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Quantum Field Theory of Black Hole Perturbations with Backreaction: I General Framework

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Abstract: In a seminal work, Hawking showed that natural states for free quantum matter fields on classical spacetimes that solve the spherically symmetric vacuum Einstein equations are KMS states of non-vanishing temperature. Although Hawking's calculation does not include the backreaction of matter on geometry, it is more than plausible that the corresponding Hawking radiation leads to black hole evaporation which is, in principle, observable. Obviously, an improvement of Hawking's calculation including backreaction is a problem of quantum gravity. Since no commonly accepted quantum field theory of general relativity is available yet, it has been difficult to reliably derive the backreaction effect. An obvious approach is to use the black hole perturbation theory of a Schwarzschild black hole of fixed mass and to quantize those perturbations. However, it is not clear how to reconcile perturbation theory with gauge invariance beyond linear perturbations. In recent work, we proposed a new approach to this problem that applies when the physical situation has an approximate symmetry, such as homogeneity (cosmology), spherical symmetry (Schwarzschild), or axial symmetry (Kerr). The idea, which is surprisingly feasible, is to first construct the non-perturbative physical (reduced) Hamiltonian of the reduced phase space of fully gauge invariant observables and only then apply perturbation theory directly in terms of observables. The task to construct observables is then disentangled from perturbation theory, thus allowing to unambiguously develop perturbation theory to arbitrary orders. In this first paper of the series we outline and showcase this approach for spherical symmetry and second order in the perturbations for Einstein–Klein–Gordon–Maxwell theory. Details and generalizations to other matter and symmetry and higher orders will appear in subsequent companion papers.

Keywords: quantum black holes; quantum gravity; quantum fields in curved spacetime

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1. Introduction

Black holes are fascinating objects. Not only are black hole binaries among the most important sources of gravitational radiation [1], supermassive black holes are good candidates for active galactic nuclei (AGN) connected with a rich astrophysical phenomenology [2]; they are also the source of numerous debates and speculations in classical and quantum gravity [3–5]. Indeed, as summarized in the seminal singularity theorems by Penrose (Nobel Prize 2020) [6], black holes clearly indicate that General Relativity is an incomplete theory and must be supplemented by quantum considerations, thus resolving the classical singularity. For instance, the classical black hole area theorem [6] combined with quantum field theory on Schwarzschild spacetime [7] leads to the speculation that black holes carry an intrinsic entropy measured by the area of the event horizon [8] which hints at a deep connection between quantum field theory, classical general relativity and thermodynamics. The fact that the entropy is apparently measured by a two-dimensional rather than three-dimensional region in spacetime leads to the speculation that general relativity is a holographic theory [9] which delivers a strong motivation for holographic approaches to quantum gravity such as the modern string theory approach based on the AdS/CFT conjecture [10].

While Hawking's original calculation only considered free quantum matter on a classical vacuum Schwarzschild spacetime of fixed, time-independent mass, which violates the Einstein equations as the corresponding energy momentum tensor is obviously non-vanishing, the presence of the corresponding black body radiation makes it more than plausible that the black hole loses mass. This is a pure quantum effect forbidden by the classical area theorem. It leads to the so-called information paradox [11] which may be sketched as follows: We imagine that the Hilbert space of the entire system made from geometry and matter can be considered as a tensor product where one factor corresponds to the observables located in the spacetime region behind the event horizon (black hole region) and the other to the observables located in the region outside of it (asymptotic region). Given an initial pure state, we can form its partial trace with respect to the black hole region which leads to a mixed state for the outside algebra. This mixed state should correspond to the KMS (temperature) state discovered by Hawking and its von Neumann entanglement entropy should correspond to the black hole entropy (or information) [12]. We use the Heisenberg picture and describe the dynamics by unitary evolution of operators acting on the the total algebra of observables while the state remains unchanged and in particular pure for the total algebra.

As the black hole shrinks due to Hawking radiation, the outside region and thus the algebra of operators located therein of outside observables grows, while the algebra of inside observables shrinks. The total algebra of all observables remains the same during the entire process since the whole system is closed. When the black hole is gone, the outside algebra becomes the total algebra again. If the semiclassical consideration that leads to the Hawking radiation picture which was derived for large black holes remains valid also for small black holes, at the end of the process we have a portion of spacetime isometric to Minkowski spacetime which means that not all of spacetime (namely the black hole region) can be reconstructed from the data available at future null infinity. Therefore, information available at past null infinity (e.g., multipole moments of ingoing radiation) is lost (e.g., the outgoing radiation only carries information about mass, charge and angular momentum), entropy is created, and the state, therefore, is not pure, i.e., we still have a KMS state. Thus, this state would be truly mixed but *now for the total algebra*. However, in the Heisenberg picture, the state does not change and remains pure which is a contradiction. Note, that the representation of the *—algebra of observables that derives from a pure state via the GNS construction is irreducible while for a mixed state, it is properly reducible, i.e., there are non-trivial invariant subspaces with corresponding projectors [13]. This means that there are drastic differences between the two situations, somehow the whole representation of the algebra has changed.

To resolve the apparent contradiction one has several possibilities, of which we mention two, see [3–5] for some of the speculations on possible mechanisms. The first possibility is that the semiclassical picture breaks down at some point and that indeed at the end of the evaporation, the state is pure, the von Neumann entropy vanishes, and information is preserved. For instance, the evaporation could be incomplete leaving a "remnant" so that there remains an inside region and the outside state can stay mixed. The second possibility is that the evaporation is complete and ends with a mixed state. Then, the corresponding projections on invariant subspaces must arise by a dynamical mechanism, i.e., the quantum dynamics cannot be unitary. The von Neumann entropy is non-vanishing, information was lost.

The reason why we repeat here this well-known discussion is to highlight two facts:

First, that black holes are ideal laboratories for quantum gravity. Any candidate theory of quantum gravity must pass the test that consists, among other things, in 1. explaining the microscopic origin of the Bekenstein–Hawking entropy, 2. resolving the black hole information paradox, 3. deriving the end product of black hole evaporation and the fate of the black hole singularity, 4. describing Hawking radiation including backreaction from first principles and 5. determining the truth value of the (weak) cosmic censorship conjecture [14] (i.e., that singularities cannot communicate with future null infinity of an asymptotically flat spacetime so that predictability from a Cauchy surface holds in classical GR). Second, that one needs a sufficiently reliable framework in order to turn these speculations into precise statements. For instance, there has been considerable progress concerning the microscopic origin of the black hole entropy of stationary black holes both in String Theory (ST) [15] and in Loop Quantum Gravity (LQG) [16]. These considerations have already led to a more useful local definition of black hole horizon which, in contrast to the event horizon, does not rely on knowing the entire spacetime [17]. As far as black hole radiation from dynamical black holes is concerned important insights have been delivered by the two dimensional exactly solvable models [18], the Vaidya metric model [19] corresponding to null radiation and the spherically symmetric scalar boson star model [20–22]. Concerning singularity avoidance of exactly spherically symmetric black holes see [23–32] and [33–36] in the canonical and covariant framework respectively.

However, it is certainly fair to say that we are very far from understanding all aspects of quantum black hole physics. As the discussion reveals, many puzzles about black holes have their origin in the attempts to extend Hawking's calculation, which was performed without taking backreaction into account, to treating the case with backreaction. The simplest of such considerations uses the Stefan-Boltzmann law to relate the power of the black hole, i.e., minus the time derivative of its mass, to its temperature which, in turn, is a function of the mass. This leads to (suppressing numerical factors)

$$M(t) = [M(0)^3 - \frac{t}{t_P}\, M_P^3]^{1/3} \tag{1}$$

where $M(0), M_P, t_P$ are initial mass, Planck mass and Planck time, respectively. Clearly (1) can at best be an approximation because $\dot{M}$ diverges at the *evaporation time* $t_E = [M(0)/M_P]^3\, t_P$ which is of the order of the age of the universe for sufficiently small primordial black holes. Thus, precisely in the last stages of the evaporation process do we expect significant deviations from (1) that lead to a resolution of the singularity and to settle the question of whether there is a remnant thus contributing to dark matter [37,38]. Such deviations are, therefore, smoking guns for quantum gravity fingerprints provided that primordial black abundances are sufficiently large [39]. In order to compute the actual time dependence of the black hole mass and the deviation from (1) we need a proper quantum gravity calculation from first principles. This is a very complex task within any approach to quantum gravity. For instance, in LQG [40–44] one would need to first find exact solutions to the quantum Einstein equations (Wheeler DeWitt equation) [45–49] which can be interpreted as black hole states and then study their relational dynamics in terms of quantum Dirac observables. Such a program is indeed conceivable in the reduced phase space approach [50]. This *non-perturbative* program is still under development and currently non-perturbative renormalization methods [51] are being applied to fix point the details of the corresponding physical (reduced) Hamiltonian.

To make progress before this step is completed, in this series of works we take a *perturbative* route. The idea is to separate the degrees of freedom into (spherically) symmetric background and non-symmetric perturbations and to expand all relevant quantities of the theory such as constraints with respect to that split. This is of course well known and there is a rich literature on the subject starting with the seminal work by Regge, Wheeler and Zerilli [52,53] in the Lagrangian setting and Moncrief [54,55] in the Hamiltonian setting. See also [56–58] for a modern account. Common to these works, however, is that the background is not considered a dynamic entity. Therefore, the phase space of the system is coordinatized just by the perturbative degrees of freedom. The constraints of the system truncated to the first order in the perturbations generate gauge transformations on this "frozen" phase space and lead to a notion of first-order gauge invariant objects. To the best of our knowledge, higher orders have not been considered, partly because the second order frozen constraints do not close under Poisson brackets in contrast to the first order ones.

Unfortunately, this kind of analysis is inappropriate precisely when we want to take the dynamical interplay between background and perturbations into account, that is, backreaction. A similar question also arises in cosmology and in [59] it was shown how to extend the action of the first order constraints to the full phase space such that they still close and define a notion of "unfrozen" gauge invariance to first order. In [59] only a partial reduction of the gauge invariance was performed, i.e., there is still a single second-order constraint that was left unreduced. This remaining single constraint trivially commutes with itself so that a consistent quantum theory can be defined [60].

To the best of our knowledge, the formalism of [59] has not been extended yet to the question of gauge invariance at higher orders or backgrounds that are not homogeneous. In [61] we developed a general framework to precisely conduct this. It turns out that the approach of [59] is embedded in a general reduction algorithm that can be performed in any order and for any Killing symmetry. It directly computes the physical (reduced) Hamiltonian perturbatively and including backreaction with respect to (Dirac) observables which are gauge invariant to all orders. The reason why it computes the fully reduced Hamiltonian and not the partially reduced constraints is that partial reduction combined with perturbation theory does not lead to a consistent algebra of perturbed leftover constraints when there is more than one which is the case, for example, when we have spherical symmetry rather than homogeneity. This way a notion of n-th order perturbative gauge invariance including backreaction, for which no consistent definition is known to the best knowledge of the author, is never necessary, perturbation theory and non-perturbative gauge invariance is disentangled. An important ingredient of [61] is a symplectic chart consisting of four sets of canonical pairs: Symmetric versus non-symmetric and gauge versus true. The (non-)symmetric gauge degrees of freedom are adapted to a similar split of the constraints into those that generate gauge transformations that do (not) preserve the symmetry and are used to reduce them. Thus, the idea to make progress on the question of backreaction in Hawking radiation is to use the framework of [61] and to compute the reduced phase space and Hamiltonian to the desired order and with the desired matter content. This reduced phase space strategy is then the basis to develop the quantum theory.

Some of the immediate questions that arise when approaching black hole perturbation theory with backreaction are the following:

1. Which black hole symmetry (or solution) should be used?
2. When considering a dynamical background, should one only allow for a dynamics of the parameters of the symmetric background solution to the Einstein (vacuum?) equations or should one allow for a dynamic of all background fields compatible with the symmetry?
3. As we want to study the late stages of the evaporation process and thus want to "look into the singularity" how can we make sure that we can explore both the interior and the exterior of the black hole when the location of the quantum horizon becomes fuzzy?

Concerning the first question, assuming that the black hole no hair theorem and suitable energy conditions on the energy-momentum tensor of admissable matter hold [6], it suffices to consider black holes of either axi-symmetry or spherical symmetry. As shown in [62–64], semiclassical considerations suggest that charge and angular momentum are radiated off much faster than mass. Hence, starting from a primordial black hole created close to the Big Bang and evaporating today, it has reached spherical symmetry long before evaporation. Thus, as we are interested in the late stages of the evaporation process, it appears to be well motivated to consider spherical symmetry. Notice, however, that the methods of [61] are immediately applicable also to axial symmetry for which much of the tedious work has been performed by Teukolsky [65,66]. Hence, to check whether these semiclassical considerations are justified, one can repeat the steps outlined in the present paper also for the Kerr case.

To explain the relevance of the second question, recall that according to Birkhoff's theorem a spherically symmetric vacuum black hole is uniquely defined by a single parameter (the mass) up to diffeomorphisms. On the other hand a spherically symmetric spacetime is uniquely defined by four functions that depend on a radial and time coordinate. Hence, one can either assume that the backreaction just affects the mass parameter making it time and radially dependent or one can assume that the backreaction affects all four functions. Of course there is some redundancy in the second description due to the presence of residual radial and temporal diffeomorphisms (as well as gauge transformations generated by the primary constraints) that act on those four functions but how these should be consistently accommodated in the presence of perturbation theory is a priori not clear. It is also not clear whether one should use the first description at all when one considers matter that gives rise to a non-vanishing spherically symmetric energy-momentum tensor (such as scalar matter) so that the vacuum solution is not an exact solution to the system.

The framework of [61] gives an unambiguous answer to this question: One has to start from the description in terms of the four functions. The matter content and the interplay between the residual gauge transformations that preserve the symmetry and those gauge transformations that do not, automatically dictate the precise reduced form of the metric.

