O(r^4). \tag{3.45}$$

Next we compute η_a . Let

$$\eta_a = r^2\eta_a^{(2)} + r^3\eta_a^{(3)} + r^4\eta_a^{(4)} + O(r^5).$$

From Lemma 3.4, we have

$$\eta_a = \frac{1}{3}r^2\beta_a + O(r^3).$$

Equation (3.6) is equivalent to

$$r^{-1}\partial_r(r\eta_a) = W_{LaL\underline{L}} + (l_a^b + r^{-1}\delta_a^b)\eta_b.$$

By Eq. (3.34), the right hand side can be expanded into

$$r\beta_a + r^2D\beta_a + r^3\left[\frac{1}{2}D^2\beta_a - \frac{1}{9}\alpha_{ab}\beta^b\right] + O(r^4).$$

Integrating, we obtain

$$\eta_a^{(3)} = \frac{1}{4}D\beta_a$$

$$\eta_a^{(4)} = \frac{1}{10} D^2 \beta_a - \frac{1}{45} \alpha_{ab} \beta^b.$$

For n_{ab} , we start with Eq. (3.5). It is equivalent to

$$r \partial_r (r^{-1} n_{ab}) = W_{Lab\underline{L}} - (l_b^c + r^{-1} \delta_b^c) n_{ac} + \nabla_a \eta_b - \eta_a \eta_b.$$

The equation becomes

$$\begin{aligned} r \partial_r (r^{-1} n_{ab}) &= r^2 [\bar{W}_{Lab\underline{L}} - \frac{1}{6} \bar{W}_{LabL} + \tilde{\nabla}_a \eta_b^{(2)}] + O(r^3) \\ &= r^2 \rho \tilde{\sigma}_{ab} + O(r^3). \end{aligned}$$

Integrating, we obtain

$$n_{ab} = \frac{1}{2} r \tilde{\sigma}_{ab} + \frac{1}{2} r^3 \rho \tilde{\sigma}_{ab} + O(r^4).$$

Lastly, we deal with Eq. (3.8) for $\sigma^{ab} n_{ab}$. We decompose

$$\begin{aligned} l^{ab} n_{ab} &= l_{ab} \sigma^{ac} \sigma^{bd} n_{cd} \\ &= (l_{ab} + \frac{\sigma_{ab}}{r}) \sigma^{ac} \sigma^{bd} (n_{cd} - \frac{\sigma_{cd}}{2r}) + \frac{1}{2} r^{-1} \sigma^{ab} l_{ab} - r^{-1} \sigma^{ab} n_{ab} + r^{-2}. \end{aligned} \tag{3.46}$$

Thus Eq. (3.8) is equivalent to

$$\begin{aligned} r^{-1} \partial_r (r \sigma^{ab} n_{ab}) &= r^{-2} + \frac{1}{2} r^{-1} \sigma^{ab} l_{ab} + (l^{ab} + r^{-1} \sigma^{ab})(n_{ab} - \frac{1}{2} r^{-1} \sigma_{ab}) \\ &\quad - \eta_a \eta^a + W_{\underline{L}\underline{L}\underline{L}\underline{L}} + \text{div}_\sigma \eta. \end{aligned}$$

Notice that

$$\begin{aligned} l_{ab} + r^{-a} \sigma_{ab} &= -\frac{1}{3} r^3 \alpha_{ab} + O(r^4) \\ n_{cd} - \frac{1}{2} r^{-1} \sigma_{cd} &= r^3 (\frac{1}{2} \rho \tilde{\sigma}_{ab} - \frac{1}{6} \alpha_{ab}) + O(r^4). \end{aligned}$$

We have

$$r^{-1} \partial_r (r \sigma^{ab} n_{ab}) = r^2 \left[\frac{1}{15} |\alpha|^2 - \frac{1}{9} |\beta|^2 \right] + \text{div}_\sigma \eta + W_{\underline{L}\underline{L}\underline{L}\underline{L}} + O(r^3).$$

Integrating this equation, we obtain the expansion for $\sigma^{ab} n_{ab}$.

$$\begin{aligned} \sigma^{ab} n_{ab} &= \frac{1}{r} + \frac{r}{2} [(\rho + (\text{div}_\sigma \eta)^{(0)})] + \frac{r^2}{3} [D\rho + (\text{div}_\sigma \eta)^{(1)}] + \frac{r^3}{4} \left[\frac{1}{2} (D^2 \rho - \frac{2}{3} |\beta|^2) \right. \\ &\quad \left. + (\text{div}_\sigma \eta)^{(2)} - \frac{1}{9} |\beta|^2 + \frac{1}{15} |\alpha|^2 \right] + O(r^4). \end{aligned}$$

We compute

$$\begin{aligned}
 (div_\sigma \eta)^{(0)} &= \frac{1}{3} \tilde{\nabla}^a (\beta_a) = \rho \\
 (div_\sigma \eta)^{(1)} &= \frac{1}{4} \tilde{\nabla}^a D\beta_a = D\rho \\
 (div_\sigma \eta)^{(2)} &= \frac{1}{10} \tilde{\nabla}^a (D^2 \beta_a) - \frac{2}{15} \tilde{\nabla}^a (\alpha_{ab} \beta^b) \\
 &= \frac{1}{2} D^2 \rho + \frac{1}{15} (|\alpha|^2 - 8|\beta|^2).
 \end{aligned}
 \tag{3.47}$$

Equation (3.47) follows from the expansion of η and the following expansion for γ_{ab}^c :

$$\gamma_{ab}^c = \tilde{\gamma}_{ab}^c + r^2 \gamma_{ab}^{(2)c} + O(r^3)
 \tag{3.48}$$

where $\tilde{\gamma}_{ab}^c$ is the Christoffel symbols for $\tilde{\sigma}_{ab}$ and $\gamma_{ab}^{(2)c} = -\frac{1}{6} \tilde{\sigma}^{cd} (\tilde{\nabla}_a \alpha_{db} + \tilde{\nabla}_b \alpha_{ad} - \tilde{\nabla}_d \alpha_{ab})$. \square

4. Small Sphere Limit of the Quasi-Local Energy in Spacetimes with Matters

Recall that the Einstein equation is

$$R_{\alpha\beta} - \frac{1}{2} R g_{\alpha\beta} = 8\pi T_{\alpha\beta}.$$

For the small sphere limit of the Wang–Yau quasi-local energy, we show that the leading order term of the quasi-local energy is precisely the stress-energy density with the order $O(r^3)$. This is true with respect to any isometric embeddings with time functions of the order $O(r^3)$. Moreover, among such embeddings, there is a solution to the optimal embedding equation when the observer is chosen correctly.

4.1. The optimal embedding equation. We study the optimal embedding equation to determine the leading order of the time function. As in [6], we will restrict ourselves to isometric embeddings close to the embedding into \mathbb{R}^3 . Namely, we suppose that the embedding is given by $X = (X_0, X_1, X_2, X_3)$ and an observer T_0 with the following expansion

$$\begin{aligned}
 X_0 &= \sum_{i=2}^{\infty} X_0^{(i)} r^i \\
 X_k &= r \tilde{X}^k + \sum_{i=3}^{\infty} X_k^{(i)} r^i \\
 T_0 &= (a^0, -a^i) + \sum_{i=1}^{\infty} T_0^{(i)} r^i.
 \end{aligned}
 \tag{4.1}$$

where $X_0^{(i)}$, $X_k^{(i)}$ and $T_0^{(i)}$ are independent of r .

Let $\tau = -X \cdot T_0$ be the time function. The optimal embedding equation is

$$\operatorname{div}(f\nabla\tau) - \Delta[\sinh^{-1}(\frac{\Delta\tau f}{|H||H_0})] = \operatorname{div}_\sigma\alpha_{H_0} - \operatorname{div}_\sigma\alpha_H, \tag{4.2}$$

where

$$f = \frac{\sqrt{|H_0|^2 + \frac{(\Delta\tau)^2}{1+|\nabla\tau|^2}} - \sqrt{|H|^2 + \frac{(\Delta\tau)^2}{1+|\nabla\tau|^2}}}{\sqrt{1+|\nabla\tau|^2}}.$$

Assuming Eq. (4.1) and using Lemma 3.5 for $|H|$ and Lemma 4 of [6] for H_0 , we have

$$|H| = \frac{2}{r} + O(r) \text{ and } |H_0| = \frac{2}{r} + O(r). \tag{4.3}$$

As a result, $f = O(r)$ and

$$\operatorname{div}(f\nabla\tau) - \Delta[\sinh^{-1}(\frac{\Delta\tau f}{|H||H_0})] = O(1).$$

From Lemma 3.5, we have $\operatorname{div}_\sigma\alpha_H = O(1)$. For $\operatorname{div}_\sigma\alpha_{H_0}$, we use Lemma 5 of [6] to conclude

$$\operatorname{div}_\sigma\alpha_{H_0} = \frac{1}{2}r^{-1}\tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(2)} + O(1).$$

However, since all other terms in Eq. (4.2) are at most $O(1)$, we conclude that

$$X_0 = \sum_{i=3}^{\infty} X_0^{(i)}r^i$$

and

$$\operatorname{div}_\sigma\alpha_{H_0} = \frac{1}{2}\tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(3)} + O(r).$$

Remark 2. We can also deduce that $X_0^{(2)}$ should vanish from the point of view of minimizing energy. Without loss of generality, we may assume $X_0^{(2)}$ is perpendicular to the kernel of the operator $\tilde{\Delta}(\tilde{\Delta} + 2)$, up to changing lower order terms in T_0 . Let \widehat{X}_r be the isometric embedding of Σ_r into the \mathbb{R}^3 . Following the discussion of [6] for the second variation of the Wang–Yau quasi-local energy and the order of $\operatorname{div}_\sigma\alpha_H$ above, we conclude

$$E(\Sigma_r, X_r, T_0) = E(\Sigma_r, \widehat{X}_r, T_0) + \frac{r^3}{4} \int_{S^2} X_0^{(2)} \tilde{\Delta}(\tilde{\Delta} + 2) X_0^{(2)} dS^2 + O(r^4),$$

where the second term is strictly positive unless $X_0^{(2)}$ vanishes.

From Eq. (4.3), it follows that

$$\lim_{r \rightarrow 0} \frac{|H|}{|H_0|} = 1$$

and we apply Theorem 2.1 of [20] to evaluate the limit of the quasi-local energy. The limit of the quasi-local energy is the linear function dual to the four-vector (e, p^1, p^2, p^3) where

$$e = \frac{1}{8\pi} \int_{\Sigma_r} (|H_0| - |H|) d\Sigma_r$$

$$p^i = \frac{1}{8\pi} \int_{\Sigma_r} X^i (div_\sigma \alpha_H - div_\sigma \alpha_{H_0}) d\Sigma_r.$$

Following the argument in [6], we show that the limit is independent of $X_0^{(3)}$ as follows. It is easy to see that e and p^i are $O(r^3)$. Furthermore, $|H_0|$ is the same up to an error of $O(r^3)$ for any isometric embedding with time functions of the order $O(r^3)$. Hence the leading order term of e is independent of the isometric embedding. For p^i , we have

$$\begin{aligned} & \frac{1}{8\pi} \int_{\Sigma_r} X_i (div_\sigma \alpha_H - div_\sigma \alpha_{H_0}) d\Sigma_r \\ &= \frac{1}{8\pi} \int_{\Sigma_r} r \tilde{X}^i (div_\sigma \alpha_H - \frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2) X_0^{(3)}) d\Sigma_r + O(r^4). \\ &= \frac{1}{8\pi} \int_{\Sigma_r} X^i (div_\sigma \alpha_H) d\Sigma_r + O(r^4). \end{aligned}$$

Hence it suffices to consider the isometric embedding into \mathbb{R}^3 to evaluate the limit.

4.2. Small sphere limit.

Theorem 4.1. *Let Σ_r be the family of affine parameter r from p , normalized by the unit timelike vector e_0 . For any family of isometric embedding X_r of Σ_r into $\mathbb{R}^{3,1}$ such that $X_0 = O(r^3)$, the limit of the quasi-local energy $E(\Sigma_r, X_r, T_0)$ as r goes to 0 satisfies*

$$\lim_{r \rightarrow 0} r^{-3} E(\Sigma_r, X_r, T_0) = \frac{4\pi}{3} T(e_0, T_0).$$

Proof. From the previous subsection, it suffices to evaluate

$$e = \frac{1}{8\pi} \int_{\Sigma_r} (H_0 - |H|) d\Sigma_r$$

$$p^i = \frac{1}{8\pi} \int_{\Sigma_r} X^i div_\sigma \alpha_H d\Sigma_r.$$

where H_0 is the mean curvature of the isometric embedding into \mathbb{R}^3 .

Lemma 4.1. *For the energy component of the limit, we have*

$$\frac{1}{8\pi} \int_{\Sigma_r} (H_0 - |H|) d\Sigma_r = \frac{4}{3} r^3 T(e_0, e_0) + O(r^4).$$

Proof. A similar equality is proved in [21]. Namely,

$$\frac{1}{8\pi} \int_{\Sigma_r} (2\sqrt{K} - |H|) d\Sigma_r = \frac{4}{3} r^3 T(e_0, e_0) + O(r^4)$$

where K is the Gaussian curvature of Σ_r . Using the Gauss equation for the image of the isometric embedding into \mathbb{R}^3 , we conclude that

$$2\sqrt{K} - H_0 = O(r^2).$$

This finishes the proof of the lemma. \square

Next we compute p^i . Using the expansion for $div_\sigma \alpha_H$ from Lemma 3.5, we have

$$\begin{aligned} p^i &= r^3 \int_{S^2} \left[\tilde{\Delta} \left[\frac{1}{2} \bar{R}_{LLLL} + \frac{1}{6} \bar{Ric}(L, L) + \frac{1}{3} \bar{Ric}(L, \underline{L}) \right] \right. \\ &\quad \left. - \bar{R}_{LLLL} - \frac{1}{3} \bar{Ric}(L, \underline{L}) - \frac{1}{6} \bar{Ric}(L, L) \right] \tilde{X}^i dS^2 + O(r^4) \\ &= r^3 \int_{S^2} \left[-2\bar{R}_{LLLL} - \bar{Ric}(L, \underline{L}) - \frac{1}{2} \bar{Ric}(L, L) \right] \tilde{X}^i dS^2 + O(r^4) \end{aligned}$$

where we apply integration by parts for the last equality.

To evaluate the above integral, we switch to the orthogonal frame $\{e_0, e_i\}$. We have

$$\begin{aligned} \int_{S^2} \left[-2\bar{R}_{LLLL} - \bar{Ric}(L, \underline{L}) - \frac{1}{2} \bar{Ric}(L, L) \right] \tilde{X}^i dS^2 &= - \int_{S^2} \bar{Ric}(e_0, e_j) \tilde{X}^j \tilde{X}^i dS^2 \\ &= -\frac{4\pi}{3} \bar{Ric}(e_0, e_i). \end{aligned}$$

This finishes the proof since $\bar{Ric}(e_0, e_i) = 8\pi T_{0i}$. \square

From the above theorem and Sect. 4 of [6], we conclude that the linearized optimal embedding is invertible if $T(e_0, \cdot)$ is timelike. The second part of Theorem 1.1 now follows from the first part and the results in Sect. 4 of [6] for the solution of the optimal embedding equation. The only formal difference is that we have an expansion in r for small r here, rather than an expansion in $\frac{1}{r}$ for r large.

Remark 3. A power series solution of the optimal embedding equation of the form (4.1) can be obtained from the results of [6, Section 4]. To show that this converges to an actual solution, we may solve the optimal embedding equation to a sufficiently higher order so that the error is small enough to apply [13, Theorem 2.1] and [12, Theorem 5.1].

5. Functions and Integrations in Terms of the Weyl Curvature at p

When we compute the small sphere limit in vacuum spacetimes, there are several functions, tensors and integrations on S^2 which appear repeatedly. We compute these quantities here for use in the later sections.

We define the functions W_0 , W_i and P_k as follows:

$$\begin{aligned}
 W_0 &= \tilde{X}^i \tilde{X}^j \bar{W}_{0i0j} = \rho \\
 W_i &= \tilde{X}^j \tilde{X}^k \bar{W}_{0kij} = \frac{1}{2}(\beta^b - 2\underline{\beta}^b) \tilde{\nabla}_b \tilde{X}^i \\
 P_k &= \frac{1}{15} \bar{W}_{0i0k} \tilde{X}^i - \frac{1}{6} W_0 \tilde{X}^k = -\frac{1}{30}(\beta^a + 2\underline{\beta}^a) \tilde{\nabla}_a \tilde{X}^k - \frac{1}{10} \rho \tilde{X}^k
 \end{aligned}
 \tag{5.1}$$

W_j are -6 -eigenfunctions and P_k are -12 -eigenfunctions of the standard Laplacian on S^2 . P_k will appear in the solution of the optimal isometric embedding equation, Lemma 6.3.

Lemma 5.1. *For P_j defined above, we have*

$$\int_{S^2} W_0 \tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} P_j \, dS^2 = 4 \int_{S^2} W_0 \tilde{X}^i P_j \, dS^2.$$

Proof. Integrating by parts,

$$\begin{aligned}
 \int_{S^2} W_0 \tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} P_j \, dS^2 &= - \int_{S^2} \tilde{\nabla}(\rho \tilde{\nabla} \tilde{X}^i) P_j \, dS^2 = 2 \int_{S^2} W_0 \tilde{X}^i P_j \, dS^2 \\
 &\quad - \int_{S^2} P_j \tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} W_0 \, dS^2.
 \end{aligned}$$

Moreover,

$$\begin{aligned}
 \tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} W_0 &= 2 \bar{W}_{0m0n} \tilde{X}^m (\delta^{in} - \tilde{X}^n \tilde{X}^i) \\
 &= -2 W_0 \tilde{X}^i + 2 \bar{W}_{0m0i} \tilde{X}^m,
 \end{aligned}$$

and $\int_{S^2} P_j \tilde{X}^m \, dS^2 = 0$. \square

We also introduce R_{ij} and S_j which will appear in Lemma 7.1 later. From the expansion of the induced metric σ_{ab} , we derive

$$\sigma^{(0)ab} = -\frac{1}{3} \alpha^{ab} \text{ and } \tilde{\sigma}^{ab} \gamma_{ab}^{(2)c} = -\frac{4}{3} \beta^c.
 \tag{5.2}$$

R_{ij} and S_j are defined as follows:

$$\begin{aligned}
 R_{ij} &= -\frac{1}{3} \alpha^{ab} \tilde{X}_a^i \tilde{X}_b^j = \sigma^{(0)ab} \tilde{X}_a^i \tilde{X}_b^j \\
 S_j &= -\frac{4}{3} \beta^c \tilde{X}_c^j = \tilde{\sigma}^{ab} \gamma_{ab}^{(2)c} \tilde{X}_c^j.
 \end{aligned}
 \tag{5.3}$$

Lemma 5.2. *R_{ij} and S_j defined in (5.3) satisfy:*

$$\begin{aligned}
 R_{ij} &= \frac{1}{3} [2 \tilde{X}^i \tilde{X}^k \bar{W}_{0i0k} + 2 \tilde{X}^j \tilde{X}^k \bar{W}_{0k0i} + \tilde{X}^i \tilde{X}^j \tilde{X}^n (\bar{W}_{0inj} + \bar{W}_{0jni}) \\
 &\quad - 2 \bar{W}_{0i0j} - \rho \delta_{ij} - \rho \tilde{X}^i \tilde{X}^j - \tilde{X}^n (\bar{W}_{0inj} + \bar{W}_{0jni})] \\
 S_j &= \frac{1}{3} (-4 \bar{W}_{0j0n} \tilde{X}^n + 4 \tilde{X}^j W_0 + 4 W_j).
 \end{aligned}$$

Proof. Direct computations. \square

We need the following lemma for the integrals of products of spherical harmonic functions.

Lemma 5.3.

$$\begin{aligned} \int_{S^2} \tilde{X}^i \tilde{X}^j dS^2 &= \frac{4\pi}{3} \delta_{ij} \\ \int_{S^2} \tilde{X}^i \tilde{X}^j \tilde{X}^k \tilde{X}^l dS^2 &= \frac{4\pi}{15} \Delta_{ijkl} \\ \int_{S^2} \tilde{X}^i \tilde{X}^j \tilde{X}^k \tilde{X}^l \tilde{X}^m \tilde{X}^n dS^2 &= \frac{4\pi}{105} (\delta_{ij} \Delta_{klmn} + \delta_{ik} \Delta_{jlmn} \\ &\quad + \delta_{il} \Delta_{jkmn} + \delta_{im} \Delta_{jkl n} + \delta_{in} \Delta_{jklm}), \end{aligned}$$

where $\Delta_{ijkl} = \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}$.