Finally concerning the third question, we must choose a coordinate system such that the metric is regular across any potential horizon, in particular the coordinate system must not depend on any dynamical parameters. In the ideal case, it should simplify the quantization of the reduced Hamiltonian as much as possible. Since the reduction process involves splitting the degrees of freedom into gauge and true degrees of freedom, these requirements select suitable gauges. For spherical symmetry we will, therefore, impose the Gullstrand–Painleveé gauge [56–58] that the spatial spherically symmetric metric be the flat Euclidean one which indeed simplifies the quantization of the reduced Hamiltonian since e.g., spatial curvature terms vanish and the Laplacian becomes the flat one with an explicitly known spectrum. In particular, the spacetime manifold has the topology of $\mathbb{R}^4$ for each asymptotic end. This moves the information about the non-trivial 4-curvature into the extrinsic curvature. Note, that GP coordinates cover either the advanced or retarded Finkelstein charts of Schwarzschild spacetime, and therefore, in the classical theory provide a convenient chart to explore both one asymptotic end and either the black hole or white hole region of the full Kruskal spacetime up until the singularity. Whether the classical singularity is resolved and replaced, for example, by a black hole–white hole transition, is then a question to be answered by the quantum theory which can be accommodated in this framework by working with two copies of GP manifolds.

The focus of the present paper is on the general structure of this program and we use the showcase of second-order perturbations of the physical Hamiltonian in the presence of scalar and Maxwell matter. We will not write out the details of the corresponding expressions which are reserved for our companion papers [67–69]. Generalizations to fermionic (in particular neutrino) matter, axial symmetry and higher orders will be the subject of future publications. The architecture of this article is as follows:

In Section 2 we basically introduce our notation and apply [61] to spherical symmetry. In particular, we review spherical tensor harmonics [70] and how they give rise to constraints C and Z, respectively, which preserve or do not preserve the symmetry, respectively. Adapted to those we have gauge canonical pairs (q, p) and (x, y), respectively, which are symmetric and non-symmetric, respectively. These are complemented by true (observable) canonical pairs (Q, P) and X, Y, respectively, which are also symmetric and non-symmetric, respectively.

In Section 3 we include a conceptual overview of many interrelated topics associated with black hole evaporation such as 1. Whether the vacuum black hole mass parameter M in fact can change at all during time evolution or rather has the status of an integration constant such as $M(0)$ in (1), 2. What replaces M as a measure of evaporation in case it is preserved, a natural candidate being the area of the apparent horizon, 3. How to describe black hole–white hole transitions within the perturbative framework, 4. What kind of Fock structures of black hole perturbative QFT are selected by the use of GP coordinates,

5. Which kind of Hawking effects are to be expected and 6. How singularity resolution would manifest itself.

In Section 4 we construct the exact reduced or physical Hamiltonian based on the GP gauge for q and the trivial gauge $x = 0$ for x following [61] which is natural in view of the algebraic structure of the constraints. This requires the full machinery of decay conditions on the background and perturbation fields and the solution of the constraints. We also construct the exact physical lapse and shift following the stability analysis of the gauge condition using the asymptotic structure at spatial infinity. This distinguishes gauge diffeomorphisms from symmetry diffeomorphisms and opens access to the full spacetime metric. The resulting expressions obtained, while non-perturbative, necessarily are implicit. To obtain explicit expressions, perturbation methods must be invoked. This entails two steps: 1. Standard non-gauge invariant perturbative expansions of the constraints and 2. Assembling different bits and pieces of those into gauge invariant contributions.

In Section 5 we perform the first step and determine the general perturbative form of the classical constraints to all orders, that is, we simply expand the constraints in their polynomial form into spherical tensor harmonics. While tedious, this step is straightforward and just involves the recoupling theory of angular momentum or equivalently harmonic analysis on the sphere. In polynomial form, the gravitational contribution to the constraints is of degree ten which is also the top degree of the perturbative expansion. Performing the sphere integral returns an expression that is exact.

In Section 6 we perform the second step and perturbatively solve the constraints $C = 0, Z = 0$, respectively, for p, y in terms of q, x, Q, P, X, Y and imposing gauges on q, x following the algorithm of [61]. While the formulae provided in [61] cover all orders, we detail the concrete expression only up to the second order. As explained in [61] certain degrees of freedom (e.g., core mass and charge) encoded in q, p are retained among the (Q, P) due to the presence of boundary terms in the constraints. These also serve to perform a second Taylor expansion in order to explicitly solve the differential equations that occur when solving for p, y.

In Section 7 we give a brief introduction to various notions of black hole horizons and argue that in the present situation with a distinguished notion of time defined by the free-falling GP observers, the apparent horizon and its area is an important quantity that captures important information about the degree of black hole evaporation. We show that the perturbative scheme developed in previous sections extends to all orders and also to the apparent horizon and its area.

In Section 8 we enter the quantum regime. Since second order perturbation theory of the reduced Hamiltonian reproduces the Regge–Wheeler and Zerilli free Hamiltonians for the perturbations in a GP spacetime of given mass, its Fock quantization is the starting point of perturbative QFT for the perturbations with the higher order terms in the reduced Hamiltonian considered as interaction terms. While we do not complete this step in the present paper we sketch all the steps towards this goal, i.e., we formulate QFT in GP spacetime. This includes a discussion of mode functions that are valid throughout the black or white hole region and an asymptotic region for each asymptotic end of the spacetime (of which there are two in the case of a black hole white hole transition). The mathematical challenge is to gain sufficient control over those mode functions in GP spacetime and to formulate junction conditions in the transition region. As a regularizing method, we consider an Einstein–Rosen type bridge of gluing a *past* ingoing GP spacetime with a *future* outgoing GP spacetime which is foliated by proper GP time Cauchy surfaces. Once established, the Fock quantization can then be applied to the apparent horizon area and its perturbation theory.

In Section 9 we touch upon the question of backreaction, i.e., interaction between symmetric and non-symmetric true degrees of freedom. This can be non-trivial already within Einstein–Maxwell theory when the mass M can change dynamically due to the details of imposing the the GP gauge. In this case one can use space adiabatic perturbation theory [71]. We used this already in application to cosmology [72]. When the matter content goes beyond that of Maxwell fields, then new challenges arise because the symmetric "slow" sector is also a field theory with infinitely many degrees of freedom, not only the "fast" non-symmetric sector.

In Section 10 we construct the conserved Noether current that follows from the reduced Hamiltonian and which can be used to compute the classical energy flux. It can also be used to construct the analog of grey body factors for the corresponding Hawking radiation in the quantum theory.

In Section 11 we summarize and give an outlook into further work under development, in particular the contact with phenomenology.

In Appendix A we review in a simple setting the Hamiltonian distinction between symmetry and gauge and how decay behaviors of fields and constraint-smearing functions as well as concepts of variational analysis come into play.

In Appendix B we apply this to vacuum black holes and show that next to the mass, there exists a second Dirac observable. The difference between symmetry and gauge diffeomorphisms explains why this is not in contradiction to Birkhoff's theorem. This is relevant because if the second variable shows up in the spacetime metric (depending on the details of the GP gauge condition) then the black hole mass M is not a constant of motion as soon as gravitational perturbations are present.

In Appendix C, we complement the GP description of Appendix B by the Kantowski–Sachs description which has recently received much interest in black hole singularity resolution scenarios and how they are matched.

In Appendix D we include elements of the analysis of generalized GP coordinates and free falling observers and foliations in black hole white hole transition spacetimes and regularized versions thereof. It contains also a consistent mechanism that reconciles the existence of the second Dirac observable without it appearing in the reduced Hamiltonian.

2. Spherical Tensor Harmonics, Symmetry and Gauge Degrees of Freedom

In the first subsection we summarize the relevant information on spherical tensor harmonics [70]. These guide our notation and serve to identify the gauge and true degrees of freedom as well as the symmetric and non-symmetric degrees of freedom. In the second subsection we interpret these in terms of the notation applied in the general framework of [61]. In the third we show how to perform the perturbative expansion of all constraints in closed form.

2.1. Spherical Tensor Harmonics

Let $\theta^1 := \theta \in [0, \pi],\ \theta^2 := \varphi \in [0, 2\pi)$ be spherical polar coordinates on S^2,

$$\Omega_{AB} := \delta^1_A\ \delta^1_B + \sin^2(\theta)\ \delta^2_A \delta^2_B;\ \ A, B, C, \ldots = 1, 2;\ \ \omega := \sqrt{\det(\Omega)};\ \ d\mu := \frac{\omega}{4\pi}\ d^2\theta;\ \ \eta_{AB} := \omega\ \epsilon_{AB} \tag{2}$$

respectively, round metric on S^2, its associated scalar density of weight one, corresponding normalized measure and skew pseudo-metric of density weight zero where $\epsilon_{12} = +1$. Let D_A be the torsion free Ω compatible covariant differential. The corresponding Riemann tensor is easily computed to be $R_{ABCD} = \eta_{AB}\ \eta_{CD}$ with Ricci tensor $R_{AB} = \Omega_{AB}$ and Ricci scalar $R = 2$. All indices are moved with Ω or its inverse where $\Omega^{AC}\ \Omega_{CB} = \delta^A_B$. We define the Laplacian $\Delta = D_A\ D^A$.

Let $L_{l,m},\ l = 0, 1, 2, \ldots; m = -l, -l+1, \ldots, l$ be the real-valued orthonormal basis of $L_2(S^2, d\mu)$ defined by Legendre polynomials. In terms of the usual complex-valued $Y_{l,m}$ with $\bar{Y}_{l,m} = Y_{l,-m}$ we have $L_{l,0} := Y_{l,0},\ \sqrt{2}\ L_{l,m} = Y_{l,m} + Y_{l,-m};\ m > 0,\ i\sqrt{2}\ L_{l,m} = Y_{l,-m} - Y_{l,m};\ m < 0$. The scalar harmonics are simply the $L_{l,m}$. We define the even "e" and odd "o" vector harmonics for $l > 0$ by

$$\sqrt{l(l+1)}\ L_{A;e,l,m} := D_A\ L_{l,m} := \sqrt{l(l+1)}\ L_{A;o,l,m} := \eta_A{}^B\ D_B\ L_{l,m} \tag{3}$$

which are orthonormal with respect to the inner product

$$< L_{\alpha,l,m}, L_{\beta,l',m'} >_{L_2^2} := \int_{S^2} d\mu \; \overline{L_{A;\alpha,l,m}} \; \Omega^{AB} \; L_{B;\beta,l',m'} = \delta_{\alpha\beta} \; \delta_{l,l'} \; \delta_{m,m'} \tag{4}$$

with $\alpha, \beta \in \{e, o\}$. The terminology used in the literature referring to "even" and "odd" is not entirely consistent. A better qualifier would be "polar" and "axial", i.e., $L_{A;e,l,m}$ does not involve the pseudo tensor η_{AB} while $L_{A;o,e,l,m}$ does. An equivalent characterization is that under reflection $\theta \mapsto \pi - \theta, \; \varphi \mapsto \varphi + \pi$ the 1-form (or the corresponding vector field) $L_{A;e/o,l,m}$ has the opposite/same intrinsic parity as $L_{l,m}$ which is $(-1)^l$. Thus, "even, odd" should not be confused with the intrinsic parity of $L_{l,m}$ which is defined to be even/odd when l is even/odd. With the understanding of "even, odd" as polar, axial the scalar perturbations are all even. The $L_{A;\alpha,l,m}$ are complete, i.e., every one form that is square integrable in the sense of (4) can be expanded in terms of them and that expansion converges to it with respect to the L_2^2 norm. This will be shown below.

Next, consider for $l \geq 0$ the horizontal "h" and for $l \geq 2$ the even "e", respectively, odd "o" symmetric (with respect to tensor indices) 2-tensor harmonics

$$\begin{aligned} \sqrt{2} \; L_{AB;h,l,m} &:= \Omega_{AB} \; L_{l,m} \\ \sqrt{2(l^2-1)(l+1)(l+2)} \; L_{AB;e,l,m} &:= (D_A \; D_B - \frac{1}{2}\Omega_{AB}\Delta) \; L_{lm} \\ \sqrt{2(l^2-1)(l+1)(l+2)} \; L_{AB;o,l,m} &:= D_{(A} \; \eta_{B)} \;{}^C D_C \; L_{lm} \end{aligned} \tag{5}$$

where both the horizontal and even 2-tensor have parity $(-1)^l$ and the odd 2-tensor has parity $(-1)^{l+1}$. The motivation for the term "horizontal" will become clear only in the next section. In the literature one refers to both the horizontal and even tensors as "even" since they are both polar while the "odd" tensors are axial. Note, that the even and odd tensors in contrast to the horizontal tensors are tracefree with respect to Ω.

The tensors (5) are orthonormal with respect to the inner product

$$< L_{\alpha,l,m}, L_{\beta,l',m'} >_{L_2^4} := \int_{S^2} d\mu \; \overline{L_{AC;\alpha,l,m}} \; \Omega^{AB} \; \Omega^{CD} \; L_{BD;\beta,l',m'} = \delta_{\alpha\beta} \; \delta_{l,l'} \; \delta_{m,m'} \tag{6}$$

with $\alpha, \beta \in \{h, e, o\}$. The $L_{AB;\alpha,l,m}$ are complete, i.e., every 2-tensor that is square integrable in the sense of (6) can be expanded in terms of them and that expansion converges to it with respect to the L_2^4 norm.

Tensor harmonics for tensors of higher rank can be constructed analogously using the building blocks $\Omega, D, L_{l,m}$. The orthonormality can be established by exploiting that D and $\tilde{D} = \eta \cdot D$ are anti-self adjoint as operators $D : \; L_2 \to L_2^2, \; L_2^2 \to L_2^4$ (derivative), $D : \; L_2^2 \to L_2, \; L_2^4 \to L_2^2$ (divergence) and similar for $\tilde{D}$. The completeness can be established relying on the completeness of the scalar harmonics as well as the fact that $-\Delta L_{l,m} = l(l+1) \; L_{l,m}$. For instance, we have for a given vector field v^A with divergence $d = D_A v^A$ and curl $c = \tilde{D}_A v^A$

$$\begin{aligned} & \Delta v^A = D_B \; D^B \; v^A = D_B \; [(D^B \; v^A - D^A \; v^B) + D^A v^B] = D_B \; (\eta^{BA} \; c) + (D^B D^A - D^A D^B) v_B + D^A \; d \\ = \; & \tilde{D}^A \; c + D^A d + R^{BA}{}_{BC} v^C = \tilde{D}^A \; c + D^A d + v^A \end{aligned} \tag{7}$$

As d, c can be expanded into scalar harmonics and $D, \tilde{D}$ annihilate the $l = 0$ contributions we find that $-(-\Delta + 1)v$ can be expanded into vector harmonics. However, the operator $-\Delta + 1$ is positive definite whence

$$v^A = -(-\Delta + 1)^{-1} [D^A d + \tilde{D}^A c] \tag{8}$$

and since $D_A \Delta f = (\Delta - 1) D_A f, \; \tilde{D}_A \Delta f = (\Delta - 1) \tilde{D}_A f$ we find that after expanding d, c into scalar harmonics labeled by $l \neq 0$ we can simply replace $(-\Delta + 1)^{-1}$ by $[l(l+1)]^{-1}$.

In our application to perturbation theory the Hilbert spaces L_2, L_2^2, L_2^4 appear naturally in the first order and some terms of second order. In other terms of second order and of higher order one encounters higher-order contractions of the $L_{l,m},\ L_{A,e/o,l,m},\ L_{AB,h/e/o,l,m}$ that are integrated over S^2 with measure μ. These can be computed by combining Clebsch–Gordan decomposition

$$L_{l,m}\ L_{l',m'} = \sum_{|l-l'|\leq \tilde{l}\leq l+l';\tilde{m}=m+m'} c_{l,m;l',m';\tilde{l},\tilde{m}}\ L_{\tilde{l},\tilde{m}'} \tag{9}$$

with expressing D_A in terms of the angular momentum operators $L_\mu,\ \mu=1,2,3$ which act diagonally or as ladder operators on the $L_{l,m}$.

Some useful identities are

$$\begin{aligned}
&D_A\Omega_{BC} = D_A\ \omega = 0 \\
&D_A\ L^A_{\alpha,l,m} = -\sqrt{l(l+1)}\ \delta^e_\alpha\ L_{l,m} \\
&D_A\ L^{AB}_{h,l,m} = \sqrt{l(l+1)/2}\ L^B_{e,l,m} \\
&D_A\ L^{AB}_{\alpha,l,m} = -\frac{1}{2}\sqrt{(l-1)(l+2)/2}\ L^B_{\alpha,l,m};\ \ \alpha=e,o \\
&D_A L_{l,m} = \sqrt{l(l+1)}\ L_{A;e,l,m} \\
&D_A L_{B;e,lm} = \sqrt{2(l-1)(l+2)}\ L_{AB;e,l,m} - \sqrt{l(l+1)/2}\ L_{AB;h,l,m} \\
&D_A L_{B;o,lm} = \sqrt{2(l-1)(l+2)}\ L_{AB;o,l,m} + \eta_{[A}{}^C\ D_{B]}\ L_{C;e,l,m}
\end{aligned} \tag{10}$$

2.2. Classification of Symmetry and Gauge Degrees of Freedom

As mentioned, for the purpose of concrete illustration we focus on the following matter content: A charged scalar field Φ with potential V which may serve to build a boson star and the Maxwell field A. In the canonical setting [14] assuming global hyperbolicity the spacetime manifold M is diffeomorphic to $\mathbb{R}\times\sigma$ where σ is a three manifold and can be foliated by Cauchy surfaces Σ_t labeled by $t\in\mathbb{R}$. What follows can be conducted in any spacetime dimension, we consider the case of four dimensions.

We thus, have the following ingredients ($\mu,\nu,\rho,\ldots=1,2,3$ are spatial tensor indices with respect to coordinates x^μ on the manifold σ):

1. Gravitational degrees of freedom: $(S^0,W_0),\ (S^\mu,W_\mu),\ (m_{\mu\nu},W^{\mu\nu})$ where S^0,S^μ are called lapse and shift functions parametrising the embeddings $\sigma\to\Sigma_t$ and m is the intrinsic metric of σ. The $W_0,W_\mu,W^{\mu\nu}$ are the respective conjugate momenta. We denote by $m^{\mu\nu}$ the inverse of $m_{\mu\nu}$ and $R[m]$ the Ricci scalar of m constructed from the torsion-free covariant differential ∇_μ compatible with $m_{\mu\nu}$.
2. Scalar degrees of freedom: (Φ,Π) where Π is the conjugate momentum of the scalar field Φ on σ which we take as a real-valued SO(2) dublett.
3. Electromagnetic degrees of freedom: $(S_0,W^0),\ (A_\mu,E^\mu)$ where S_0 is the temporal component of the 4-connection and A_μ is its spatial component. Again, W^0,E^a are the conjugate momenta and $B^\mu=\epsilon^{\mu\nu\rho}\ \partial_\nu\ A_\rho,\ E^\mu$ are referred to as magnetic and electric fields, respectively. We also refer to $F_{\mu\nu}:=2\partial_{[\mu}A_{\nu]}$ as the curvature of A_μ.
4. Primary constraints: $B_0:=W_0,\ B_\mu:=W_\mu,\ B^0:=W^0$
5. Secondary constraints:

$$
\begin{aligned}
V_0 &:= V_0^E + V_0^{KG} + V_0^M \\
V_0^E &:= \frac{1}{\sqrt{\det(m)}} [m_{\mu\rho}\, m_{\nu\lambda} - \frac{1}{2} m_{\mu\nu}\, m_{\rho\lambda}]\, W^{\mu\nu}\, W^{\rho\lambda} - \sqrt{\det(m)}\, R[m] \\
V_0^{KG} &:= \frac{||\Pi||^2}{2\sqrt{\det(m)}} + \frac{1}{2}\sqrt{\det(m)}\, m^{\mu\nu}\, [D_\mu \Phi]^T\, [D_\nu \Phi] + \sqrt{\det(m)}\, U(||\Phi||^2) \\
V_0^M &:= \frac{m_{\mu\nu}}{2\sqrt{\det(m)}} [E^\mu\, E^\nu + B^\mu\, B^\nu] \\
V_\mu &:= V_\mu^E + V_\mu^{KG} + V_\mu^M \\
V_\mu^E &:= -2\, \nabla_\nu W^\nu{}_\mu \\
V_\mu^{KG} &:= \Pi^T\, \Phi_{,\mu} \\
V_\mu^M &:= E^\nu (\partial_\mu A_\nu) - (E^\nu\, A_\mu)_{,\nu} \\
G &:= G^M + G^{KG} := \partial_\mu\, E^\mu + \Pi^T\, \epsilon\, \Phi
\end{aligned}
\tag{11}
$$

where ϵ is the skew matrix in 2 dimensions, $D = d + \epsilon A$, $||\Phi||^2 = \Phi^T \Phi$ of which the potential U is a polynomial (e.g., mass term) and ∇ is the covariant differential determined by m. Here, V_0 is referred to as the Hamiltonian constraint, V_μ as the spatial diffeomorphism constraints and G as the Gauss constraint. We have labeled the respective contributions due to Einstein, Klein–Gordon and Maxwell fields, respectively, by E, KG, M, respectively.

6. Unreduced Hamiltonian (v^0, v^μ, v_0 are velocities that remain undetermined by the Legendre transform)

$$H = \int_\sigma d^3x\, [v^0\, B_0 + v^\mu\, B_\mu + v_0\, B^0 + S^0\, V_0 + S^\mu\, V_\mu + S_0\, G] \tag{12}$$

7. Symplectic potential (we normalize by the unit sphere area and d is the exterior differential on field space)

$$4\pi\, \Theta = \int_\sigma d^3z\, [W_0\, dS^0 + W_\mu\, dS^\mu + W^0\, dS_0 + W^{\mu\nu}\, dm_{\mu\nu} + \Pi^T\, d\Phi + E^\mu\, dA_\mu] \tag{13}$$

The Hamiltonian density is a linear combination of all constraints as it is always true for generally covariant field theories. As there is a "boundary" at spatial infinity, one has to add boundary terms to (12) ensuring that (12) continues to be differentiable and convergent also when the functions S^0, S_μ, S_0 do not vanish at infinity but we will not display them here as we will automatically encounter them in a later stage of the analysis. The velocities v^0, v^μ, v_0 are arbitrary "Lagrange multipliers" that one could not solve for when performing the Legendre transform. The stabilization (preservation in time) of the primary constraints B_0, B_μ, B^0 implies the secondary constraints D_0, D_μ, G. Their stabilization leads to no new constraints because their Poisson algebra closes: The hypersurface deformation algebra generated by the V_0, V_μ closes by itself while V_0, G are invariant under G and the V_μ, G close among themselves. All the primary constraints are obviously close to each other (they are Abelian since they involve only momenta W_0, W_μ, W^0) and they have vanishing Poisson brackets with the secondary constraints because these do not involve the variables S^0, S^μ, S_0.

Before proceeding it is convenient to get rid of the primary constraints B_0, B_μ, B^0 by gauge fixing the variables S^0, S^μ, S_0 conjugate to W_0, W_μ, W^0. This is accomplished by imposing suitable gauge conditions $K = (K^0, K^\mu, K_0)$ on the variables $(m_{\mu\nu}, W^{\mu\nu}), (\Phi, \Pi), (A_\mu, E^\mu)$. In order that these conditions are stable under the gauge flow, the variables S^0, S^μ, S_0 become given functions $S_* = (S^0_*, S^\mu_*, S^*_0)$ of $(m_{\mu\nu}, W^{\mu\nu}), (\Phi, \Pi), (A_\mu, E^\mu)$ and are thus also fixed. The reduced Hamiltonian acts only on the subset of true degrees of freedom, i.e., those among $(m_{\mu\nu}, W^{\mu\nu}), (\Phi, \Pi), (A_\mu, E^\mu)$ not determined by $K = 0$ and $V = (V_0, V_\mu, G) = 0$ and is determined by first computing the Poisson bracket between functions of the true degrees of freedom and the unreduced Hamiltonian and then evaluating the result at

$S = S_*, K = V = 0$. It follows that the terms proportional to $B = (B_0, B_\mu, B^0)$ can be ignored from the outset. The correspondingly simplified Hamiltonian coincides with (12) except that the terms proportional to B_0, B_μ, B^0 are dropped and that S^0, S^a, S_0 acquire now the status of arbitrary smearing functions of the constraints that appear (12) on that reduced phase space which will later be fixed by the stability requirement for the gauge fixing condition.

We now make contact with the general framework [61]. To conduct this, we must introduce two splits of the degrees of freedom into i. symmetric ones and non-symmetric ones on the one hand and ii. gauge and observable (true) ones on the other. The symmetry split is essentially dictated by the decomposition of the fields into tensor harmonics. In particular, it induces a symmetry split among the fields S^0, S^μ, S_0. Their symmetry split induces a symmetry split of the secondary constraints V_0, V_μ, G which then suggests a natural additional gauge split on all configuration and momentum variables.

Accordingly, we begin with the spherical harmonics decomposition using the polar coordinate system $z^A := \theta^A,\ A = 1,2$ (see the previous subsection) and one radial coordinate $z^3 := r$ for each asymptotic end where $z^\mu = r(\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta))$ are the usual Cartesian coordinates at spatial infinity. We have the following symmetry split of the functions S^0, S^μ, S_0

$$\begin{aligned} S^0 &=: f^v + \sum_{l>0,|m|\le l} g^{v,l,m}\ L_{l,m} \\ S^3 &=: f^h + \sum_{l>0,|m|\le l} g^{h,l,m}\ L_{l,m} \\ S^A &=: 0 + \sum_{l>0,|m|\le l,\ \alpha\in\{e,o\}} g^{\alpha,l,m}\ L^A_{\alpha,l,m}, \quad A = 1,2 \\ S_0 &=: f^M + \sum_{l>0,|m|\le l} g^{M,l,m}\ L_{l,m} \end{aligned} \tag{14}$$

where the labels "v" and "h" mean "vertical" and "horizontal", respectively, and capture the fact that the Hamiltonian and spatial diffeomorphism constraints, respectively, generate spacetime diffeomorphisms transversal (vertical) and tangential (horizontal) to the Cauchy surfaces. The functions $f^v,\ g^{v,l,m},\ f^h,\ g^{h,l,m},\ g^{\alpha,l,m},\ f^M, g^{M,l,m}$ depend only on the radial coordinate r. The contributions to S^0, S^3, S_0 given by the functions f^v, f^h, f^M are, therefore, spherically symmetric and thus are referred to as "symmetric" smearing functions while the contributions to S^0, S^3, S^A, S_0 defined by the functions $g^{v,l,m}, g^{h,l,m}, g^{\alpha,l,m}, g^{M,l,m}$ are not spherically symmetric and thus are referred to as "non-symmetric" smearing functions.

We perform an analogous split for the fields $m_{\mu\nu},\ W^{\mu\nu},\ \Phi, \Pi, A_\mu, E^\mu$

$$\begin{aligned} m_{33} &=: q^v_E + \sum_{l>0,|m|\le l} x^{v,l,m}_E\ L_{l,m} \\ m_{3A} &=: 0 + \sum_{l>0,|m|\le l,\alpha\in\{e,o\}} x^{\alpha,l,m}_E\ L_{A;\alpha,l,m} \\ m_{AB} &= q^h_E\ \Omega_{AB} + \sum_{l>0,|m|\le l} x^{h,l,m}_E\ L_{AB;h,l,m} + \sum_{l>1,|m|\le l,\alpha\in\{e,o\}} X^{\alpha,l,m}_E\ L_{AB;\alpha,l,m} \\ W^{33} &=: \omega\ [p^E_v + \sum_{l>0,|m|\le l} y^E_{v,l,m}\ L_{l,m}] \\ W^{3A} &=: \frac{\omega}{2}\ [0 + \sum_{l>0,|m|\le l,\alpha\in\{e,o\}} y^E_{\alpha,l,m}\ L^A_{\alpha,l,m}] \end{aligned} \tag{15}$$

$$
\begin{aligned}
W^{AB} &=: \omega\, [\frac{p_h^E}{2}\, \Omega^{AB} + \sum_{l>0,|m|\le l} y^E_{h,l,m}\, L^{AB}_{h,l,m} + \sum_{l>1,|m|\le l,\alpha\in\{e,o\}} Y^E_{\alpha,l,m}\, L^{AB}_{\alpha,l,m}] \\
\Phi &=: Q_{KG} + \sum_{l>0,|m|\le l} X^{l,m}_{KG}\, L_{l,m} \\
\Pi &=: \omega\, [P^{KG} + \sum_{l>0,|m|\le l} Y^{KG}_{l,m}\, L_{l,m}] \\
A_3 &=: q_M + \sum_{l>0,|m|\le l} x^{l,m}_M\, L_{l,m} \\
A_C &=: 0 + \sum_{l>0,|m|\le l,\alpha\in\{e,o\}} X^{\alpha,l,m}_M\, L_{C;\alpha,l,m} \\
E^3 &=: \omega\, [p^M + \sum_{l>0,|m|\le l} y^M_{l,m}\, L_{l,m}] \\
E^C &=: \omega\, [0 + \sum_{l>0,|m|\le l,\alpha\in\{e,o\}} Y^M_{\alpha,l,m}\, L^C_{\alpha,l,m}]
\end{aligned}
$$

We have paid attention to the fact that the momenta conjugate to the respective configuration variables are respective dual tensors that carry density weight one rather than zero and thus have pulled out a factor of $\omega = \sqrt{\det(\Omega)}$ (see the previous section). The labels E, KG, M mean Einstein, Klein–Gordon, Maxwell degrees of freedom, respectively. We have grouped the coefficient functions of the tensor harmonics that appear in (15) and which only depend on the radial coordinate r into the following four groups following the general notation of [61]:

1. symmetric gauge $\{(q^a, p_a)\} := \{(q^v_E, p^E_v), (q^h_E, p^E_h), (q_M, p^M)\}$
2. symmetric true: $\{(Q^A, P_A)\} := \{(Q_{KG}, P^{KG}\}$
3. non-symmetric gauge ($l > 0, |m| \le l,\ \alpha \in \{v, h, e, o\}$): $\{(x^j, y_j)\} := \{(x^{\alpha,l,m}_E,\ y^E_{\alpha,l,m}),$ $(x^{l,m}_M,\ y^M_{l,m})\}$
4. non-symmetric true ($\alpha \in \{e, o\}$ and $l > 0$ for KG, M while $l > 1$ for E): $\{(X^J, Y_J)\} :=$ $\{(X^{\alpha,l,m}_E,\ Y^E_{\alpha,l,m}),\ (X^{l,m}_{KG},\ Y^{KG}_{l,m}),\ X^{\alpha,l,m}_M,\ Y^M_{\alpha,l,m})\}$.