Proof. We repeatedly use $\tilde{\Delta} \tilde{X}^i = -2X^i$ and $\tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} \tilde{X}^j = \delta_{ij} - \tilde{X}^i \tilde{X}^j$ to compute the Laplacian of the integrand and then integrate by parts. For example, the integration of

$$\tilde{\Delta}(\tilde{X}^i \tilde{X}^j) = -6\tilde{X}^i \tilde{X}^j + 2\delta_{ij}$$

gives the first formula. \square

6. The Optimal Isometric Embedding

Assuming Eq. (4.1) for the isometric embedding, we determine $X_0^{(3)}$ and $X_i^{(3)}$ from the optimal embedding equation in this section. We show that $X_i^{(3)}$ is determined purely by the induced metric via the isometric embedding. However, for each T_0 , there is a corresponding solution $X_0^{(3)}$ of the leading order term of the optimal embedding equation depending on the choice of T_0 . This is different from the non-vacuum case of the small sphere limit or the large sphere limit, where only one choice of the $T_0^{(0)}$ would allow the leading order term of the optimal embedding equation to be solvable.

Lemma 6.1.

$$X_i^{(3)} = -\frac{1}{3} \beta^c \tilde{\nabla}_c \tilde{X}^i + \frac{1}{2} \rho \tilde{X}^i = \frac{1}{3} \bar{W}_{0i0j} \tilde{X}^j + \frac{1}{3} \bar{W}_{0kji} \tilde{X}^j \tilde{X}^k + \frac{1}{6} \tilde{X}^i \tilde{X}^j \tilde{X}^k \bar{W}_{0j0k}$$

satisfies the linearized isometric embedding equation

$$\sum_i \partial_a \tilde{X}^i \partial_b X_i^{(3)} + \partial_b \tilde{X}^i \partial_a X_i^{(3)} = \frac{1}{3} \alpha_{ab}. \tag{6.1}$$

Proof. To solve the linearized isometric embedding equation, we write

$$X_i^{(3)} = N \tilde{X}^i + P^a \tilde{X}_a^i.$$

Differentiating, we have

$$(X_i^{(3)})_b = N_b \tilde{X}^i + N \tilde{X}_b^i + \tilde{\nabla}_b P^a \tilde{X}_a^i - P_b \tilde{X}^i. \tag{6.2}$$

In terms of N and P^a , Eq. (6.1) is

$$2N\tilde{\sigma}_{ab} + \tilde{\nabla}_a P_b + \tilde{\nabla}_b P_a = \frac{1}{3}\alpha_{ab}. \tag{6.3}$$

By (3.25), we check that $N = \frac{1}{2}\rho$ and $P^a = -\frac{1}{3}\beta^a$ satisfy the above equation. This finishes the proof of the lemma. \square

Lemma 6.2. *Let f be the function as defined in Eq. (2.1). We have*

$$f = \frac{W_0}{a^0}r + O(r^2).$$

Proof.

$$f = \frac{|H_0| - |H|}{a^0} + O(r^2),$$

where

$$|H_0| = \frac{2}{r} + 2W_0r + O(r^2) \quad \text{and} \quad |H| = \frac{2}{r} + W_0r + O(r^2)$$

from the result in [5]. \square

Lemma 6.3. *For the observer $T_0 = (a^0, -a^1, -a^2, -a^3)$, the solution of the optimal embedding equation gives*

$$X_0^{(3)} = -\frac{1}{3}W_0 + \frac{a^i}{a^0}P_i.$$

Proof. We compute

$$div(f\nabla\tau) - \Delta(\sinh^{-1}(\frac{f\Delta\tau}{|H||H_0|})) = \tilde{\nabla}^a(f^{(1)}\tilde{\nabla}_a\tau^{(1)}) - \frac{1}{4}\tilde{\Delta}(f^{(1)}\tilde{\Delta}\tau^{(1)}) + O(r).$$

After simplification, the right hand side, up to a term of $O(r)$ is $-6f^{(1)}\tau^{(1)} + 2\tilde{\nabla}\tau^{(1)}$. $\tilde{\nabla}f^{(1)}$, or $60\frac{a^i}{a^0}P_i$, by the definition of P_i in (5.1).

Setting the Ricci curvature to 0 in Lemma 3.5, we conclude

$$div_\sigma\alpha_H = -4W_0 + O(r).$$

Recall that

$$div_\sigma\alpha_{H_0} = \frac{1}{2}\tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(3)} + O(r).$$

The top order term of the optimal isometric embedding equation is thus

$$\frac{1}{2}\tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(3)} = -4W_0 + 60\frac{a^i}{a^0}P_i.$$

The lemma follows since W_0 is a -6 -eigenfunction and P_i are -12 -eigenfunctions. \square

Corollary 2. *For any isometric embedding into $\mathbb{R}^{3,1}$ with $O(r^3)$ time function, we have*

$$|H_0| = \frac{2}{r} + 2W_0r + O(r^2).$$

Remark 4. By Lemma 4 of [6], the result is the same for any isometric embedding into $\mathbb{R}^{3,1}$ with $O(r^3)$ time function. For the embedding into \mathbb{R}^3 , this is computed in [5].

For each choice of $T_0^{(0)}$, we will compute $8\pi E(\Sigma_r, X_r(T_0), T_0)$ which is given by

$$\int_{\Sigma_r} f(1+|\nabla\tau|^2)+(\Delta\tau) \sinh^{-1}\left(\frac{f\Delta\tau}{|H||H_0|}\right)d\Sigma_r + \int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_{H_0} d\Sigma_r - \int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_H d\Sigma_r. \tag{6.4}$$

We evaluate the three integrals in the next three sections, respectively and put the results together in Sect. 10. Then we minimize the energy among all $T_0^{(0)}$ in Sect. 11.

7. The Energy Component

In this section, we evaluate the first integral in Eq. (6.4):

$$\int_{\Sigma_r} f(1+|\nabla\tau|^2) + (\Delta\tau) \sinh^{-1}\left(\frac{f\Delta\tau}{|H||H_0|}\right)d\Sigma_r.$$

It suffices to evaluate $\int_{\Sigma_r} f[1+|\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H||H_0|}]d\Sigma_r$ since for x small,

$$\sinh^{-1}(x) = x + O(x^3).$$

Denote the expansion of the physical data by

$$\begin{aligned} \sigma_{ab} &= r^2 \tilde{\sigma}_{ab} + r^4 \sigma_{ab}^{(4)} + r^5 \sigma_{ab}^{(5)} + O(r^6) \\ |H| &= \frac{2}{r} + rh^{(1)} + r^2 h^{(2)} + r^3 h^{(3)} + O(r^4) \\ \alpha_H &= r^2 \alpha_H^{(2)} + r^3 \alpha_H^{(3)} + r^4 \alpha_H^{(4)} + O(r^5). \end{aligned}$$

Furthermore, for the embedding $X_r(T_0)$ from Sect. 6, we have

$$\begin{aligned} |H_0| &= \frac{2}{r} + rh_0^{(1)} + r^2 h_0^{(2)} + r^3 h_0^{(3)} + O(r^4) \\ \alpha_{H_0} &= r^2 \alpha_{H_0}^{(2)} + r^3 \alpha_{H_0}^{(3)} + r^4 \alpha_{H_0}^{(4)} + O(r^5). \end{aligned}$$

First we derive the following lemma.

Lemma 7.1.

$$\begin{aligned} |\nabla\tau|^2 &= \sum_{ij} a^i a^j (\delta^{ij} - \tilde{X}^i \tilde{X}^j) + g_1 r^2 + O(r^3) \\ (\Delta\tau)^2 &= 4 \sum_{ij} a^i a^j (\tilde{X}^i \tilde{X}^j) r^{-2} + g_2 + O(r), \end{aligned}$$

where

$$\begin{aligned} g_1 &= a^i a^j (R_{ij} + 2\tilde{\nabla} \tilde{X}^i \tilde{\nabla} X_j^{(3)}) + 2a^0 a^i \tilde{\nabla} \tilde{X}^i \tilde{\nabla} X_0^{(3)} \\ g_2 &= 4a^i a^j \tilde{X}^i (S_j - \tilde{\Delta} X_j^{(3)}) - 4a^0 a^i \tilde{X}^i \tilde{\Delta} X_0^{(3)}, \end{aligned}$$

and R_{ij} and S_j are defined in Eq. (5.3).

Proof. We have

$$\tau = \sum_i a^i \tilde{X}^i r + (a^i X_i^{(3)} + a^0 X_0^{(3)})r^3 + O(r^4)$$

since $T_0 = (a^0, -a^i) + O(r)$. As a result,

$$\begin{aligned} |\nabla\tau|^2 &= \sum_{ij} a^i a^j (\delta^{ij} - \tilde{X}^i \tilde{X}^j) \\ &\quad + r^2 \left[\sigma^{(0)ab} (a^i \tilde{X}_a^i) (a^j \tilde{X}_b^j) + 2(a^i \tilde{\nabla} \tilde{X}^i) (a^j \tilde{\nabla} X_j^{(3)} + a^0 \tilde{\nabla} X_0^{(3)}) \right] + O(r^3), \end{aligned}$$

and the formula follows from equations (3.2), (3.23), and (5.3). Similarly,

$$\begin{aligned} (\Delta\tau)^2 &= 4 \sum_{ij} a^i a^j (\tilde{X}^i \tilde{X}^j) r^{-2} + 4(a^i \tilde{X}^i) (a^j \tilde{\sigma}^{ab} \gamma_{ab}^{(2)c} \tilde{X}_c^j) \\ &\quad - 4(a^i \tilde{X}^i) (a^j \tilde{\Delta} X_j^{(3)} + a^0 \tilde{\Delta} X_0^{(3)}) + O(r), \end{aligned}$$

where

$$\begin{aligned} &4(a^i \tilde{X}^i) (a^j \tilde{\sigma}^{ab} \gamma_{ab}^{(2)c} \tilde{X}_c^j) - 4(a^i \tilde{X}^i) (a^j \tilde{\Delta} X_j^{(3)} + a^0 \tilde{\Delta} X_0^{(3)}) \\ &= 4a^i a^j \tilde{X}^i S_j - 4(a^i \tilde{X}^i) (a^j \tilde{\Delta} X_j^{(3)} + a^0 \tilde{\Delta} X_0^{(3)}) \\ &= 4a^i a^j \tilde{X}^i (S_j - \tilde{\Delta} X_j^{(3)}) - 4a^0 a^i \tilde{X}^i \tilde{\Delta} X_0^{(3)}. \end{aligned}$$

□

With the above lemma, we compute $f(1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H||H_0|})$.