The labels $a, b, c, \ldots;\ A, B, C, \ldots;\ j, k, l, \ldots;\ J, K, L, \ldots$ take the corresponding values which include the value of the coordinate r. The unfortunate doubling of the labels $A, B, C, \ldots = 1, 2$ of components of tensors on S^2 with the range $A, B, C, \ldots = r \in [0, \infty)$ for Q^A, P_A does not cause confusion because we will get rid of the spherical harmonics right away so that they play no role any more below.

When plugging the decomposition (15) into the symplectic potential (13) we find due to $\omega\, d^3z = 4\pi\, dr\, d\mu$ and the normalization of the spherical harmonics with respect to μ (see the previous subsection)

$$
\begin{aligned}
&\Theta = p_a\, dq^a + P_A\, dQ^A + y_j\, dx^j + Y_J\, dX^J \qquad (16)\\
= &\int_0^\infty dr\, \{[p^E_v\, dq^v_E + p^E_h\, dq^h_E + p^M\, dq_M] + [(P^{KG})^T\, dQ_{KG}]\} \\
&+ \sum_{l>0,|m|\le l} [(\sum_{\alpha\in\{v,h,e,o\}} y^E_{\alpha,l,m}\, dx^{\alpha,l,m}_E) + y^M_{l,m}\, dx^{l,m}_M] \\
&+ \sum_{l>0,|m|\le l} [(Y^{KG}_{l,m})^T\, dX^{l,m}_{KG}] + \sum_{\alpha\in\{e,o\}} [\sum_{l>1,|m|\le l} Y^E_{\alpha,l,m}\, dX^{\alpha,l,m}_E + \sum_{l>0,|m|\le l} Y^M_{\alpha,l,m}\, dX^{\alpha,l,m}_M]\}
\end{aligned}
$$

which shows that the pairs listed in the decomposition $(q, p), (Q, P), (x, y), (X, Y)$ are indeed conjugate so that we have, for instance

$$\{y^E_{\alpha,l,m}(r), x^{\alpha',l',m'}_E(r')\} = \delta^{(1)}(r, r')\, \delta^{\alpha'}_\alpha\, \delta^{l'}_l\, \delta^{m'}_m \qquad (17)$$

etc., (in particular, Poisson brackets between fields from different species E, KG, M vanish) where $\delta^{(1)}(r, r')$ is the δ distribution on the positive real line if we consider one asymptotic end.

2.3. Perturbative Decomposition

When plugging the decompositions (14) and (15) into the Hamiltonian (12) one would like to integrate out the angle dependence. This is immediately possible for the contributions to H from spatial diffeomorphism and Gauss constraint V_μ, G (recall that we could already delete the piece depending on v^0, v^μ, v_0) because these are homogeneous polynomials of degree three and two, respectively, in the fields (14) and (15) and just requires to apply the normalization of the spherical harmonics and the Clebsch–Gordan decomposition. However, the contribution to H from V_0 is non-polynomial in the metric field (all other degrees of freedom enter polynomially). While one could, in principle, try to integrate out the angular dependence of the non-polynomial constraints directly and non-perturbatively, it is not known whether one can conduct this in closed form. Moreover, as we are interested in perturbation theory with respect to the non-symmetric degrees of freedom x, y, X, Y, we may as well perform the perturbative expansion before the angular integration. One then obtains a perturbation series which is infinite but only due to field $m_{\mu\nu}$, the series is finite as far as the other fields are concerned and each term in that series can be integrated into the closed form using again Clebsch–Gordan theory.

One can avoid this infinite series as follows: The Hamiltonian constraint V_0 depends on $\sqrt{\det(m)}^{\pm 1}$ in order that each term has net density weight unity. If we multiply V_0 by $\sqrt{\det(m)}$ then only $\det(m)$ appears which is a cubic polynomial in m. Then, $\sqrt{\det(m)}\ [V_0^M + V_0^{KG}]$ and the piece of $\sqrt{\det(m)}\ V_0^E$ not involving the Ricci scalar is already polynomial. The Ricci scalar contains a term linear that is derived and a term quadratic but without derivatives in the Christoffel symbol $\Gamma^\mu_{\nu\rho} = m^{\mu\lambda}\ \Gamma_{\lambda\nu\rho}$ where $\Gamma_{\lambda\nu\rho}$ is homogeneously linear and these terms are contracted with the inverse metric. Thus, $\tilde{V}_0 := \sqrt{\det(m)}^5\ V_0$ is polynomial in all variables. It is quadratic in all momenta $W^{\mu\nu},\ \Pi,\ E^\mu$, quadratic in A_μ and quadratic in Φ if U is just a mass term, otherwise higher if U is a higher-order polynomial. Since $\det(m)\ m^{\mu\nu}$ is a polynomial of degree two, in $\tilde{V}_0^E$ all terms are of order eight in $m_{\mu\nu}$, in $\tilde{V}_0^{KG}$ the term independent of, respectively, dependent on Π has degree eight (or higher if there is a nonquadratic potential), respectively, six and $\tilde{V}_0^M$ has degree seven in $m_{\mu\nu}$. Thus, $\tilde{V}_0$ is polynomial in all fields. Since the smearing function S^0 is arbitrary, we can absorb $\sqrt{\det(m)}^{-5}$ into it, thererby defining $\tilde{S}^0 = [\det(m)]^{-5/2} S^0$ which has density weight minus five. Then, we can still use the first formula in (14) with S^0 replaced by $\tilde{S}^0$ if we multiply its right hand side by ω^{-5}.

To see that this is allowed, note while the "rescaling" of S^0, V_0 by $\gamma := \det(m)]^{5/2} > 0$ does have a non-trivial effect on both the constraint and the smearing function, it has absolutely no effect on the reduced Hamiltonian which is what we are interested in. To see the latter, recall that given gauge fixing conditions say of the form $G = K - \tau$ (K are functions on the phase space, τ are some time dependent coordinate conditions) for constraints C with smearing functions f the reduced Hamiltonian H_r acting on functions F of the true degrees of freedom is computed by the formula $\{H_r, F\} = \{C(f), F\}_{C=G=f-\hat{f}=0}$ where $f = \hat{f}$ solves $\{C(f), G\} = \dot{\tau}$. Since $C, \tilde{C} = \gamma C$ have the same zeroes, the gauge fixing is the same and the matrices γ cancel in H_r because $\hat{\tilde{f}} = \gamma^{-1}\hat{f}$ when $C = 0$.

With this understanding, all constraints are finite polynomials in all fields (of top degree twelve, e.g., for a charged scalar field and for at most quadratic potential otherwise of degree nine plus the degree of the potential) and plugging in (14), (15) allows us to carry out all angular integrals in closed form, thereby yielding an *exact* closed expression for the Hamiltonian written as a polynomial of degree two in all p, P, y, Y; of degree two in x_M, X_M; of degree two or the degree of the potential in Q_{KG}, X_{KG}; of degree at most nine in q_E, x_E. Thus, we obtain an expression for H that is known *non-perturbatively*. However, note that this perfectly allowed reformulation of H in terms of $\tilde{V}_0$ (relying on the assumed non-degeneracy of $\det(m)$) which enables us to carry out all angular integrals, does not prevent the *exact* reduced or physical Hamiltonian from being non-polynomial in Q, P, X, Y. This is because in its computation [61] we must solve for the momenta p, y which appear non-linearly (namely quadratically) in $\tilde{V}_0$ and thus their solution leads to square roots. The algorithm of [61] computes that square root perturbatively in X, Y which thus involves again an infinite series. Nevertheless, the computational effort when working with $\tilde{S}^0, \tilde{V}_0$ is significantly smaller than when working with S^0, V_0 because 1. the number of necessary Clebsch–Gordan decompositions required are finite and can be performed in closed form, hence there are no perturbative errors at this stage and 2. since $\tilde{V}_0$ does not involve an infinite series while V_0 does, the perturbative solution of $\tilde{V}_0$ in terms of x, y, X, Y is tremendously simplified. Of course, whether one works with D_0 or $\tilde{V}_0$, the perturbative solution to both constraints including the angular integrals is the same, it is just that $\tilde{V}_0$ is significantly more convenient.

With these preparations and dropping the tilde in $\tilde{S}^0, \tilde{D}_0$ again we can thus write the Hamiltonian in the form

$$H = f^a\, C_a + g^j\, Z_j := \int_{\mathbb{R}_0^+} dr\, \{[f^v\, C_v + f^h\, C_h + f^M\, C_M] + \sum_{l>0,|m|\le l} [\sum_{\alpha\in\{v,h,e,o,M\}} g^{\alpha,l,m}\, Z_{\alpha,l,m}]\,\} \tag{18}$$

where ($\alpha \in \{e, o\},\ l > 0$)

$$\begin{aligned} &C_v :=< 1, V_0/\omega^6 >_{L_2},\ C_h :=< 1, V_3/\omega >_{L_2},\ C_M :=< 1, G/\omega >_{L_2}, \\ &Z_{v,l,m} =< L_{l,m}, V_0/\omega^6 >_{L_2},\ Z_{h,l,m} =< L_{l,m}, V_3/\omega >_{L_2}, \\ &Z_{\alpha,l,m} =< L_{\alpha,l,m}, V_./\omega >_{L_2^2};\ \alpha \in \{e, o\},\ Z_{M,l,m} =< L_{l,m}, G/\omega >_{L_2} \end{aligned} \tag{19}$$

where we refer to C_a, Z_j, respectively, as the symmetric and non-symmetric constraints, respectively. Note, however, that each of them depends on all degrees of freedom and thus Poisson brackets of C_a, Z_j, respectively, also affect x, y, X, Y and q, p, Q, P, respectively.

To compute the inner producs (19) we expand the polynomials C_a, Z_j into their homogeneous pieces $C_{a(n)}, Z_{j(n)}$, respectively, where the notation means that, e.g., $C_{a(n)}$ is a homogeneous polynomial of degree $n \ge 0$ in x, y, X, Y. Then, the integrals over S^2 in (19) involve n or $n+1$ tensor harmonics, respectively, for the contribution $C_{a(n)}, Z_{j(n)}$, respectively. Since $< 1, L_{l,m} >_{L_2} = 0,\ l \ne 0$ it follows immediately the simple but very powerful observation that

$$C_{a(1)} = Z_{j(0)} = 0 \tag{20}$$

which turns out to be crucial in order for the perturbative construction algorithm for the physical Hamiltonian to work. On the other hand, the contributions from $C_{a(0)}, C_{a(n)}; n \ge 2$, $Z_{j(n)}; n \ge 1$ are in general, not vanishing. One computes them explicitly using Riemann tensor calculus and harmonic analysis on the sphere as well as Clebsch–Gordan decomposition. Explicitly one finds for vanishing Klein–Gordan potential U that

$$\begin{aligned} &C_{v(n)},\ 1 \ne n \le 12;\ C_{h(n)},\ 1 \ne n \le 2;\ C_{M(n)}; n = 0, 2,\ Z_{v,l,m(n)},\ 0 < n \le 12; \\ &Z_{\alpha,l,m(n)},\ \alpha \in \{h, e, o\}, 0 < n \le 2;\ Z_{M,l,m(n)},\ n = 1, 2 \end{aligned} \tag{21}$$

are non-vanishing and can be computed in closed-form.

3. Concepts of Quantum Black Hole Perturbation Theory

The purpose of this section is to review several concepts of (quantum) black hole perturbation theory in a non-technical fashion before we go into technical details in later sections. The aim is to explain these notions and their interrelations in order to erect a consistent conceptual picture.

3.1. Observables, Backreaction and Black Hole Evaporation

By backreaction, we understand the interaction between the spherically symmetric and spherically asymmetric true degrees of freedom. The symmetric and asymmetric true degrees of freedom, respectively, are basically the $l = 0$ and $l \geq 1$ multipole moments of the various observable (or true) fields (geometry and matter) as described in the previous section. With this understanding of backreaction, the following issue arises: Consider first the Einstein–Maxwell sector, i.e., there is no additional, e.g., scalar matter "hair". Then, by Birkhoff's theorem [6], the symmetric sector (no radiation, i.e., no multipoles) is uniquely described by two variables, namely the black hole mass M and charge Q. These arise as integration constants when solving the perturbative Einstein equations also when the multipoles are non-vanishing. The physical Hamiltonian then will be a functional of the asymmetric true degrees of freedom denoted by X, Y for the Einstein–Maxwell sector and a function of M, Q, say $H[M, Q; X, Y]$. By construction, M, Q have vanishing Poisson brackets with X, Y and among themselves. Therefore, M, Q would be constants of motion with respect to H and while there is gravitational and electromagnetic radiation described by X, Y, certainly M, Q would be unchanged by the dynamics described by H, in particular, M, Q could not evaporate. This is in contrast to the situation in cosmology where the physical Hamiltonian, e.g., deparametrized with respect to the homogeneous mode of a scalar field ϕ, does depend on the scale factor *a and* its conjugate momentum p_a so that there *is* backreaction in the above sense between a, p_a and the inhomogeneous modes of both matter and geometry [72]. In spherical symmetry, the situation for M changes, e.g., when introducing neutral scalar matter and for Q it changes when, e.g., introducing charged scalar matter. In that case, M, Q are simply absorbed into true symmetric (in this case) scalar matter degrees of freedom with which there is non-trivial backreaction.