Lemma 7.2.

$$\begin{aligned} &f(1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H||H_0|}) \\ &= a^0 r (h_0^{(1)} - h^{(1)}) + a^0 r^2 (h_0^{(2)} - h^{(2)}) \\ &\quad + a^0 r^3 \left[(h_0^{(3)} - h^{(3)}) + \frac{(W_0)(g_1 + \frac{g_2}{4} - \frac{3}{2} W_0 \sum_{ij} a^i a^j \tilde{X}^i \tilde{X}^j)}{2(a^0)^2} \right] + O(r^4). \end{aligned}$$

Proof. From Lemma 7.1, we have

$$1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H_0|^2} = (a^0)^2 + r^2 (g_1 + \frac{g_2}{4} - h_0^{(1)} \sum_{ij} a^i a^j \tilde{X}^i \tilde{X}^j),$$

and thus

$$|H_0| \sqrt{1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H_0|^2}} = a^0 \left[\frac{2}{r} + r(h_0^{(1)} + \frac{g_1 + \frac{g_2}{4} - h_0^{(1)} \sum_{ij} a^i a^j \tilde{X}^i \tilde{X}^j}{(a^0)^2}) \right] + O(r^2).$$

$|H|\sqrt{1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H|^2}}$ and $1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H_0||H|}$ can be computed similarly and $f(1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H||H_0|})$ is equal to

$$\begin{aligned} & \left(\frac{4}{r} + (h_0^{(1)} + h^{(1)})r\right)[(h_0^{(1)} - h^{(1)})r + (h_0^{(2)} - h^{(2)})r^2 + (h_0^{(3)} - h^{(3)})r^3] \\ & \times \frac{1 + |a|^2 + r^2[g_1 + \frac{g_2}{4} - \frac{(h_0^{(1)} + h^{(1)})}{2} \sum_{ij} a^i a^j \tilde{X}^i \tilde{X}^j]}{a^0 \left\{ \frac{4}{r} + r[h_0^{(1)} + h^{(1)} + \frac{2g_1 + \frac{g_2}{2} - 2(h_0^{(1)} + h^{(1)}) \sum_{ij} a^i a^j \tilde{X}^i \tilde{X}^j}{(a^0)^2}] \right\}}. \end{aligned}$$

Finally we plug in $h_0^{(1)} = 2W_0$ and $h^{(1)} = W_0$. \square

Lemma 7.3.

$$\begin{aligned} & \lim_{r \rightarrow 0} r^{-5} \int_{\Sigma_r} f\left(1 + |\nabla\tau|^2 + \frac{(\Delta\tau)^2}{|H||H_0|}\right) d\Sigma_r \\ & = a^0 \int_{S^2} (h_0^{(3)} - h^{(3)}) dS^2 - \frac{3a^i a^j}{4a^0} \int_{S^2} W_0^2 \tilde{X}^i \tilde{X}^j dS^2 \\ & + \frac{a^i a^j}{2a^0} \int_{S^2} (W_0)[R_{ij} + 2\tilde{\nabla}\tilde{X}^i \cdot \tilde{\nabla}(X_j^{(3)} + P_j) + \tilde{X}^i(S_j - \tilde{\Delta}X_j^{(3)} + 12P_j)] dS^2. \end{aligned}$$

Proof. For the volume form, we have $d\Sigma_r = r^2 dS^2 + O(r^5)$ from the expansion of metric in Lemma 3.5. As a result, it suffices to use $r^2 dS^2$ for the volume form.

For the mean curvature in $\mathbb{R}^{3,1}$,

$$|H_0| = 2\sqrt{K} + O(r^3)$$

since $X_0 = O(r^3)$. Hence, using the result of [21], we conclude that for $i = 1, 2$

$$\int_{S^2} (h_0^{(i)} - h^{(i)}) dS^2 = 0.$$

Thus

$$\begin{aligned} \int_{S^2} W_0(g_1 + \frac{g_2}{4}) dS^2 & = a^i a^j \int_{S^2} W_0[R_{ij} + 2\tilde{\nabla}\tilde{X}^i \tilde{\nabla}(X_j^{(3)} + P_j) \\ & + \tilde{X}^i(S_j - \tilde{\Delta}X_j^{(3)} + 12P_j)] dS^2 \\ & - a^i a^0 \int_{S^2} W_0(\frac{2}{3}\tilde{\nabla}\tilde{X}^i \tilde{\nabla}W_0 + 2\tilde{X}^i W_0) dS^2. \end{aligned}$$

The second integral on the right hand side vanishes by parity. \square

7.1. *Computation of $\int (h_0^{(3)} - h^{(3)})$.* Suppose X is the isometric embedding of σ into $\mathbb{R}^{3,1}$ of the form

$$\begin{aligned} X_0 &= r^3 X_0^{(3)} + O(r^4) \\ X_i &= r \tilde{X}^i + r^3 X_i^{(3)} + r^4 X_i^{(4)} + r^5 X_i^{(5)} + O(r^6), \end{aligned}$$

where $X_0^{(3)}$ and $X_i^{(3)}$ are given by Lemma 6.1 and Lemma 6.3, respectively.

Let X' be the isometric embedding of σ into \mathbb{R}^3 where

$$\begin{aligned} (X_0)' &= 0 \\ (X_i)' &= r \tilde{X}^i + r^3 X_i'^{(3)} + r^4 X_i'^{(4)} + r^5 X_i'^{(5)} + O(r^6). \end{aligned}$$

Let A' be the second fundamental form the embedding X' and \mathring{A}' be its traceless part.

$$\mathring{A}'_{ab} = r^3 \mathring{A}'_{ab}{}^{(3)} + O(r^4)$$

Suppose the Gauss curvature K of σ has the following expansion:

$$2\sqrt{K} = \frac{2}{r} + k^{(1)}r + k^{(2)}r^2 + k^{(3)}r^3 + O(r^4). \tag{7.1}$$

We have

Proposition 7.1. *The integral $\int_{S^2} (h_0^{(3)} - h^{(3)})dS^2$ can be written as follows:*

$$\begin{aligned} \int_{S^2} (h_0^{(3)} - h^{(3)})dS^2 &= \frac{1}{2} \int_{S^2} |\mathring{A}'{}^{(3)}|_{\tilde{\sigma}}^2 dS^2 + \int (k^{(3)} - h^{(3)})dS^2 - \frac{2}{3} \int_{S^2} W_0^2 dS^2 \\ &\quad - 30 \frac{a^i a^j}{(a^0)^2} \int_{S^2} P_i P_j dS^2. \end{aligned}$$

Proof. We first rewrite

$$\int_{\Sigma_r} (|H_0| - |H|)d\Sigma_r = \int_{\Sigma_r} (|H_0| - 2\sqrt{K})d\Sigma_r + \int_{\Sigma_r} (2\sqrt{K} - |H|)d\Sigma_r.$$

Using the result of [21], we have

$$\int_{\Sigma_r} (2\sqrt{K} - |H|)d\Sigma_r = r^5 \int_{S^2} (k^{(3)} - h^{(3)})dS^2.$$

To evaluate $\int_{\Sigma_r} (|H_0| - 2\sqrt{K})d\Sigma_r$, recall that $|H_0|^2$ is given by

$$|H_0|^2 = -(\Delta X_0)^2 + \sum_{i=1}^3 (\Delta X_i)^2. \tag{7.2}$$

Let H'_0 be the mean curvature of X' . Similarly, $|H'_0|$ is given by

$$|H'_0|^2 = \sum_{i=1}^3 (\Delta(X_i)')^2. \tag{7.3}$$

The Gauss equation reads

$$4K = (H_0')^2 - 2|\mathring{A}'|^2. \tag{7.4}$$

We compute from (7.2), (7.4), and (7.3) that

$$|H_0|^2 - 4K = 2|\mathring{A}'|^2 - (\Delta X_0)^2 + \sum_{i=1}^3 (\Delta X_i)^2 - \sum_{i=1}^3 (\Delta X_i')^2,$$

where

$$\Delta X_0 = \Delta(r^3 X_0^{(3)} + O(r^4)) = r \tilde{\Delta} X_0^{(3)} + O(r^2)$$

and

$$\begin{aligned} \sum_{i=1}^3 (\Delta X_i)^2 - \sum_{i=1}^3 (\Delta(X_i'))^2 &= \sum_{i=1}^3 \Delta(X_i - X_i') \Delta(X_i + X_i') \\ &= -4r^2 \tilde{X}^i \tilde{\Delta}(X_i^{(5)} - X_i'^{(5)}) + O(r^3). \end{aligned}$$

As a result, we have

$$\begin{aligned} &\int_{S^2} (h_0^{(3)} - h^{(3)}) dS^2 \\ &= \frac{1}{2} \int_{S^2} |\mathring{A}'^{(3)}|_{\tilde{\sigma}}^2 dS^2 - \frac{1}{4} \int_{S^2} (\tilde{\Delta} X_0^{(3)})^2 dS^2 - \int_{S^2} \tilde{X}^i \tilde{\Delta}(X_i^{(5)} - X_i'^{(5)}) dS^2 \\ &\quad + \int_{S^2} (k^{(3)} - h^{(3)}) dS^2. \end{aligned}$$

To evaluate the second last terms, we need

Lemma 7.4. *If we choose $X_i^{(3)} = X_i'^{(3)}$ and $X_i^{(4)} = X_i'^{(4)}$, $X_i^{(5)}$ and $X_i'^{(5)}$ are related by*

$$2\tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla}(X_i^{(5)} - X_i'^{(5)}) = |\tilde{\nabla} X_0^{(3)}|^2.$$

Proof. This follows directly from the expansion of the metric and the isometric embedding equation. \square

The proposition now follows from the expression of $X_0^{(3)}$ in Lemma 6.3. \square

7.1.1. *Computing $\int |\mathring{A}'^{(3)}|_{\tilde{\sigma}}^2 dS^2$.* The notation in this subsection is slightly different from before. Let X be the isometric embedding of σ into \mathbb{R}^3 where

$$X = r\tilde{X} + r^3 X^{(3)} + O(r^4)$$

and

$$\sigma = r^2 \tilde{\sigma} + r^4 \sigma_{ab}^{(4)} + O(r^5).$$

Let ν be the unit normal of X . Suppose

$$\nu = \tilde{X} + r^2 \nu^{(2)}.$$

We have

$$v^{(2)} = -\langle \tilde{X}, X_a^{(3)} \rangle \tilde{\sigma}^{ab} \tilde{X}_b.$$

The second fundamental form h_{ab} of X has the following expansion

$$h_{ab} = r \tilde{\sigma}_{ab} - r^3 \langle \tilde{X}, \tilde{\nabla}_a \tilde{\nabla}_b X^{(3)} \rangle + O(r^4).$$

The traceless part \hat{A}_{ab} of h_{ab} has the following expansion

$$\hat{A}_{ab} = r^3 \hat{A}_{ab}^{(3)} + O(r^4).$$

Lemma 7.5.

$$\hat{A}_{ab}^{(3)} = (\tilde{X}_a^i \tilde{X}_b^j + \tilde{X}_b^i \tilde{X}_a^j) \left(-\frac{1}{4} W_0 \delta_{ij} - \frac{1}{2} W_{0i0j} \right).$$

Proof. We compute

$$\hat{A}_{ab}^{(3)} = -\langle \tilde{X}, \tilde{\nabla}_a \tilde{\nabla}_b X^{(3)} \rangle + \frac{1}{2} \tilde{\sigma}_{ab} \langle \tilde{X}, \tilde{\Delta} X^{(3)} \rangle - \sigma_{ab}^{(4)}.$$

A direct computation shows

$$\langle \tilde{X}, \tilde{\nabla}_a \tilde{\nabla}_b X^{(3)} \rangle = (\tilde{X}_a^i \tilde{X}_b^j + \tilde{X}_b^i \tilde{X}_a^j) \left[\frac{1}{2} \delta_{ij} \left(-\frac{5}{6} W_0 + \frac{2}{3} W_k \tilde{X}^k \right) + \frac{1}{6} (\bar{W}_{0i0j} - 2 \tilde{X}^k \bar{W}_{0jki}) \right]$$

$$\langle \tilde{X}, \tilde{\Delta} X^{(3)} \rangle = -2W_0 + \frac{4}{3} W_k \tilde{X}^k$$

$$\sigma_{ab}^{(4)} = \frac{1}{3} (\tilde{X}_a^i \tilde{X}_b^j + \tilde{X}_b^j \tilde{X}_a^i) (W_{0i0j} + \frac{1}{2} W_0 \delta_{ij} + \tilde{X}^k W_{0ikj}).$$

Finally, we note that $\sum_k W_k \tilde{X}^k = 0$. \square

This leads to the following.