Thus, it would seem that in the Einstein–Maxwell theory M, Q could not evaporate, *not even in the quantized theory* which would include a quantization of $H[M, Q; X, Y]$. While for Q this is expected as photons do not carry a charge, for M this is non-trivial: In the classical theory it is a manifestation of the black hole area theorem since Maxwell matter obeys the weak energy condition. However, in the quantum theory where the weak energy condition is typically violated locally, one would not expect that M does not evaporate. In particular, in Einstein–Maxwell theory the above argument suggests that even including backreaction *there is no dynamic mechanism for black hole evaporation* which is in contradiction to the semiclassical argument that the existence of Hawking radiation predicts black hole evaporation irrespective of the matter species.

Two ways out of that conclusion suggest themselves:

1. The first way out is based on the observation that Birkhoff's theorem treats *all* spacetime diffeomorphisms as gauge transformations. However, in the Hamiltonian framework one makes a finer distinction between diffeomorphisms that generate nonobservable gauge transformations and those that are observable symmetry transformations. If one adopts that Hamiltonian point of view which is consequential within this purely Hamiltonian treatment of black holes, then additional observables, namely momenta P_M, P_Q conjugated to P, Q are unlocked. If the spacetime metric depends at least on both (M, P_M) then M is no longer conserved even in pure Einstein–Maxwell theory and can possibly evaporate in the quantum theory. We will see that P_Q does not enter the spacetime metric while P_M does or does not, depending on the way that the expression that defines P_M is made compatible with the chosen gauge fixing condition.
2. The second way out is to accept the absence of P_M from the reduced Hamiltonian and consists of interpreting M not as the dynamical mass but just as an integration constant, namely the initial mass $M(0)$ in (1). The role of the dynamical mass must then be played by another object. It cannot be the ADM mass which is basically the reduced Hamiltonian which is, therefore, also conserved. The natural notion of dynamical mass is the square root of the area of the apparent horizon with respect to the foliation selected by the gauge fixing conditions (equivalent to the selection of an observer congruence), which coincides with the notion of irreducible mass for the case that apparent and event horizon coincide.

In the following two subsections, we will spell out some of the details of these two possibilities. In the main part of the paper, we adopt the second point of view as it appears to be less sensitive to the choice of gauge fixing condition but keep the first point of view in mind for potential future applications. Some of the possible technical implementations of the first viewpoint can be found in Appendices A–C.

3.1.1. Dirac Observable Conjugate to the Mass

In [23,73,74] it was observed that the reduced phase space of a spherically symmetric vacuum black hole is not described by just the mass M but also its conjugate momentum P_M and a scaling parameter κ. Both M, P_M are Dirac observables, that is, functionals of the canonical variables of a vacuum black hole (or the symmetric degrees of freedom) that have vanishing Poisson brackets with the constraints. Moreover, M, P_M are canonically conjugate. The number κ enters the physical Hamiltonian $H = \kappa\ M$. In Appendices A and B we explain in non-technical terms why this happens: Essentially, one can perform a canonical transformation to conjugate variables m, p_m and the constraints impose that $m' = 0$. This leaves an integration constant $m = M$ as the solution. One then shows that $P_M := \int\ dr\ p_m$ is gauge invariant, and thus cannot be gauged away and is conjugate to M. Finally, the transformations that stabilize any choice of gauge consistent with the value P_M have the generator κM where κ is arbitrary. The existence of κ can be understood from the fact that $C(r) = m'(r) = 0$ is equivalent to $\tilde{C}(r) = m(r) - m(0) = 0$ which is identically satisfied at $r = 0$ thus the constraints $C(r)$ are redundant. Equivalently, when solving the stability condition for transformations preserving a gauge compatible with P_M one must solve a differential equation for the smearing function of the constraint which has a free integration constant which is κ. All of this has to be conducted with due care paying attention to decay conditions, boundary terms, finiteness of both symplectic structure and constraint integrals and functional differentiability of the constraints, see Appendix A.

In [23,73] it is explained why the existence of P_M is not in conflict with Birkhoff's theorem: Indeed, Birkhoff's theorem says that in asymptotically flat regions of spherically symmetric spacetimes one can pass to coordinates in which P_M vanishes. By carefully investigating the required temporal diffeomorphism, one observes that this diffeomorphism is asymptotically non-trivial and thus is to be considered as a *symmetry* transformation rather than a *gauge* transformation [75] in the Hamiltonian setting. Thus, the existence of P_M comes about due to the different notions of gauge in the Lagrangian (as used in Birkhoff's theorem) and Hamiltonian setting, respectively. To make our exposition self-contained, we will review this subtle difference in gauge in Appendices A and B. A similar observation was made in [76] in the context of cosmological models.

Note, that the existence of a two-dimensional rather than one-dimensional reduced phase space of the spherically symmetric vacuum sector is also natural from the point of view of symplectic reduction of phase spaces with respect to first-class constraints which always returns an even-dimensional reduced phase space at least in the case of finite-dimensional unreduced phase spaces. The idea would then be that the reduced Hamiltonian depends on both M, P_M and X, Y so that $H[M, P_M; X, Y]$ mediates an interaction between both types of degrees of freedom. In the quantum theory, that interaction can then be treated, e.g., using the methods of space adiabatic perturbation theory [71] (SAPT), a generalization of the Born–Oppenheimer approximation scheme that can deal with the situation that the interaction depends on both slow degrees of freedom M, P_M rather than just one, similar to the analysis performed for cosmology [72]. The SAPT scheme then would produce an effective Hamiltonian for M, P_M that would take this notion of backreaction into account.

To make this work, one has to supply a missing ingredient to the works [23,73,74], namely to explain how the functionals $M[q, p], P_M[q, p]$ of the spherically symmetric intrinsic metric q and its conjugate momentum p can give rise to prescribed values M, P_M when one solves the constraints for p with some choice of gauge for q installed. Since the constraints can be solved for $p(r) = p(r; M, q)$ for general q where M is an integration constant, apparently the only solution to this problem appears to be that the gauge for q must depend on both M, P_M or at least on P_M. But then the following puzzle arises: Since the physical Hamiltonian is essentially the black hole mass M, while M is a constant of physical motion, P_M is not. This would mean that the metric q, even in the absence of the perturbations X, Y and outside the horizon is potentially not static and the effect is not necessarily small as $\dot{P}_M = O(1)$ and thus $|P_M|$ is unbounded in time. Below, we offer three possible resolutions to this puzzle which all rests on the fact that the formal expression for $P_M[q, p]$ is actually an ill-defined integral, which requires a more careful definition, for the standard choices of gauge. The three resolutions differ in the way that this integral is regularized given a choice of gauge. The choice of gauge we employ, respectively, will be closely related to the (generalized) Gullstrand–Painlevé gauge (GPG) [56–58] which we review in Appendix C. This gauge choice is motivated by the fact that it is both adapted to the spherical symmetry of the problem and natural from the point of view of QFT in curved spacetimes (Hawking radiation) and black hole–white hole transitions as we explain further below.

A. Since $\tilde{P}_M[q, p] := P_M[q, p] - f(M)$ is still conjugate to M for any function f of M, it is possible to obtain a finite expression by choosing the exact Gullstrand–Painlevé gauge (GPG) [56–58] which is independent of both M, P_M, except for an arbitrarily small neighborhood of the origin where the metric is singular anyway. The coordinate size L of that neighborhood does not grow with time and can be chosen to be at most Planck size so that this deviation is hidden behind the horizon even for Planck size black holes. Yet, the deviation can be chosen to depend on L, M, P_M in such a way that the prescribed value for P_M is obtained from $\tilde{P}_M[q, p]$ on the reduced phase space (i.e., both constraints and this gauge are installed). This will be described in Appendix C. A variant of this is to glue two asymptotic ends along the cylinder $r = l < 2M$. Then, it turns out that the corresponding vacuum solution reaches the Einstein–Rosen bridge solution $l = 2M$ exponentially fast, see Appendix B.

B. Another way to regularize the integral is to take the principal values of the integral which has singularities at $r = M, r = \infty$. We consider the generalized GPG [56–58] which depends on an additional parameter e corresponding to the energy of a timelike radial geodesic observer on which more will be said below. It is then possible to regularize the integral such that $c\, P_M = \text{arth}(e/e_0)$ for some fixed numerical value c, e_0. Then, as $|P_M|$ grows, e approaches a constant value e_0, more rapidly the larger $|c|$ is, e.g., $e_0 = 1$ which is the exact GPG. Thus, while e is not a constant of physical motion, it quickly reaches a quasi-constant value e_0.

C. We can pick the exact GPG and still regularize the integral such that the given value of P_M results.

Option C is the simplest and while P_M exists it does not show up in the gauge fixed q, its value is simply a regularization ambiguity. For the electric charge, this is automatically the case, i.e., the momentum P_Q conjugate to Q does not enter the gauge fixed metric, and therefore, the reduced Hamiltonian. Option B is quasi-equivalent to option C rapidly in time. Option A in the first variant is almost (locally in space) the exact GPG, it has the disadvantage to make perturbative calculations more complicated. Common to these options is that P_M either does not show up in q at all (option C) or is quasi absent either with time (option B) or spatially locally (option A, first variant) or the interior of the black hole is removed so that P_M becomes a function of M (option A, second variant). In that sense, the backreaction on M via the interaction between M, P_M, X, Y is either exact or quasi absent.

Note, that the generalized GPG with parameter e_0 are spacetime diffeomorphic to the standard SS coordinate solution for $r > 2M$ but the required temporal diffeomorphism involves in all options a rescaling of the time coordinate (i.e., the lapse is asymptotically different from unity). Hence, it is asymptotically non-trivial and should, therefore, not be considered a gauge transformation.

To see which of these three options is preferred one may invoke the mathematical argument to have a match with the Kantowski–Sachs (KS) picture which underlies most of the treatments of the quantum black hole with LQG methods (LQBH) [23–36] building on the huge amount of experience with the treatment of quantum cosmology with LQG methods (LQC) [77,78]. We will review this in Appendix D. Note, however, two caveats with that argument: First, the equivalence of both pictures is due to the fact that the GPG vacuum solution is stationary while the KS vacuum solution is homogenous so that one can just switch the roles of time and space. This is no longer true with matter coupling unless the spherically symmetric matter sector also leads to only stationary solutions (such as TOV spacetimes with perfect fluid energy-momentum tensors and suitable equations of state between pressure and energy density [14]). Second, the mathematical equivalence between the KS picture and the generalized GPG picture rests on considering all spacetime diffeomorphisms as gauge transformations and thus, is insensitive precisely to the issue of the status of existence of P_M which relies on a finer classification of diffeomorphisms.

Nevertheless, it is of interest to understand the correspondence between the two pictures in the Hamiltonian setting: In the KS picture one considers the Hamiltonian analysis of homogeneous, spherically symmetric but anisotropic KS cosmologies which depend on two scale factors A, B and their conjugate momenta p_A, p_B. The spatial diffeomorphism constraint vanishes identically and there is only one remaining Hamiltonian constraint. Hence, this is a mechanical system with a 4d phase space and one (necessarily first-class) constraint so that the counting of degrees of freedom is very simple: The reduced phase is 2d and there are exactly two algebraically independent and canonically conjugate Dirac observables. One can develop both the relational observables and true degrees of freedom picture and compute the physical reduced Hamiltonian. The solutions of the physical equations of motion show that on shell the scale factors and lapse are exactly those of the Schwarzschild interior solution with the switch between radial and temporal coordinate understood, up to one exception: While the first observable is associated with the mass, the second corresponds to a rescaling of the time coordinate and can be interpreted as a "clock ticking rate". It is exactly the same scaling parameter κ that occurs also in the above GPG picture (which covers both the interior and exterior of the black hole). Accordingly, in the KS picture the possibility for P_M to show up in the physical metric never occurs. It follows that the two pictures agree if we pick for the GPG picture option C i.e., we install the exact GPG and ascribe P_M to a regularization freedom.

It is quite interesting to see how this happens: In the KS picture, we start from a finite-dimensional phase space with a very transparent counting of degrees of freedom. On the other hand, in the generalized GPG picture we start with a field theory, i.e., an infinite dimensional phase space before the constraint treatment and there is a complicated set of issues such as spatial fall-off conditions, boundary terms, solving spatial differential equations, etc., arise. Because of this the construction of the reduced phase spaces and physical Hamiltonians is quite different. In the cosmological KS picture, the physical Hamiltonian simply results from gauge fixing conditions and the effective equations of motion for the corresponding true degrees of freedom while in the GPG picture, it is the boundary term that must be added to make the constraints functionally differentiable that drives the dynamics of the true degrees of freedom. In the KS picture, we have two true degrees of freedom or Dirac observables M, κ, in the GPG picture we have two observables M, P_M and an additional integration constant κ which arises due to constraint redundancy while in the KS picture, there can be no such redundancy. In option C above we can discard P_M as it does not show up anywhere in the metric and then both pictures match as far as the surviving parameters, namely M, κ, are concerned. However, while M, κ have non-vanishing brackets in the KS picture, in the GPG picture κ is considered a phase space independent constant. The resolution of this apparent contradiction is as follows: In the KS picture, the physical Hamiltonian and M, κ are *explicitly time dependent* with respect to KS time T. However, in solutions of the equations of motion they become constants of motion. In contrast, in the exact GPG picture the physical Hamiltonian is conservative, i.e., like M, P_M is not explicitly time-dependent with respect to GPG time τ. In solutions, also M is a constant of motion and κ was a time-independent constant from the outset. Note, that since essentially the KS time T is the radial variable, T independence in the KS picture translates into radial independence which again brings both pictures into congruence.