Lemma 7.6.

$$\int_{S^2} |\hat{A}^{(3)}|_{\tilde{\sigma}}^2 dS^2 = 3 \int_{S^2} W_0^2 dS^2.$$

Proof. Using Lemma 5.3, it is clear that

$$\int_{S^2} W_0^2 dS^2 = \frac{8\pi}{15} \sum_{ij} W_{0i0j}^2.$$

On the other hand,

$$\begin{aligned} & \int_{S^2} |\hat{A}^{(3)}|_{\tilde{\sigma}}^2 dS^2 \\ &= \frac{1}{4} \int_{S^2} [\tilde{\sigma}_{ab} W_0 + \bar{W}_{0i0j} (\tilde{X}_a^i \tilde{X}_b^j + \tilde{X}_b^i \tilde{X}_a^j)] \tilde{\sigma}^{ac} \tilde{\sigma}^{bd} [\tilde{\sigma}_{cd} W_0 + \bar{W}_{0k0l} (\tilde{X}_c^k \tilde{X}_d^l + \tilde{X}_c^l \tilde{X}_d^k)] dS^2 \\ &= \frac{1}{4} \int_{S^2} \left[2W_0^2 + 4W_0(\delta^{kl} - \tilde{X}^k \tilde{X}^l) \bar{W}_{0k0l} + 4\bar{W}_{0i0j} \bar{W}_{0k0l} (\delta^{ik} - \tilde{X}^i \tilde{X}^k) (\delta^{jl} - \tilde{X}^j \tilde{X}^l) \right] dS^2 \\ &= \frac{1}{4} \int_{S^2} \left[2W_0^2 + \frac{4}{3} \bar{W}_{0i0j} \bar{W}_{0i0j} \right] dS^2 \\ &= 3 \int_{S^2} W_0^2 dS^2. \end{aligned}$$

\square

7.1.2. Computing $\int (k^{(3)} - h^{(3)})dS^2$.

Lemma 7.7.

$$\int_{S^2} (k^{(3)} - h^{(3)})dS^2 = -\frac{3}{4} \int_{S^2} W_0^2 dS^2 - \frac{1}{60} \int_{S^2} |\alpha|^2 dS^2 + \frac{11}{45} \int_{S^2} |\beta|^2 dS^2. \tag{7.5}$$

Proof. First we compute $\int k^{(3)}dS^2$. From Eq. (7.1), we have

$$K = \frac{1}{r^2} + k^{(1)} + k^{(2)}r + [k^{(3)} + \frac{(k^{(1)})^2}{4}]r^2 + O(r^3).$$

We also have

$$d\Sigma_r = (r^2 - \frac{1}{180}r^6|\alpha|^2)dS^2 + O(r^7)$$

from the expansion of $\sigma^{ab}l_{ab}$ in Lemma 3.11. By the Gauss–Bonnet theorem $\int_{\Sigma_r} K d\Sigma_r = 4\pi$. Collecting the $O(r^4)$ terms from the left hand side, we have

$$\int_{S^2} k^{(3)} + \frac{(k^{(1)})^2}{4} dS^2 = \frac{1}{180} \int_{S^2} |\alpha|^2 dS^2.$$

Furthermore, $k^{(1)} = 2W_0$. Hence

$$\int_{S^2} k^{(3)} dS^2 = - \int_{S^2} W_0^2 dS^2 + \frac{1}{180} \int_{S^2} |\alpha|^2 dS^2.$$

For $h^{(3)}$, we have

$$h^{(3)} = (\sigma^{ab}n_{ab})^{(3)} - \frac{1}{90}|\alpha|^2 - \frac{(\sigma^{ab}n_{ab}^{(1)})^2}{4}.$$

Using Lemmas 3.11 and 3.9, we conclude

$$\begin{aligned} \int_{S^2} (k^{(3)} - h^{(3)})dS^2 &= -\frac{3}{4} \int_{S^2} W_0^2 dS^2 + \frac{1}{60} \int_{S^2} |\alpha|^2 dS^2 - \int_{S^2} (\sigma^{ab}n_{ab})^{(3)} dS^2 \\ &= -\frac{3}{4} \int_{S^2} W_0^2 dS^2 - \frac{1}{60} \int_{S^2} |\alpha|^2 dS^2 + \frac{11}{45} \int_{S^2} |\beta|^2 dS^2. \end{aligned} \tag{7.6}$$

□

8. Computing the Reference Hamiltonian

In this section, we compute the limit of the second integral in Eq. (6.4):

$$\int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_{H_0} d\Sigma_r.$$

For simplicity, we denote \bar{W}_{0m0n} by D_{mn} .

Proposition 8.1.

$$\lim_{r \rightarrow 0} r^{-5} \int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_{H_0} d\Sigma_r = \frac{4}{3} \int_{S^2} a^0 W_0^2 dS^2 - 10 \frac{a^i a^j}{a^0} \int_{S^2} \tilde{X}^i W_0 P_j dS^2.$$

Proof. We use the optimal embedding equation for the image of the isometric embedding of Σ_r to compute the integral. The equation reads

$$\operatorname{div}_\sigma \alpha_{H_0} = -(\widehat{H} \widehat{\sigma}^{ab} - \widehat{\sigma}^{ac} \widehat{\sigma}^{bd} \widehat{h}_{cd}) \frac{\nabla_b \nabla_a \tau'}{\sqrt{1 + |\nabla \tau'|^2}} + \operatorname{div}_\sigma \left(\frac{\nabla \tau'}{\sqrt{1 + |\nabla \tau'|^2}} \cosh \theta_0 |H_0| - \nabla \theta_0 \right) \tag{8.1}$$

where

$$\tau' = r^3 X_0^{(3)} + r^4 X_0^{(4)} + r^5 X_0^{(5)} + O(r^6) \text{ and } \sinh \theta_0 = \frac{-\Delta \tau'}{|H_0| \sqrt{1 + |\nabla \tau'|^2}}.$$

It suffices to compute the expansion of $\operatorname{div}_\sigma \alpha_{H_0}$ up to $O(r^3)$ error terms. For this purpose, we can approximate $\sqrt{1 + |\nabla \tau'|^2}$ by 1 and θ_0 by $\frac{-\Delta \tau'}{|H_0|}$. We have

$$\begin{aligned} \operatorname{div}_\sigma \alpha_{H_0} &= -[\widehat{H} \widehat{\sigma}^{ab} - \widehat{\sigma}^{ac} \widehat{\sigma}^{bd} \left(\frac{\widehat{H}}{2} \sigma_{cd} + r^3 \dot{A}'_{cd} \right)] \nabla_b \nabla_a \tau' \\ &\quad + \operatorname{div}_\sigma (|H_0| \nabla \tau') + \Delta \left(\frac{\Delta \tau'}{|H_0|} \right) + O(r^3). \end{aligned}$$

Recall

$$|H_0| = \widehat{H} + O(r^2) = \frac{2}{r} + 2W_0 r + O(r^2).$$

We have

$$\begin{aligned} \operatorname{div}_\sigma \alpha_{H_0} &= r^3 \widehat{\sigma}^{ac} \widehat{\sigma}^{bd} \dot{A}'_{cd} \nabla_b \nabla_a \tau' + \left(\frac{1}{r} + W_0 r \right) \Delta \tau' + \nabla H_0 \nabla \tau' \\ &\quad + \frac{r}{2} \Delta [(1 - W_0 r^2) \Delta \tau'] + O(r^3) \\ &= \frac{1}{2} (r^{-2} \Delta) (r^{-2} \Delta + 2) (X_0^{(3)} + r X_0^{(4)} + r^2 X_0^{(5)}) \\ &\quad + r^2 [\tilde{\sigma}^{ac} \tilde{\sigma}^{bd} \dot{A}'_{cd} \tilde{\nabla}_b \tilde{\nabla}_a X_0^{(3)} + W_0 \tilde{\Delta} X_0^{(3)} + 2 \tilde{\nabla} W_0 \tilde{\nabla} X_0^{(3)} \\ &\quad - \frac{1}{2} \tilde{\Delta} (W_0 \tilde{\Delta} X_0^{(3)})] + O(r^3). \end{aligned}$$

We compute

$$\begin{aligned} &\int_{\Sigma_r} (a^i \tilde{X}^i r + r^3 a^\alpha X_\alpha^{(3)}) \operatorname{div}_\sigma \alpha_{H_0} d\Sigma_r \\ &= \int_{\Sigma_r} (a^i \tilde{X}^i r + r^3 a^\alpha X_\alpha^{(3)}) \left\{ \frac{1}{2} (r^{-2} \Delta) (r^{-2} \Delta + 2) (X_0^{(3)} + r X_0^{(4)} + r^2 X_0^{(5)}) \right. \\ &\quad + r^2 \left[\dot{A}'_{ab} \tilde{\nabla}^b \tilde{\nabla}^a X_0^{(3)} + 2W_0 \tilde{\Delta} X_0^{(3)} + 2 \tilde{\nabla} W_0 \tilde{\nabla} X_0^{(3)} \right. \\ &\quad \left. \left. - \frac{1}{2} (\tilde{\Delta} + 2) (W_0 \tilde{\Delta} X_0^{(3)}) \right] \right\} d\Sigma_r + O(r^6) \end{aligned}$$

$$\begin{aligned}
 &= r^5 \int_{S^2} \frac{-a^i S_i}{2} \tilde{\Delta} X_0^{(3)} + \frac{1}{2} a^\alpha X_\alpha^{(3)} \tilde{\Delta} (\tilde{\Delta} + 2) X_0^{(3)} + a^i \tilde{X}^i (\hat{A}_{ab}^{\prime(3)} \tilde{\nabla}^b \tilde{\nabla}^a X_0^{(3)} \\
 &\quad + 2W_0 \tilde{\Delta} X_0^{(3)} + 2\tilde{\nabla} W_0 \tilde{\nabla} X_0^{(3)}) dS^2 + O(r^6).
 \end{aligned}$$

Using Lemmas 5.1, 5.2, 6.1 and 6.3,

$$\begin{aligned}
 \int_{S^2} \frac{-a^i S_i}{2} \tilde{\Delta} X_0^{(3)} dS^2 &= \int_{S^2} \frac{1}{3} (-4a^i D_{in} \tilde{X}^n + 4a^i W_0 \tilde{X}^i + 4a^i W_i) (-W_0 + 6\frac{a^j P_j}{a^0}) dS^2 \\
 &= 8\frac{a^i a^j}{a^0} \int_{S^2} W_0 \tilde{X}^i P_j dS^2 - \frac{4}{3} a^i \int_{S^2} W_i W_0 dS^2, \\
 \int_{S^2} \frac{1}{2} a^\alpha X_\alpha^{(3)} \tilde{\Delta} (\tilde{\Delta} + 2) X_0^{(3)} dS^2 &= \int_{S^2} (\frac{2}{5} a^i D_{in} \tilde{X}^n - \frac{1}{3} a^i W_i - \frac{1}{3} a^0 W_0) (-4W_0 + 60\frac{a^j P_j}{a^0}) dS^2 \\
 &= \frac{4}{3} \int_{S^2} a^i W_i W_0 dS^2 + \frac{4}{3} \int_{S^2} a^0 W_0^2 dS^2,
 \end{aligned}$$

and

$$\begin{aligned}
 \int_{S^2} a^i \tilde{X}^i (2W_0 \tilde{\Delta} X_0^{(3)} + 2\tilde{\nabla} W_0 \tilde{\nabla} X_0^{(3)}) dS^2 &= -2\frac{a^i a^j}{a^0} \int_{S^2} W_0 \tilde{\nabla} \tilde{X}^i \tilde{\nabla} P_j dS^2 \\
 &= -8\frac{a^i a^j}{a^0} \int_{S^2} W_0 \tilde{X}^i P_j dS^2.
 \end{aligned}$$

Finally, we compute $\int a^i \tilde{X}^i \tilde{\sigma}^{ac} \tilde{\sigma}^{bd} \hat{A}_{cd}^{\prime(3)} \tilde{\nabla}_b \tilde{\nabla}_a X_0^{(3)}$. From Lemma 6.3, we have

$$\begin{aligned}
 \int_{S^2} a^i \tilde{X}^i \hat{A}_{ab}^{\prime(3)} \tilde{\nabla}^b \tilde{\nabla}^a X_0^{(3)} dS^2 &= \frac{a^i a^j}{a_0} \int_{S^2} \tilde{X}^i \hat{A}_{ab}^{\prime(3)} \tilde{\nabla}^b \tilde{\nabla}^a P_j dS^2 \\
 &= \frac{a^i a^j}{a_0} \int_{S^2} [\tilde{\nabla}^b \tilde{\nabla}^a \tilde{X}^i \hat{A}_{ab}^{\prime(3)} + 2\tilde{\nabla}^a \tilde{X}^i \tilde{\nabla}^b \hat{A}_{ab}^{\prime(3)} \\
 &\quad + \tilde{X}^i \tilde{\nabla}^b \tilde{\nabla}^a \hat{A}_{ab}^{\prime(3)}] P_j dS^2.
 \end{aligned}$$

The first term vanishes since $\hat{A}_{ab}^{\prime(3)}$ is traceless. For the second and third terms, we use

$$\tilde{\nabla}^b \hat{A}_{ab}^{\prime(3)} = \tilde{\nabla}_a W_0$$

which can be derived from the Codazzi equation. As a result,

$$\begin{aligned}
 \int_{S^2} a^i \tilde{X}^i \hat{A}_{ab}^{\prime(3)} \tilde{\nabla}^b \tilde{\nabla}^a X_0^{(3)} dS^2 &= \frac{a^i a^j}{a_0} \int_{S^2} (2\tilde{\nabla}^a \tilde{X}^i \tilde{\nabla}_a W_0 - 6\tilde{X}^i W_0) P_j dS^2 \\
 &= -10\frac{a^i a^j}{a_0} \int_{S^2} \tilde{X}^i W_0 P_j dS^2,
 \end{aligned}$$

where we apply Lemma 5.1 and integration by parts for the last equality. \square

9. Computing the Physical Hamiltonian

In this section, we compute the limit of the third integral in Eq. (6.4):

$$\int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_H d\Sigma_r.$$

Proposition 9.1.

$$\lim_{r \rightarrow \infty} r^{-5} \int_{\Sigma_r} \tau \operatorname{div}_\sigma \alpha_H d\Sigma_r = \int_{S^2} \left[\frac{4a^0}{3} W_0^2 + \frac{2}{3} a^i W_i W_0 - (a^i \tilde{X}^i) |\beta|^2 \right] dS^2.$$

Proof. Recall that

$$\operatorname{div}_\sigma \alpha_H = -\frac{1}{2} \Delta \ln(-\sigma^{ab} l_{ab}) + \frac{1}{2} \Delta \ln(\sigma^{ab} n_{ab}) - \operatorname{div}_\sigma \eta.$$

The expansions for $\sigma^{ab} l_{ab}$, $\sigma^{ab} n_{ab}$ and $\operatorname{div}_\sigma \eta$ are obtained in Lemma 3.11. First we compute

$$\begin{aligned} \int_{\Sigma_r} \tau \Delta \ln(-\sigma^{ab} l_{ab}) d\Sigma_r &= \int_{S^2} (a^i \tilde{X}^i) r \Delta \left[\frac{2}{r} - \frac{r^3}{45} |\alpha|^2 \right] r^2 dS^2 + O(r^6) \\ &= -r^5 \int_{S^2} (a^i \tilde{X}^i) \tilde{\Delta} \frac{1}{90} |\alpha|^2 dS^2 + O(r^6) \\ &= \frac{1}{45} r^5 \int_{S^2} (a^i \tilde{X}^i) |\alpha|^2 dS^2 + O(r^6). \end{aligned}$$

Next we compute the term involving $\operatorname{div}_\sigma \eta$. From Eq. (3.47), we have

$$\begin{aligned} \int_{\Sigma_r} \tau \operatorname{div}_\sigma \eta d\Sigma_r &= \int_{S^2} (a^i \tilde{X}^i r + r^3 a^\beta X_\beta^{(3)}) \{ \rho + r D \rho \\ &\quad + r^2 \left[\frac{D^2 \rho}{2} + \frac{|\alpha|^2 - 8|\beta|^2}{15} \right] \} r^2 dS^2 + O(r^6) \\ &= r^5 \int_{S^2} \left\{ (a^i \tilde{X}^i) \frac{1}{15} (|\alpha|^2 - 8|\beta|^2) + a^\beta X_\beta^{(3)} \rho \right\} dS^2 + O(r^6), \end{aligned}$$

where Lemma 3.9 is used in the last equality. We compute

$$\int_{S^2} a^\beta X_\beta^{(3)} W_0 dS^2 = \int_{S^2} \left(-\frac{a^0}{3} W_0 - \frac{a^i}{3} W_i \right) W_0 dS^2.$$

Lastly, we compute $\int_{\Sigma_r} \tau \Delta \ln(\sigma^{ab} n_{ab}) d\Sigma_r$.

$$\begin{aligned} &\int_{\Sigma_r} \tau \Delta \ln(\sigma^{ab} n_{ab}) d\Sigma_r \\ &= \int_{\Sigma_r} \Delta [r a^i \tilde{X}^i + r^3 a^\beta X_\beta^{(3)}] \ln(1 + r^2 (\sigma^{ab} n_{ab}))^{(1)} \\ &\quad + r^3 (\sigma^{ab} n_{ab})^{(2)} + r^4 (\sigma^{ab} n_{ab})^{(3)} d\Sigma_r + O(r^6) \end{aligned}$$

$$\begin{aligned}
 &= \int_{S^2} [-2a^i \tilde{X}^i r + r^3(2a^0 W_0 + 2a^i W_i - a^i S_i - \frac{4}{5} a^i D_{ij} \tilde{X}^j)] \{r^2(\sigma^{ab} n_{ab})^{(1)} \\
 &\quad + r^3(\sigma^{ab} n_{ab})^{(2)} \\
 &\quad + r^4[(\sigma^{ab} n_{ab})^{(3)} - \frac{1}{2}((\sigma^{ab} n_{ab})^{(1)})^2]\} dS^2 + O(r^6).
 \end{aligned}$$

Using Lemma 3.11 for the expansion of $\sigma^{ab} n_{ab}$ and applying Lemma 3.9, we conclude

$$\begin{aligned}
 &\int_{\Sigma_r} \tau \Delta \ln(\sigma^{ab} n_{ab}) d\Sigma_r \\
 &= r^5 \int_{S^2} \{(2a^i W_i + 2a^0 W_0 - a^i S_i - \frac{4}{5} a^i D_{ij} \tilde{X}^j) W_0 \\
 &\quad - 2a^i \tilde{X}^i [(\sigma^{ab} n_{ab})^{(3)} - \frac{1}{2} W_0^2]\} dS^2 + O(r^6) \\
 &= r^5 \int_{S^2} [(2a^i W_i + 2a^0 W_0 - a^i S_i) W_0 + a^i \tilde{X}^i (\frac{22}{45} |\beta|^2 - \frac{1}{15} |\alpha|^2)] dS^2 + O(r^6).
 \end{aligned}$$

The proposition follows from collecting terms and Eq. (3.32). \square

10. Evaluating the Energy

We now evaluate the energy for an observer $T_0 = (\sqrt{1 + |a|^2}, -a_1, -a_2, -a_3)$ using Lemma 7.3 and Propositions 7.1, 8.1 and 9.1. It is easy to observe that the energy takes the following form

$$\sum_{\alpha} A_{\alpha} a^{\alpha} + \sum_{ij} A_{ij} \frac{a^i a^j}{a^0}.$$

The following lemma, which follows from Lemma 5.3, is useful for evaluating the above integrals. Recall that we denote \bar{W}_{0m0n} by D_{mn} .