To summarize: For the rest of this paper, we will follow option C when considering nonvacuum spacetimes. This means that the mass parameter M is a constant of physical motion and can, therefore, be called the "remnant mass" because the physical Hamiltonian reduces to it when perturbations and matter are absent. There is no dynamical mechanism that can change M because while the second Dirac observable P_M exists it does not enter the physical Hamiltonian. We work in the exact GPG. Still, we may use the above-introduced cut-off $l = r$ as a regularization method when we compute the black hole white hole transition mode functions, see Section 8.

3.1.2. Apparent Horizon Area

Consider then M as an integration constant. It happens to coincide in the exactly spherically symmetric case with many different definitions of mass in general spacetimes that have been discussed in the literature such as the ADM mass [75] or the irreducible mass [6,14]. The ADM mass is expected to be the leading term of the physical Hamiltonian H for small perturbations and thus is, in particular, preserved (together with M if P_M is absent in the metric), hence "evaporation of H" is again not possible. However, the irreducible mass with respect to the apparent horizon serves as a suitable more direct measure of backreaction. Recall that given a foliation of (M, g) by spacelike hypersurfaces $\tau \mapsto \Sigma_\tau$ a compact 2-surface $S_\tau \subset \Sigma_\tau$ without a boundary is called an outer marginally trapped if $\theta_+ = 0,\ \theta_- < 0$ where $\theta_\pm$ are the expansions of the null normals $l_\pm = n \pm s$ with $g(n, n) = -1,\ g(s, s) = +1,\ g(n, s) = 0$ with future-oriented timelike unit normal n to Σ_τ and the outward-oriented spacelike unit normal s to S_τ and tangential to Σ_τ. The outermost trapped surface (two-dimensional) is called the apparent horizon $\mathfrak{H}_\tau$ at τ and the union of apparent horizons as τ varies is called trapped horizon (three-dimensional) $\mathfrak{H}$. Finally, the irreducible mass M_τ at τ is the square root of the area A_τ of $\mathfrak{H}_\tau$ (up to a constant factor; abusing terminology, the actual definition refers to the event horizon rather than the apparent horizon).

Following [79] it is not difficult to show, see Section 7, that indeed one can uniquely determine A_τ to arbitrary order in perturbation theory directly in the Hamiltonian setting and thus obtain a notion of time-dependent mass that can possibly evaporate. This notion of mass is also operationally preferred as an astrophysicist would recognize a black hole as a marginally outer trapped region (which is the condition that the light rays leaving S_τ orthogonally are marginally converging). Now, the following issue arises: Under a combination of the usual assumptions, namely that the classical Einstein equations hold, that the energy conditions for the energy-momentum tensor are satisfied, the validity of cosmic censorship and global hyperbolicity, classical GR makes two predictions: First, that the existence of trapped surfaces implies the existence of a singularity and second, if that singularity is a black hole (rather than a naked one forbidden by cosmic censorship) then the trapped surface is within the black hole region. Therefore, if the astronomer is outside the black hole region, they will indeed measure the event horizon as the sphere of no escape. From that point of view, the apparent horizon appears to be of no use except that one expects it to be a good approximation (or at least a lower bound) of the event horizon. The apparent horizon has the advantage of being less teleological than the event horizon but it has the disadvantage of being foliation dependent. We do not share that criticism but rather accept that the notion of irreducible mass *is* observer-dependent and here the foliation is selected by the (generalized) Gull–Strand–Painlevé gauge which we motivate in the next subsection. We refer the reader to the rich literature on apparent horizons and its specialisations (e.g., dynamical and isolated horizons) [17].

Now, again by classical GR the area of the event horizon cannot decrease; therefore, in classical GR there is no evaporation possible. We need quantum theory to have evaporation by violating at least one of the assumptions of classical GR. The most obvious one is the violation of the energy conditions, recalling similar quantum violations of classical (energy) inequalities in QFT in flat spacetime [80]. In that case, one can have trapped regions which evolve dynamically while there is no event horizon at all if, for example, the singularity is resolved, as the existence of trapped regions no longer implies the existence of a singularity (assuming that the classical reasoning can be applied at all, at least in a semiclassical sense). Even if there still is an event horizon, the violation of the energy conditions now no longer implies the apparent horizon to lie in the black hole region, it can even lie outside. This picture is confirmed in exactly solvable 2d models such as the CGHS black hole solutions including matter [18].

Now, in perturbation theory the zeroth order is a spherically symmetric vacuum black hole if there is no spherically symmetric matter hair and that spacetime does have a singularity and an event horizon. The second order describes the perturbations as propagating on that singular spacetime and can, e.g., serve to start a Fock quantization of the system. Therefore, it appears strange to perturb a singular spacetime with an event horizon if one expects that in quantum theory the non-perturbative spacetime is in fact free of singularities, and therefore, does not have an event horizon, that is, it seems that black hole perturbation methods are unable to capture the actual non-singular nature of the quantum theory. Our point of view here is that the causal structure of the spacetime including its singularities and horizons is itself subject to perturbation theory. Hence, even in the second order one would compute the expectation value with respect to an initial state (using the Heisenberg picture) of the (perturbed) metric tensor, curvature tensor, reduced Hamiltonian, apparent horizon and its area, etc., using their classical expressions and substitute them by the corresponding operator-valued distributions. Altogether, this describes a new effective spacetime metric to which we may apply the usual classical GR definitions of singularities and horizons to calculate a quantum corrected Penrose diagram (at least in regions where that effective metric has small quantum fluctuations). This process can be iterated at higher orders of perturbation theory and presents a drastic form of backreaction. It goes beyond the semiclassical Einstein equations in which one defines the Einstein tensor as the expectation value of the matter energy-momentum tensor $G(g) :=< T(g) >$ and tries to find a self-consistent metric g solving this equation [81] because here the (perturbations of) the metric are also quantized in the Heisenberg picture (the Heisenberg equations follow from the reduced Hamiltonian, to any order in perturbation theory, using the Gell–Mann and Low formula if we use Fock quantization). A possible mechanism for violation of energy conditions is due to normal ordering prescriptions of $< T(g) >$.

If the singularity disappears in this process, what forms and evaporates is then not the event horizon but the apparent horizon, see also [82,83]. Therefore, perhaps one should in fact set $M = 0$ at zeroth order i.e., start with Minkowski space and follow the above process from formation to evaporation although it is unclear whether starting from $M = 0$ and Minkwoski space Fock spaces for the perturbations and an initial coherent state peaked at gravitational collapse initial data one really obtains a collapse–evaporation process in the quantum theory. For the sake of generality in this paper, we handle the general $M > 0$ case but motivated by the quantum theoretical considerations feel free to regularize the singular $M > 0$ background spacetime when needed.

It is remarkable that the innocent-looking integration constants M, Q have such a tremendous impact on the whole quantization process. Namely, they decide whether second-order perturbation theory we consider Fock representations on singular or non-singular spacetimes, with or without horizons. We close the discussion by mentioning the following observations:

A. The components of the spacetime metric g are specific functions of M, X, Y. These arise as follows: One imposes the GPG, fixing the components of the spatial metric m different from X, solves the constraints for the components of p different from Y and solves for lapse S^0 and shift S^a using the stability condition of the imposed gauge under gauge transformations. The irreducible mass then is also a specific function $m = m[M, X, Y]$ of these true degrees of freedom. As we will show in Section 7 we have $m = M + m_2[M, X, Y] + m_3[M, X, Y] + \ldots$ where m_n is of n-th order in X, Y. Now, even if radiation described by X, Y is *produced* only in a compact spacetime region R, since X, Y have to obey wave equations, that radiation is generically non-vanishing in the entire causal future $J_+(R)$ of that region (the causal future is of course also influenced by the amount of radiation present as it perturbs the metric). Given a foliation of (M, g) by Cauchy surfaces Σ_τ let τ_0 be the latest foliation parameter such that $\Sigma_\tau \cap R \neq \emptyset$. Then, still $\Sigma_\tau \cap J_+(R) \neq \emptyset$ for all $\tau \geq \tau_0$. Thus, a timelike observer with eigentime τ will eventually enter $J_+(R)$, however, for sufficiently large timelike distances from R the signal described by X, Y will be weak. Thus, the spatial metric m returns to almost strict GPG for sufficiently large τ because it is a spatially *local* function of X, namely $q - g^{\mathrm{GPG}} = X$. On the other hand, the solution of p, N, N^a at given τ is a spatially *non-local* function of X, Y involving integrals over the entire hypersurface Σ_τ. This is because the constraint and stability equations are PDE's and not algebraic equations. Since $\Sigma_\tau \cap J_+(R)$ becomes larger in volume the later τ is, these integrals can counterbalance the decay of X, Y and lead to strong deviations of lapse and shift from their pre-radiation values which are $S^0 = 1$ and $S^a = \delta^a_3\sqrt{2M/r}$ for all $\tau \geq \tau_0$ in the causally allowed region of spacetime. As a measure of this deviation, we may introduce the effective mass by $\sqrt{2m_{\mathrm{eff}}(r,\tau)/r} := \int_{S^2} d\Omega(y) S^3[M, X, Y](r, y, \tau)$ which, therefore, can deviate from M for all $\tau \geq \tau_0$ and can potentially vanish, therefore, describing the evaporation effect. Since the spatial integral over a fixed τ hypersurface captures non-linear contributions from the "gravition" fields X, Y related to their data in R by the corresponding retardation, this may be considered as an instance of a non-linear memory effect [84].

B. The apparent horizon at τ is defined by a radial profile function $\rho : S^2 \to \mathbb{R}_+;$ which depends on X, Y which become quantum fields. In that sense the coordinate location of the apparent horizon becomes quantized, subject to quantum fluctuations. This, on the one hand, is very similar to the construction of quantum reference frames [85,86] and on the other hand, intuitively explains why the black hole area theorem can be violated in the quantum theory: Even if an event and apparent horizon coincide, in suitable states the fluctuations can be very large so that the location of the apparent horizon becomes fuzzy.

C. In the classical theory, if the metric does not depend on the observable P_M conjugate to M, and possibly also the quantum theory it is conceivable that significant evaporation, apart from minuscule quantum fluctuations, only arise if we take interactions into account. These arise only beyond second-order perturbation theory due to either self-interactions of X, Y or interactions between X, Y and the matter degrees of freedom. The reason is that in the second order geometry, matter fluctuations decouple and all field species effectively propagate on a GPG background with fixed M. As that background is GP time independent, each mode function that solves the corresponding classical equations of motion is $\propto e^{i\omega\tau}$ for some $\omega \in \mathbb{R}$ and thus periodic in GP time with periodicity determined by ω. If the classical or quantum field is only excited for a finite number of such ω then all notions of mass depending on the fluctuations will be (quasi-)periodic rather than decaying functions of time which would rather require a superposition (integral) of an infinite number of modes. In second order there can be an interaction between matter and geometry fluctuations if the electric charge does not vanish (or if the Klein–Gordon potential has a linear term) but such a quadratic interaction can be decoupled by a canonical transformation and the time dependence would still be quasi-periodic. This indicates that having a manifestly gauge invariant formalism at one's disposal that allows to unambiguously compute the effects of higher order perturbations of the true degrees of freedom is probably very crucial in order that significant evaporation effects are turned on even if only a finite number of modes are excited.

3.2. Foliations and Hawking Radiation

The physical Hamiltonian can be expanded to any order in X, Y and in quadratic order suggests a Fock representation of X, Y corresponding to a free field on a spacetime whose metric depends parametrically on M. This requires that the $\tau =$ const. surfaces of the foliation defined by the gauge fixing conditions are actually complete Cauchy surfaces, i.e., they have a timelike normal and every inextendible causal curve must cross each Σ_τ precisely once. Moreover, as we wish to explore the fate of the singularity and the possibility of black to white hole transitions, the spacetime covered cannot only be an asymptotic region but must also deal with the interior of the black hole parametrized by M and possibly another exterior region.

All of this rules out using standard Schwarzschild time, as the Killing field ∂_t orthogonal to the $t = const.$ slices is spacelike for $r < 2M$ and there is a coordinate singularity at $r = 2M$. As a physical selection criterion for the gauge fixing and the corresponding foliation, we use the principle of general relativity, that is, the equivalence principle: The Fock vacuum (zero particle vector state) selected by the Hamiltonian should be the one of an observer in geodesic motion since this observer comes as close as possible to an inertial observer in flat spacetime. Since the spacetime parametrized by M is spherically symmetric we employ that symmetry property and consider radial unit timelike geodesics adapted to spherical symmetry. These carry two parameters e, ρ in addition to the directional angles. Here, $e := -g(\xi, u) \in \mathbb{R}_+$ is the asymptotic energy per mass where $\xi = \partial_t$ is the Killing vector field corresponding to Schwarzschild time t and $u = \partial_\tau$ is the unit timelike tangent along the affinely parametrized geodesics with eigentime parameter τ, i.e., $g(u, u) = -1,\ \nabla_u u = 0$. The parameter $\rho \in \mathbb{R}$ labels the geodesic and has the meaning that at eigentime $\tau = \rho$ the geodesic hits the singularity $r = 0$ where r is the Schwarzschild radial coordinate. The parameter e which is the same for the whole geodesic congruence is a function of M, P_M as detailed in Appendix C which would be of interest if we would use option B of the previous subsection and is, therefore, a Dirac observable as one would expect from its geometrical meaning. For $e \neq 1$ the corresponding coordinates are called generalized GP coordinates while $e = 1$ corresponds to the standard or exact GPG. As motivated in the previous subsection we will use $e = 1$ in what follows but briefly comment on the case $e \neq 1$ for possible future use. Since the geodesics are complete (τ has infinite range) only for $|e| > 1$ it is sufficient to consider only the case $e \geq 1$.