Lemma 10.1.

$$\int_{S^2} W_0 \tilde{X}^i \tilde{X}^j dS^2 = \frac{8\pi}{15} D_{ij} \tag{10.1}$$

$$\int_{S^2} W_0^2 dS^2 = \frac{8\pi}{15} \sum_{ij} D_{ij}^2 \tag{10.2}$$

$$\int_{S^2} W_i \tilde{X}^j \tilde{X}^l dS^2 = \frac{4\pi}{15} (\bar{W}_{0lij} + \bar{W}_{0jil}) \tag{10.3}$$

$$\int_{S^2} W_0 W_i dS^2 = \frac{8\pi}{15} \sum_{jl} D_{jl} \bar{W}_{0lij}. \tag{10.4}$$

Proof. These follow from the definitions of W_0 and W_i as well as Lemma 5.3. \square

First we compute A_0 . Collecting the coefficients, we have

$$\begin{aligned} A_0 &= \frac{1}{12} \int_{S^2} W_0^2 dS^2 - \frac{1}{60} \int_{S^2} |\alpha|^2 dS^2 + \frac{11}{45} \int_{S^2} |\beta|^2 dS^2 \\ &= \frac{1}{12} \int_{S^2} W_0^2 dS^2 + \frac{1}{9} \int_{S^2} |\beta|^2 dS^2. \end{aligned}$$

Equation (3.31) is used in the last equality.

Lemma 10.2.

$$\int_{S^2} |\beta|^2 dS^2 = \frac{12\pi}{15} \sum D_{ij}^2 + \frac{6\pi}{15} \sum \bar{W}_{ijk0}^2.$$

Proof.

$$\begin{aligned} \int_{S^2} |\beta|^2 dS^2 &= \int_{S^2} \bar{W}_{Lir0} \bar{W}_{Lir0} dS^2 - \int_{S^2} \bar{W}_{0rr0} \bar{W}_{0rr0} dS^2 \\ &= \int_{S^2} \bar{W}_{0ir0} \bar{W}_{0ir0} dS^2 + \int_{S^2} \bar{W}_{rir0} \bar{W}_{rir0} dS^2 - \int_{S^2} W_0^2 dS^2 \\ &= \frac{20\pi}{15} D_{ij} D_{ij} + \frac{4\pi}{15} \bar{W}_{jik0} \bar{W}_{min0} (\delta_{jk} \delta_{mn} + \delta_{jm} \delta_{kn} + \delta_{jn} \delta_{mk}) - \frac{8\pi}{15} D_{ij} D_{ij} \\ &= \frac{12\pi}{15} D_{ij} D_{ij} + \frac{4\pi}{15} \bar{W}_{jik0} (\bar{W}_{jik0} + \bar{W}_{kij0}), \end{aligned}$$

where Lemma 10.1 is used in the second last equality. The lemma follows from the first Bianchi identity, since

$$\bar{W}_{ijk0} \bar{W}_{ijk0} = -\bar{W}_{ijk0} (\bar{W}_{jki0} + \bar{W}_{kij0}) = 2\bar{W}_{jik0} \bar{W}_{kij0}.$$

□

Thus, we have proved that

Proposition 10.1.

$$A_0 = \frac{4\pi}{15} \left(\frac{1}{6} \sum_{ijk} \bar{W}_{0ijk}^2 + \frac{1}{2} \sum_{ij} D_{ij}^2 \right).$$

Next we compute A_j . Collecting the coefficients, we have

$$A_j = \int_{S^2} \tilde{X}^i |\beta|^2 dS^2 - \frac{2}{3} \int_{S^2} W_i W_0 dS^2. \tag{10.5}$$

We compute

$$\begin{aligned} \int_{S^2} \tilde{X}^i |\beta|^2 dS^2 &= \int_{S^2} \tilde{X}^i \bar{W}_{Ljr0} \bar{W}_{Lkr0} (\delta^{jk} - X^k X^j) dS^2 \\ &= \int_{S^2} \tilde{X}^i \bar{W}_{Ljr0} \bar{W}_{Ljr0} dS^2 - \int_{S^2} \tilde{X}^i \bar{W}_{0rr0} \bar{W}_{0rr0} dS^2 \\ &= \frac{8\pi}{15} D_{jm} \bar{W}_{0mij}. \end{aligned}$$

As a result, we have

Proposition 10.2.

$$A_i = \frac{4\pi}{15} \left(\frac{2}{3} D_{jm} W_{0mi}\right).$$

At the end, we have

Proposition 10.3.

$$A_{ij} = -\frac{2\pi}{45} \delta_{ij} \sum_{m,n} D_{mn}^2. \tag{10.6}$$

Proof. To compute A_{ij} , we combine Lemma 7.3 and Proposition 7.1, 8.1 and 9.1 and derive

$$\begin{aligned} A_{ij} &= \int_{S^2} \frac{W_0}{2} [R_{ij} + 2\tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} (X_j^{(3)} + P_j) + \tilde{X}^i (S_j - \tilde{\Delta} (X_j^{(3)} + 12P_j))] dS^2 \\ &\quad - \frac{3}{4} \int_{S^2} W_0^2 \tilde{X}^i \tilde{X}^j dS^2 - 30 \int_{S^2} P_i P_j dS^2 - 10 \int_{S^2} \tilde{X}^i W_0 P_j dS^2. \end{aligned} \tag{10.7}$$

We compute

$$\begin{aligned} &\int_{S^2} \frac{W_0}{2} [R_{ij} + 2\tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} (X_j^{(3)} + P_j) + \tilde{X}^i (S_j - \tilde{\Delta} X_j^{(3)} + 12P_j)] dS^2 \\ &= \int_{S^2} \frac{W_0}{6} [2\tilde{X}^i \tilde{X}^k \bar{W}_{0j0k} + 2\tilde{X}^j \tilde{X}^k \bar{W}_{0k0i} - 2\bar{W}_{0i0j} - W_0 \delta_{ij} - W_0 \tilde{X}^i \tilde{X}^j] dS^2 \\ &\quad + \int_{S^2} W_0 \tilde{\nabla} \tilde{X}^i \cdot \tilde{\nabla} \left(\frac{2}{5} \bar{W}_{0j0n} \tilde{X}^n\right) \\ &\quad + \int_{S^2} W_0 \tilde{X}^i \left(\frac{2}{3} \tilde{X}^j W_0 - \frac{2}{3} \bar{W}_{0j0n} \tilde{X}^n + \frac{2}{5} \bar{W}_{0j0n} \tilde{X}^n\right) dS^2 \\ &= \int_{S^2} \frac{W_0}{6} [2\tilde{X}^i \tilde{X}^k \bar{W}_{0j0k} + 2\tilde{X}^j \tilde{X}^k \bar{W}_{0k0i} - 2\bar{W}_{0i0j} - W_0 \delta_{ij} - W_0 \tilde{X}^i \tilde{X}^j] dS^2 \\ &\quad + \int_{S^2} W_0 \tilde{X}^i \left(\frac{2}{3} \tilde{X}^j W_0 - \frac{2}{3} \bar{W}_{0j0n} \tilde{X}^n\right) dS^2 \\ &= \frac{1}{2} \int_{S^2} W_0^2 \tilde{X}^i \tilde{X}^j dS^2 - \frac{1}{6} \delta_{ij} \int_{S^2} W_0^2 dS^2. \end{aligned}$$

Moreover,

$$\begin{aligned} -30 \int_{S^2} P_i P_j dS^2 &= 5 \int_{S^2} W_0 \tilde{X}^i P_j dS^2 \\ &= \frac{1}{3} \int_{S^2} W_0 \bar{W}_{0j0n} \tilde{X}^i \tilde{X}^n dS^2 - \frac{5}{6} \int_{S^2} W_0^2 \tilde{X}^i \tilde{X}^j dS^2, \end{aligned}$$

and thus

$$A_{ij} = \frac{7}{12} \int_{S^2} W_0^2 \tilde{X}^i \tilde{X}^j dS^2 - \frac{1}{6} \delta_{ij} \int_{S^2} W_0^2 dS^2 - \frac{1}{3} \int_{S^2} W_0 \bar{W}_{0j0n} \tilde{X}^i \tilde{X}^n dS^2.$$

Applying the last formula in Lemma 5.3, we obtain

$$\int_{S^2} W_0^2 \tilde{X}^m \tilde{X}^n dS^2 = \frac{4\pi}{3 \cdot 5 \cdot 7} (2\delta_{mn} \sum_{ij} D_{ij}^2 + 8 \sum_i D_{im} D_{in}).$$

□

11. Minimizing the Energy

In this section, we study the existence and uniqueness of observers $T_0 = (a^0, -a^1, -a^2, -a^3)$ that minimize the energy computed in Sect. 10. In Lemma 6.3, we solve the leading order term of the optimal embedding equation. In this section, we show that by minimizing the quasi-local energy, the optimal embedding equation can be solved to higher orders.

Throughout the section, we denote the surface Σ_r simply by Σ and the isometric embedding X_r by X . We consider pairs (X, T_0) with the following expansion:

$$\begin{aligned} X_0 &= \sum_{i=3}^{\infty} X_0^{(i)} r^i \\ X_k &= r \tilde{X}^k + \sum_{i=3}^{\infty} X_k^{(i)} r^i \\ T_0 &= (a^0, -a^i) + \sum_{i=1}^{\infty} T_0^{(i)} r^i. \end{aligned} \tag{11.1}$$

For such pairs, we have

$$E(\Sigma, X, T_0) = \sum_{i=5}^{\infty} E(\Sigma, X, T_0)^{(i)} r^i.$$

Similar to [6], the $O(r^k)$ part of the optimal embedding equation is of the form

$$\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2) X_0^{(k+3)} = M_k(X_0^{(3)}, \dots, X_0^{(k+2)}, T_0^{(0)}, \dots, T_0^{(k)}).$$

The equation is solvable if

$$\int_{S^2} M_k(X_0^{(3)}, \dots, X_0^{(k+2)}, T_0^{(0)}, \dots, T_0^{(k)}) \tilde{X}^i dS^2 = 0.$$

We need the following lemma about the above integral.

Lemma 11.1.

$$\int_{S^2} M_k(X_0^{(3)}, \dots, X_0^{(k+2)}, T_0^{(0)}, \dots, T_0^{(k)}) \tilde{X}^i dS^2$$

is independent of $X_0^{(k+2)}$ and $T_0^{(j)}$ for $j \geq k - 1$.