At each fixed e, the family of ingoing geodesics labeled by ρ, θ, ϕ is a geodesic congruence which covers the Schwarzschild (SS) and black hole (BH) portion of the Kruskal extension of the spacetime and the family of outgoing geodesics labeled by ρ, θ, ϕ is a geodesic congruence which covers the mirror Schwarzschild (BSS) and white hole (WH) portion of the Kruskal extension of the spacetime. It turns out that these geodesics intersect the spacelike surface $r = 0$ orthogonally when $e = 1$ and that the $\tau = const.$ slices Σ_τ which carry coordinates ρ, θ, φ are spacelike surfaces that intersect the singularity tangentially when $e = 1$. If we restrict these surfaces to SS and BH or MSS and WH only, then they are not Cauchy surfaces for these portions because they end at the singularity. We can turn them into Cauchy surfaces in two ways: The first possibility is to restrict to say the SS and BH portion and use part of the singularity to complete Σ_τ in a C^1 manner to a Cauchy surface. This spacetime has topology $\mathbb{R} \times \mathbb{R}_+ \times S^2$ covered by τ, r, θ, φ coordinates. However, to use part of the singularity surface $r = 0$ as the Cauchy surface is problematic as the metric is singular on an entire 3d submanifold of that Cauchy surface and because the so extended Cauchy surfaces actually overlap at the singularity surface. Thus, one would rather extend the Cauchy surface into the BH part slightly off the $r = 0$ surface after hitting the singularity and such that they do not overlap (there is of course considerable freedom in doing so). The second possibility is to glue a SS and BH portion belonging to a "past universe" to an MSS and WH portion of a "future universe". We conduct this by gluing an ingoing geodesic labeled by ρ in SS+BH to an outgoing geodesic labeled by ρ in MSS+WH. In this way we can foliate the entire set SS+BH+WH+MSS by "free falling Cauchy surfaces" describing a black hole white hole transition between two universes. This spacetime has topology $\mathbb{R}^2 \times S^2$ covered by $\tau, \rho, \theta, \varphi$ coordinates. All $\rho = const.$ geodesics start at past timelike infinity of the past universe as $\tau \to -\infty$ and end in the future timelike infinity of the future universe as $\tau \to +\infty$. All $\tau = const.$ Cauchy surfaces end in the two asymptotic ends, i.e., the spatial infinity of SS in the past universe and of MSS in the future universe. They intersect the singularity in a single point only. Accordingly, it is mathematically preferred to use the entire SS+BH+WH+MSS portion. It is the common domain of dependence of all free-falling Cauchy surfaces and thus this spacetime region is globally hyperbolic if we do not exclude the singularity $r = 0$. In Appendix C we have collected the background material associated with this construction.

Note, that due to the singular behavior of the metric at $r = 0$ there is a priori no reason to assume that the mass M is the same in the future and past universe, respectively, and for the same reason the clock ticking rate κ is not necessarily the same. For reasons of continuity of the geodesic $\rho =$ const. we consider only the equal value case for both M, κ.

In SS+BH+WH+MSS the metric can be described using global coordinates $\tau, \rho, \theta, \varphi$ except for the singularity at $\rho = \tau$ and it remains to be investigated whether certain observables are nevertheless singularity free across $\rho = \tau$ in the quantum theory. For instance, the mode functions that enter the construction of the Fock representation have to solve a stationary equation of Schrödinger type involving a potential that is singular at $r = 0$. However, such a situation is common in quantum mechanics (e.g., the hydrogen atom) and not necessarily an obstacle to solve the corresponding stationary Schrödinger equation.

Note, that the construction can be repeated indefinitely to the future and the past by gluing these transition spacetimes labeled by $I \in \mathbb{Z}$ along the various horizons $r_I = 2M$, $\bar{r}_I = 2M$ where r_I is the radial coordinate in the I-th SS+BH and $\bar{r}_I$ in the I-th MSS+WH part. However, that extended spacetime is no longer globally hyperbolic even when ignoring the singularities because while each transition block is the common domain of dependence on all its free-falling leaves, for instance the timelike geodesics start and end in the past and future timelike infinity of that block and do not enter other blocks. Thus, boundaries between the blocks are Cauchy horizons. Alternatively, one can complete such a transition block along the $r = 2M$ and $\bar{r} = 2M$ boundaries by two Minkowski space Penrose diagram triangles in the past and the future where the vertical long side of the triangles represent $r = 0$ and $\bar{r} = 0$, respectively, before/after the formation/evaporation of the black/white hole, see Appendix C for the details. That completed spacetime continues to be globally hyperbolic.

Returning to one block, given such a foliation, one has to determine the solutions of the classical equations of motion for X, Y dictated by the quadratic part of the Hamiltonian (mode functions). For the case $e = 1$ and $r > M$ these are known as Heun functions [87] and there are techniques available to extend them to $0 < r \leq M$ [88,89]. Thus, in principle, we can construct the mode functions of the Fock representation selected by the radially free-falling observers. This works for either the SS+BH or the MSS+WH portions separately. If these two descriptions can be meaningfully joined we can discuss black hole–white hole transitions as discussed in the next subsection, otherwise we have to restrict to only one of these portions keeping in mind the necessity to extend the free-falling equal proper time surfaces to Cauchy surfaces in this case. In both cases, we call the corresponding vacuum the *geodesic* vacuum. As a congruence of geodesic observers defines a Riemann normal coordinate system wrt which the metric is locally Minkowski, we expect the two-point function of the geodesic vacuum of Hadamard form [90] when we pick the asymptotic form of the mode functions at the spatial infinities to correspond to a flat space Hadamard state.

One can then describe two kinds of Hawking effects in the usual way: The first type is to use the t = const. foliation of the SS portion to define the Fock structure with respect to an asymptotically static observer, express the quantum fields X, Y restricted to SS with respect to the mode functions of the $\tau = const.$ and $t = const.$ foliations, respectively, and derive the Bogolubov coefficients from the equality of the two expansions. This is similar to the Unruh effect with the role of the inertial, respectively, accelerated obserer of Minkowski spacetime played by the τ, respectively, t foliation observer in the curved spacetime parametrized by M, i.e., one uses two *different* foliations in a portion of spacetime. The second type is to use the observation that in ρ, τ coordinates the vector field ∂_τ is not Killing but everywhere timelike and orthogonal to the foliation (the metric depends only on the combination $\rho - \tau$ so that the Killing vector field is $\partial_\rho + \partial_\tau$, however, it is not timelike everywhere). Accordingly one can use the notion of adiabatic vacua [90–93] familiar from cosmology to describe particle production between different $\tau = const$. slices within the *same* foliation of spacetime.

3.3. Black Hole–White Hole Transition and Singularity Resolution

In the literature on quantum black holes inspired by LQG [23–36] one argues that the singularity is removed in two possible ways:

I. In the first scenario, so far restricted to vacuum spacetimes, one uses that the BH and WH portions of the spacetime are described by a Kantowski–Sachs cosmology in suitable coordinates, i.e., the metric is spatially homogeneous and described by two scale factor functions A, B of BH resp. WH "time" $r, \bar{r}$ joined at $r = \bar{r} = 0$ (recall that the radius is timelike in the interior; one can consider the time coordinate $T := -r$ in BH and $T := \bar{r}$ in WH to work with a single "time" coordinate) subject to the condition $A^2 = 1 - 2M/B,\ B^2 = r^2, \bar{r}^2$, respectively. Instead of imposing these conditions we can consider a phase space with canonical pairs $(A, p_A),\ (B, p_B)$ and a Hamiltonian constraint C such that the symplectic reduction of that constrained system recovers the above form of A, B where $2M$ plays the role of an integration constant. See Appendix D for some of the details of this construction. Then, one quantizes the unconstrained phase space using a Narnhofer–Thirring type of representation [94] of the corresponding Weyl algebra inspired by LQG by the same logic applied in LQC [77,78]. Then, one must impose C as a quantum constraint which in this representation is only possible if one modifies C by replacing A, B by suitable linear combinations of Weyl elements which are not all strongly continuous in this representation, e.g., A becomes $\sin(\lambda A)/\lambda$ for small λ in the simplest proposal. One finds that the singularity $B^2 = 0$ is resolved and replaced by a minimal positive value of Planck area order in the "effective equation" approximation sketched below. That is, the quantum metric becomes regular.

II. In the second scenario, so far restricted to spherically symmetric spacetimes with dust matter, one uses coordinates that cover both the interior and exterior of potential black holes. The dust fields are used as material reference systems and one passes to a reduced phase space formulation. The remaining gauge invariant, spherically symmetric metric fields are then quantized in a LQG type of representation similar to in the first scenario. This involves again an approximation of fields by Weyl elements called "polymerization" and one mostly studies the "effective equations", i.e., the classical equations of motion that result from the "polymerized" classical, reduced Hamiltonian. One also here finds singularity resolution in this restricted sense.

The intention of the present work is to extend these results beyond the spherically symmetric (vacuum) sector, beyond the effective description and to use standard matter rather than dust. In that respect the second option is more adapted to the present approach because it is conceptually and technically unclear how to deal with the switch between time and radial coordinates in a canonical quantization (which rests on foliations of the entire spacetime) when passing between the interior and exterior of the black hole. Following the second option, in the present approach one can identify the role of the symmetric true observables with the reduced phase space of the purely spherically symmetric models covered by the second option above and follow their LQG type of quantization. If the quantum theory would be truly non-singular (not only at the effective level) then the quantum spacetime would be non-singular and we could in principle straightforwardly extend X, Y between the BH, and WH portions and discuss BH–WH transitions in a singularity-free manner although solving the corresponding mode functions would become quite involved.

Besides those options, here we explore a less radical possibility: If we avoid the polymerization, which generically is accompanied by "discretization ambiguities", then the symmetric sector of the theory, which is typically non-polynomial in the symmetric true degrees of freedom, describes classically singular spacetimes. Its quantization is, therefore, challenging and must be addressed by independent methods. In Section 6 we sketch a possible approach. It rests on the presence of the integration constant M which allows an expansion of the reduced Hamiltonian in powers of M^{-1} (inverse core mass expansion). The coefficients are then nested radial integrals of the polynomial energy–momentum density of the symmetric sector which can be quantized, e.g., using Fock space techniques. The non-symmetric sector couples to the symmetric sector but can be treated also with this inverse core mass expansion. Therefore, in principle, the system can be treated, e.g., with perturbative Fock space techniques. Still, the mode functions to be solved when defining the Fock representations are derived from differential equations with singular coefficient functions which are obtained from the lowest order in the inverse core mass expansion. Specifically, the metric expressed in τ, ρ coordinates covers a spherically symmetric vacuum spacetime which is singular at $\rho = \tau$ where the leaves of the geodesic foliation intersect the singularity. Accordingly, the corresponding wave equations for X, Y are also singular at $\rho = \tau$. If they can be meaningfully continued across $\rho = \tau$ we can discuss black hole white hole transitions just using standard Fock space techniques. We intend to use a mixture of the machinery of Heun functions [87,95] and the orthonormal basis of the one particle Hilbert space developed in [96] that allow to deal with potentials that contain arbitrarily negative powers of $r, \bar{r}$ in order to define a dense domain of the corresponding Schrödinger type operator and to meaningfully analyze the possibility of a BH to WH transition and a singularity resolution.

3.4. Quantum Penrose Diagramme

In the sketched Fock space approach, eventually, the reduced Hamiltonian for the true degrees of freedom is a perturbative expansion in the X, Y which at quadratic order is that of a free quantum field in the exact GP spacetime of mass M. But that does not mean that the quantum theory describes this spacetime. Rather, the quadratic part of the Hamiltonian just starts the Fock space representation. After this, interesting observables such as the apparent horizon area or the metric coefficients become operator-valued distributions. In the Heisenberg picture, we can, in principle, construct their (perturbative) Heisenberg evolution with respect to the reduced Hamiltonian (truncated at the desired order) and we can compute the vacuum expectation values of those. These expectation values now define a "quantum metric" which will differ from the GP metric we started from and that just served to initiate the quantization. We can then compute the resulting "quantum Penrose diagram" from that quantum metric that captures, at least in part, the quantum corrections to the GP spacetime that one started from. Accordingly, the singular GP spacetime with mass M that initiates the quantization could, in principle, be replaced by a non-singular quantum spacetime via this process.

4. Choice of Gauge Condition and Associated Reduced Hamiltonian

In the first subsection, we motivate the choice of gauge condition adapted to spherical symmetry. In the second we specify the decay behavior of the fields with respect to the chosen system of coordinates. This is somewhat different from the usual decay behavior in terms of the coordinates of an asymptotic observer at rest as the shift function approaches zero more slowly at spatial infinity. In the third, we show that the chosen gauge can be locally installed modulo the usual global issues. In the fourth we solve the constraints *non-perturbatively* in a neighborhood of the chosen gauge cut in implicit form, that is, modulo explicitly solving a system of ordinary differential equations; however, we provide an iteration method for solving it. In the fifth, we compute the corresponding reduced Hamiltonian implicitly but non-perturbatively by solving the stability conditions for lapse and shift functions thereby obtaining the dependence of the full spacetime metric on the true degrees of freedom and exploiting the explicit decay conditions. We will follow the general program outlined in [61].

While all formulae of this section are implicit only, they provide the the fundamental starting point for the explicit perturbative scheme that is developed in the subsequent sections.

4.1. Exact and Generalised Gullstrand–Painlevé Gauge

As outlined in [61] it is important to impose gauge conditions that involve only configuration coordinates on the phase space. This is because otherwise the choice of gauge would not be disentangled from the (perturbative) solution of the constraints for the momentum variables which, in turn, determines the reduced Hamiltonian. Therefore, the gauge condition must not depend on the mass of the black hole. Next, as we wish to be independent of the matter content, this forces us to impose conditions on the three metrics $m_{\mu\nu}$. Furthermore, as we wish to explore the black hole interior, we should impose gauge conditions on $m_{\mu\nu}$ which ensures that the metric is regular across any possible horizons. Therefore, the gauge condition must be regular on the entire three manifold σ which we choose to be $\sigma = \mathbb{R}^3$ for each asymptotic component. At the same time the gauge condition should of course not be in conflict with the possible presence of a black hole (nonvanishing mass) and must be consistent with the available gauge freedom, i.e., the gauge must not eliminate physical degrees of freedom that cannot be removed by a true gauge transformation. This is a subtle point which for completeness is reviewed in Appendices A–C. Finally, there are practical considerations, which prefer gauge conditions which simplify the computations of covariant derivatives and curvature associated with $m_{\mu\nu}$ as much as possible because $m_{\mu\nu}$ features prominently in all couplings between matter and geometry in the Hamiltonian constraint.

These guidelines motivate the **(Generalized) Gullstrand–Painlevé Gauge** (GGPG) $G_\mu = 0, \ \mu = 0,1,2,3$ where [56,57]

$$G_3 := q_3 - e^{-2}, \ G_A := q_A, \ G_0 := q_0 - r^2 \tag{22}$$

which have proved very powerful for exactly spherically symmetric classical and quantum LTB spacetimes [97–99]. Here, $e^2 \geq 1$ is a parameter that cannot be removed by a Hamiltonian gauge transformation (it can be by a Lagrangian one, see Appendix C). These coordinates and their relations to timelike geodesic congruences and simultaneity foliations are reviewed in Appendix C. We refer to the exact Gullstrand–Painlevé gauge (GPG) as the one corresponding to $e^2 = 1$.