Proof. The optimal embedding equation reads

$$div_{\sigma}(f \nabla \tau) - \Delta(\sinh^{-1}(\frac{f \Delta \tau}{|H||H_0|})) = div_{\sigma} \alpha_{H_0} - div_{\sigma} \alpha_H.$$

For the right hand side, $div_{\sigma} \alpha_H$ is independent of (X, T_0) . $div_{\sigma} \alpha_{H_0}$ is independent of T_0 . While it depends on X , $X_0^{(k+2)}$ contributes

$$\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2) X_0^{(k+2)} r^{k-1} + O(r^{k+1})$$

to the right hand side and does not contribute to M_k . For the left hand side, $|H|$ is independent of (X, T_0) . $X_0^{(k+2)}$ only contributes to $|H_0|$ by terms of the order $O(r^{k+2})$ and does not contribute to M_k . For $T_0^{(k-1)} = (b^0, -b^i)$, it contributes to τ by

$$b^i \tilde{X}^i r^{k-1} + O(r^k).$$

As in the proof of Lemma 6.3, this contributes to the left hand side by a linear combination of -12 -eigenfunctions. \square

Remark 5. Here are some examples to illustrate the above lemma. Set $k = 1$, the $O(r)$ order of the optimal embedding equation is

$$\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(4)} = M_1(X_0^{(3)}, T_0^{(0)}, T_0^{(1)}). \tag{11.2}$$

By the lemma, it is solvable for any choice of $X_0^{(3)}$, $T_0^{(0)}$ and $T_0^{(1)}$. On the other hand, set $k = 2$, the $O(r^2)$ order of the optimal embedding equation is

$$\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(5)} = M_2(X_0^{(3)}, X_0^{(4)}, T_0^{(0)}, T_0^{(1)}, T_0^{(2)}). \tag{11.3}$$

Its solvability depends only on $T_0^{(0)}$ and $X_0^{(3)}$. In fact, it only depends on the choice of $T_0^{(0)}$ since $X_0^{(3)}$ is determined by $T_0^{(0)}$ using Lemma 6.3.

The structure of the higher order terms of the optimal embedding equation is the same. Namely, the $O(r^k)$ order of the optimal embedding equation is

$$\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2)X_0^{(k+3)} = M_2(X_0^{(3)}, \dots, X_0^{(k+2)}, T_0^{(0)}, \dots, T_0^{(k)}) \tag{11.4}$$

but the solvability depends only on the choice of $T_0^{(i)}$ for $i \leq k - 2$. We expect there is a unique choice such that the equation is solvable.

Let $E(\Sigma, X(T_0), T_0)$ be the quasi-local energy of Σ with embedding $X(T_0)$ and observer T_0 where $X(T_0)$ is the isometric embedding of Σ into $\mathbb{R}^{3,1}$ determined by Lemma 6.1 and Lemma 6.3. We have

$$E(\Sigma, X(T_0), T_0) = \sum_{i=5}^{\infty} E(\Sigma, X(T_0), T_0)^{(i)} r^i,$$

where

$$E(\Sigma, X(T_0), T_0)^{(5)} = \frac{1}{90} \left\{ \left(\frac{1}{2} \sum_{k,m,n} \bar{W}_{0kmn}^2 + \sum_{m,n} \bar{W}_{0m0n}^2 \right) a^0 + 2 \sum_i \sum_{m,n} \bar{W}_{0m0n} \bar{W}_{0min} a^i + \sum_{m,n} \frac{\bar{W}_{0m0n}^2}{2a^0} \right\}.$$

We show that generically, there is a unique minimizer T_0 of $E(\Sigma, X(T_0), T_0)^{(5)}$. Moreover, for the minimizer, Eq. (11.3) is solvable. We start with the following lemma.

Lemma 11.2. *Let $V = (\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2, 2 \sum \bar{W}_{0m0n} \bar{W}_{0min})$. V is future directed non-spacelike. Moreover, V is timelike unless in some orthonormal frame, we have*

$$(D_{ij}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -b \end{pmatrix} \quad (E_{ij}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & b \\ 0 & b & 0 \end{pmatrix} \tag{11.5}$$

where

$$\bar{W}_{0ijk} = \epsilon^{jkn} E_{in}.$$

Remark 6. D and E are both symmetric traceless 3 by 3 matrices. Together, they capture all the ten independent components of the Weyl curvature at a point.

Proof. It suffices to show that

$$(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2)^2 \geq 4 \sum_i (\sum_{m,n} \bar{W}_{0m0n} \bar{W}_{0min})^2. \tag{11.6}$$

We pick an orthonormal frame which diagonalizes D . Suppose

$$(D_{ij}) = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -(a+b) \end{pmatrix}.$$

In this case, the only components of E that appear on the right hand side are the off-diagonal entries. Let

$$\bar{W}_{0131} = c \quad \bar{W}_{0212} = d \quad \bar{W}_{0121} = e$$

and the inequality follows from

$$(c^2 + d^2 + e^2 + a^2 + b^2 + ab)^2 - [(a - b)^2 c^2 + (2b + a)^2 d^2 + (2a + b)^2 e^2] \geq 0,$$

where we discard terms of the form W_{0123} , namely the entries on the diagonal of E , from the left hand side of equation (11.6). However

$$\begin{aligned} & (c^2 + d^2 + e^2 + a^2 + b^2 + ab)^2 - ((a - b)^2 c^2 + (2b + a)^2 d^2 + (2a + b)^2 e^2) \\ &= c^2(a + b)^2 + (c^2 + ab)^2 + d^2 a^2 + (d^2 - b^2 - ab)^2 + e^2 b^2 + (e^2 - a^2 - ab)^2. \end{aligned}$$

Hence the vector $(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2, 2 \sum \bar{W}_{0m0n} \bar{W}_{0min})$ is future directed non-spacelike. If the vector is indeed null, then the diagonal of E is 0 and $c(a + b)$, $(c^2 + ab)$, da , $(d^2 - b^2 - ab)$, eb and $(e^2 - a^2 - ab)$ must all vanish. Then, up to switching the indices, D_{ij} and E_{ij} must be the ones indicated in the statement of the lemma. \square

Corollary 3. *The energy functional $E(\Sigma, X(T_0), T_0)^{(5)}$ is non-negative. Moreover, it is positive and proper when V is timelike.*

Hence, when V is timelike, there is at least one observer $T_0 = (a^0, -a^i)$ which minimizes $E(\Sigma, X(T_0), T_0)^{(5)}$. We show that under the same condition, the minimizer is unique.

Lemma 11.3. *Assume V is timelike then there is a unique $T_0 = (\bar{a}^0, -\bar{a}^i)$ that minimizes $E(\Sigma, X(T_0), T_0)^{(5)}$.*

Proof. It suffices to show that $E(\Sigma, X(T_0), T_0)^{(5)}$ is a strictly convex function of (a^1, a^2, a^3) since a convex function cannot have two critical points. Recall $E(\Sigma, X(T_0), T_0)^{(5)}$ is

$$\frac{1}{90} \left\{ \left(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2 \right) a^0 + 2 \sum \bar{W}_{0m0n} \bar{W}_{0min} a^i + \frac{1}{2} \sum \bar{W}_{0m0n}^2 \frac{1}{a^0} \right\}.$$

Since $\partial_{a^i} a^0 = \frac{a^i}{a^0}$, the first derivative of $90E(\Sigma, X(T_0), T_0)^{(5)}$ with respect to a^i is

$$\left(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2 \right) \frac{a^i}{a^0} + 2 \sum \bar{W}_{0m0n} \bar{W}_{0min} - \frac{1}{2} \sum \bar{W}_{0m0n}^2 \frac{a^i}{(a^0)^3}$$

and the second derivative is

$$\begin{aligned} & \left(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2 \right) \left(\frac{1}{a^0} - \frac{(a^i)^2}{(a^0)^3} \right) - \frac{1}{2} \sum \bar{W}_{0m0n}^2 \left(\frac{1}{(a^0)^3} - \frac{3(a^i)^2}{(a^0)^5} \right) \\ &= \left(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \sum \bar{W}_{0m0n}^2 \right) \left(\frac{1}{a^0} - \frac{(a^i)^2}{(a^0)^3} \right) - \frac{1}{2} \sum \bar{W}_{0m0n}^2 \left(\frac{1}{(a^0)^3} - \frac{(a^i)^2}{(a^0)^5} \right) \\ & \quad + \frac{\sum \bar{W}_{0m0n}^2 (a^i)^2}{(a^0)^5} \\ &\geq \left(\frac{1}{2} \sum \bar{W}_{0kmn}^2 + \frac{1}{2} \sum \bar{W}_{0m0n}^2 \right) \left(\frac{1}{a^0} - \frac{(a^i)^2}{(a^0)^3} \right) \end{aligned}$$

This is positive unless the Weyl curvature tensor vanishes at p . \square

As a result, there is a unique observer $\bar{T}_0 = (\bar{a}^0, -\bar{a}^i)$ such that for any other T_0 ,

$$E(\Sigma, X(T_0), T_0)^{(5)} \geq E(\Sigma, X(\bar{T}_0), \bar{T}_0)^{(5)}.$$

Lemma 11.4. *For every pair (X, T_0) with expansion given in Eq. (4.1),*

$$E(\Sigma, X, T_0)^{(5)} \geq E(\Sigma, X(\bar{T}_0), \bar{T}_0)^{(5)}.$$

Proof. It suffices to show that

$$E(\Sigma, X, T_0)^{(5)} \geq E(\Sigma, X(T_0), T_0)^{(5)}.$$

However, tracing through the dependence of $E(\Sigma, X, T_0)^{(5)}$ on X , we have

$$E(\Sigma, X, T_0)^{(5)} - E(\Sigma, X(T_0), T_0)^{(5)} = M(X_0^{(3)}) - M(X_0^{(3)}(T_0)),$$

where

$$M(f) = \int_{S^2} \left[\frac{1}{4} f \tilde{\Delta}(\tilde{\Delta} + 2)f + fg \right] dS^2$$

for some function g on S^2 . This is a convex functional of f and the $X_0^{(3)}(T_0)$ obtained in Lemma 6.3 is its critical point. \square

Finally, we show that Eq. (11.3) is solvable for the minimizer $(\bar{a}^0, -\bar{a}^i)$. We may assume that we pick some $T_0^{(1)}, T_0^{(2)}, X_0^{(3)}$ and $X_0^{(4)}$ such that the top order term of the optimal embedding equation and Eq. (11.2) are solved. From Lemma 11.4, we have

$$\partial_{a^i} E(\Sigma, X(\bar{T}_0), T_0)^{(5)} = 0.$$

However,

$$\partial_{a^i} \tau = \tilde{X}^i r + O(r^2).$$

We conclude that

$$\begin{aligned} \partial_{a^i} E(\Sigma, X(\bar{T}_0), T_0)^{(5)} = & \pm \int_{S^2} \tilde{X}^i \left[\frac{1}{2} \tilde{\Delta}(\tilde{\Delta} + 2) X_0^{(5)} \right. \\ & \left. - M_2(X_0^{(3)}, X_0^{(4)}, T_0^{(0)}, T_0^{(1)}, T_0^{(2)}) \right] dS^2. \end{aligned}$$

As a result,

$$\int_{S^2} \tilde{X}^i M_2(X_0^{(3)}, X_0^{(4)}, T_0^{(0)}, T_0^{(1)}, T_0^{(2)}) dS^2 = 0.$$

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