The notation is as follows: We have chosen Cartesian coordinates $x^\mu, \ \mu = 1,2,3$ on $\sigma = \mathbb{R}^3$ with corresponding radial coordinates $z^3 := r$ and angular coordinates $z^A, \ A = 1,2$; $z^1 = \theta, \ z^2 = \varphi$ and the components q_{33}, q_{3A}, q_{AB} are with respect to z^3, z^A. Then,

$$q_3 := m_{33}, \ q_A := m_{3A}, \ q_0 := \frac{1}{2}\Omega^{AB} \, m_{AB} \tag{23}$$

The latter is the trace with respect to the background metric Ω on S^2. The GGPG implies that the dynamical configuration degrees of freedom are

$$q^\perp_{AB} = X_{AB} = q_{AB} - \Omega_{AB} \, q_0 \tag{24}$$

The conjugate momenta are

$$P^3 := W^{33}, \ P^A := 2 \, W^{3A}, \ P^0 := \Omega_{AB} \, W^{AB}, \ P^{AB}_\perp = Y^{AB} := W^{AB} - \frac{1}{2}\Omega^{AB} \, P^0 \tag{25}$$

Note, that the non-vanishing Poisson brackets are

$$\begin{aligned} &\{P^3(z), q_3(z')\} = \{P^0(z), q_0(z')\} = \delta(z,z'), \ \ \{P^A(z), q_B(z')\} = \delta^A_B \, \delta(z,z'), \\ &\{P^{AB}_\perp(z), q^\perp_{CD}(z')\} = [\delta^A_{(C} \, \delta^B_{D)} - \frac{1}{2}\Omega^{AB}\Omega_{CD}] \, \delta(z,z') \end{aligned} \tag{26}$$

The GGPG suggests to solve the constraints for the momenta P^3, P^A, P^0 to which we turn in the next subsection.

For completeness, we repeat here the argument why the GGPG can always be installed by a spacetime diffeomorphism when the metric is spherically symmetric (but not necessarily stationary), that is, of the form

$$ds^2 = -f\, d\hat{T}^2 + g\, dX^2 + 2\, h\, d\hat{T}\, dX + k^2\;\; d\Omega^2,\; d\Omega^2 := \Omega_{AB}\, dz^A\, dz^B \tag{27}$$

where f, g, h, k are the functions of $\hat{T}, X$ and $g, k > 0, f + h^2\, g^{-1} > 0$ in order for the metric to be regular and of signature $-1, +1, +1, +1$. We first set $T := \hat{T},\; r := k(\hat{T}, X)$ and invert $\hat{T} = T,\; X = K(T, r)$. Then, upon substitution (27) acquires the form

$$ds^2 = -F\, dT^2 + G\, dr^2 + 2\, H\, dT\, dr + r^2\;\; d\Omega^2, \tag{28}$$

where now F, G, H are functions of T, r. Next, we set $T = T(\tau, r)$ and find

$$ds^2 = -F\, \dot{T}^2\, d\tau^2 + [G - F\, (T')^2 + 2\, H\, T']\;\; dr^2 + 2\, [H\, T' - F\, \dot{T}\, T']\, d\tau\, dr + r^2\;\; d\Omega^2, \tag{29}$$

where $\dot{T} = dT/d\tau,\; T' = dT/dr$. The GGPG can now be completed by solving the non-linear ODE (at a fixed τ)

$$G - F\, (T')^2 + 2\, H\, T' = e^{-2} \tag{30}$$

where G, F, H are functions of $T(t, r)$ and r. The solution of (30) is unique up to a sign and to addition of a function $T_0(\tau)$. Plugging in that solution we find

$$\begin{aligned} ds^2 &= -A\, d\tau^2 + 2\, B\;\; d\tau\, dr + e^{-2}\, d\vec{x}^2 + r^2(1 - e^{-2})d\Omega^2 \\ &= -[A + B^2 e^2]\, d\tau^2\; + e^{-2}\;\; \delta_{\mu\nu}\, [dx^\mu + B\, e^2\, n^\mu d\tau]\, [dx^\nu + B\, e^2\, n^\nu d\tau] + r^2(e^{-2} - 1)d\Omega^2 \end{aligned} \tag{31}$$

where $n^\mu = x^\mu / r$ which shows that the metric is regular and of Lorentzian signature if $A + B^2/e^2 > 0$ which can be ensured using the freedom of choosing T_0.

It is illustrative [56–58] to transform the Schwarzschild form of the line element for $r > 2M$ ($2M$ is the Schwarzschild radius) to GGP form which can be conducted using $T_0(t) = t$. One finds (see Appendix C) that $A = e^{-2}[1 - \frac{2M}{r}],\; B = \mp e^{-2}\, \sqrt{e^2 - 1 + \frac{2M}{r}}$ i.e., $A + B^2\; e^2 = 1$. It follows that lapse and shift are $N = 1,\; N^3 = e^2\, B,\; N^A = 0$. The sign corresponds to a congruence of outgoing/ingoing timelike geodesics for which τ is the eigentime.

The GGP form can be analytically extended beyond $r > 2M$ and covers the advanced ($B > 0$) and retarded ($B < 0$) Finkelstein portions of the Kruskal extension and thus makes it a suitable coordinate system for our purposes of exploring the interior of the black hole. In fact, we will explore the possibility to glue two such spacetimes to a Black Hole White Hile Transition (BHWHT) spacetime constructed more explicitly in Appendix C and for which we require two asymptotic ends covered by two different radial coordinates $r, \bar{r}$ for the part of the spacetime containing the black and white hole, respectively.

An important feature of the exact GPG (i.e., $e^2 = 1$) is that in the foliation defined by the GP time T the spatial sections are *flat*. This tremendously simplifies all subsequent calculations in perturbation theory and the canonical quantization of the system. The complete information about the non-vanishing 4-curvature, therefore, does not reside in the intrinsic 3-curvature but the extrinsic curvature, e.g., $K_{33} = -\frac{1}{2N}\, [\mathcal{L}_{\vec{N}} q]_{33} = -B'$. The price to pay is that the line element is stationary but not static in these coordinates. Of course the GP or GGP coordinates do not remove the singularity at $r = 0$. This cannot be achieved by the classical theory but potentially by the quantum theory, which is what we wish to explore.

That the GGPG can always be installed when the 3-metric is spherically symmetric by a coordinate transformation that preserves spherical symmetry (i.e., does not depend on angular coordinates) does not show that the GGPG can also be always installed when the 3-metric is not spherically symmetric. In what follows we will show that this is nevertheless the case where coordinate transformations that violate spherical symmetry can be exploited to achieve just that. We will conduct this directly in the Hamiltonian formalism. As a prerequisite this requires us to carefully state the decay behavior of the fields at spatial infinity because these decide which kind of transformations are to be considered as gauges and which as symmetry. See Appendix A for an illustrative toy model that exhibits this phenomenon in a mathematically transparent setting and its implications already for the exactly spherically symmetric vacuum sector in Appendix B.

4.2. Decay Behaviour of the Fields at Spatial Infinity

We consider two asymptotic ends with radial coordinates $r, \bar{r}$ glued at $r = \bar{r} = 0$. Thus, $r = 0$ is not a boundary of the spatial slices $\tau =$ const. and no boundary conditions need to be stated there.

In the gravitational sector we have to state the decay behavior of the canonical pairs (m_{33}, W^{33}), (m_{3A}, W^{3A}), (m_{AB}, W^{AB}). As before we split (dropping the subscript $_E$ for notational simplicity)

$$m_{33} = q^v + x^v,\; m_{3A} = q_A + x_A,\; m_{AB} = q^h\, \Omega_{AB} + X_{AB}$$
$$\frac{W^{33}}{\omega} = p_v + y_v,\; \frac{W^{3A}}{\omega} = \frac{1}{2}\,[p^A + y^A],\; \frac{W^{AB}}{\omega} = \frac{1}{2}\Omega^{AB}\,[p_h + y_h] + Y^{AB} \tag{32}$$

with $q_A = p^A \equiv 0$. The fields q^v, p_v, q^h, p_h coordinate the purely spherically symmetric sector and do not carry any angular dependence. By contrast, the fields $x^v, y_v, x_A, y^A, h^h, y_h$, X_{AB}, Y^{AB} capture the total angular dependence and have no spherically symmetric $l = 0$ modes when expanded into scalar, vector and tensor harmonics. The symplectic potential reads (for two asymptotic ends, $z = \theta(z)r - \theta(-z)\bar{r}$)

$$\Theta = \int_{-\infty}^{\infty} dz\; [\sum_{\alpha\in\{v,h\}} p_\alpha\; dq^\alpha + \sum_{\alpha\in\{v,h,e,o\},1\le l\ge|m|} y_{\alpha,l,m}\; dx^{\alpha,l,m} + \sum_{\alpha\in\{e,o\},2\le l\ge|m|} Y_{\alpha,l,m}\; dX^{\alpha,l,m}] \tag{33}$$

It is customary to state the fall-off conditions in tandem with parity conditions [100] but in (33) there are no parity conditions to state any longer as all functions displayed depend only on r, i.e., they are parity invariant. Since all functions displayed are independent of each other, every single term must be convergent. Therefore, since we wish not to rely on possible cancellation effects from the two infinities as the background solution does not display such an effect, the weakest condition that we can impose is that the individual terms of the form $p\; dq,\; y\; dx,\; Y\; dX$ decay stronger than r^{-1}, say as $r^{-1+\epsilon},\; \epsilon > 0$.

In the purely spherically symmetric sector reviewed in Appendix B we find that the general solution of the constraints is given in terms of $\gamma^2 := q^v,\; \delta^2 := q^h,\; p_\gamma := 2\gamma p_v, p_\delta = 2\;\delta\; p_h$ by

$$\{\frac{p_\gamma^2}{16\delta} + \delta[1 - (\frac{\delta'}{\gamma})^2]\}' = 0,\;\; p_\delta = \gamma\; p_\gamma'/\delta' \tag{34}$$

where γ, δ are still arbitrary functions of r provided that $\gamma \neq 0, \delta' = d\delta/dr > 0$. Denoting the integration constant by $m = 2M$ the solution of (34) in the GPGG const.$= \gamma^2 = e^{-2} \le 1$, $\delta = r$ is given by

$$p_\gamma = \pm 4\sqrt{m\; r + [\gamma^{-2} - 1]\; r^2},\;\; p_\delta = \pm 2\gamma \frac{m + 2[\gamma^{-2} - 1]r}{\sqrt{m\; r + [\gamma^{-2} - 1]\; r^2}} \tag{35}$$

which for the exact GPG $\gamma \equiv 1$ simplifies to

$$p_\gamma = \pm 4\sqrt{m\; r},\;\; p_\delta = 2\sqrt{\frac{m}{r}} \tag{36}$$

Thus, the choice between GGPG and exact GPG makes a drastic difference for the decay behavior of the momenta in the vacuum case: For generic $0 < \gamma^2 < 1$ we have $p_\gamma = O(r)$, $p_\delta = O(1)$ while for $\gamma^2 \equiv 1$ we have $p_\gamma = O(r^{1/2}),\; p_\delta = O(r^{-1/2})$. Likewise, as explained in Appendix C.6, the choice between GGPG and GPG has a drastic consequence for the dynamics of M in the presence of metric perturbations and or matter: While in the GGPG, M can change dynamically, in the exact GPG it cannot.

Since in the GGPG the fields p_v, p_h decay much slower and because $d\ q_v =\propto d\ \gamma^2 = O(1)$ even does not decay at all to leading order (as γ^2 is dynamical in this case), the definition of the reduced phase space consistent with the GGPG is much more delicate than in the case of the strict GPG. In the present paper we will, therefore, consider only the decay behavior in the strict GPG. We will return to the GGPG case in a forthcoming manuscript.

As in the strict GPG the sperically symmetric spatial background metric is the flat Euclidean metric $dr^2 + r^2\ d\Omega^2$ we can motivate the choice of decay behavior from the usual decay behavior stated in the standard Cartesian coordinates at spatial infinity

$$m^{\mathsf{Cart}}_{ab} = \delta_{ab} + \frac{f^e_{ab}(\Omega)}{r} + \frac{f^o_{ab}(\Omega)}{r^2},\ W^{ab}_{\mathsf{Cart}} = \frac{F^{ab}_o(\Omega)}{r^2} + \frac{F^{ab}_e(\Omega)}{r^3}, \tag{37}$$

where $f^{e/o}_{ab}(\Omega),\ F^{ab}_{e/o}(\Omega)$ are even/odd parity tensors depending only on the angular coordinates. Then, with $\vec{x} = r\vec{n}(\Omega), z^1 = \theta, z^2 = \phi, z^3 = r$

$$\begin{aligned}
m^{\mathsf{Sph}}_{\mu\nu} &= \frac{\partial x^a}{\partial z^\mu}\ \frac{\partial x^a}{\partial z^\mu} m^{\mathsf{Cart}}_{ab} \\
W^{\mu\nu}_{\mathsf{Sph}} &= |\det([\frac{\partial x}{\partial z}])|\ \frac{\partial z^\mu}{\partial x^a}\ \frac{\partial z^\nu}{\partial x^b} W^{ab}_{\mathsf{Cart}} \\
m_{33} &= 1 + \frac{f^e_{33}(\Omega)}{r} + \frac{f^o_{33}(\Omega)}{r^2} \\
m_{3A} &= 0 + f^e_{3A}(\Omega) + \frac{f^o_{3A}(\Omega)}{r} \\
m_{AB} &= r^2\ \Omega_{AB} + r\ f^e_{AB}(\Omega) + f^o_{AB}(\Omega) \\
\frac{W^{33}}{\omega} &= F^{33}_o(\Omega) + \frac{F^{33}_e(\Omega)}{r} \\
\frac{W^{3A}}{\omega} &= \frac{F^{3A}_o(\Omega)}{r} + \frac{F^{AB}_e(\Omega)}{r^2} \\
\frac{W^{AB}}{\omega} &= \frac{F^{AB}_o(\Omega)}{r^2} + \frac{F^{AB}_e(\Omega)}{r^3}
\end{aligned} \tag{38}$$

Note, that this transformation between Cartesian coordinates x^a at fixed Schwarzschild time t is to be supplemented by the transition to GP time τ which is given by $\tau = t \mp f(r)$, $f' = \sqrt{R/r}\ [1 - \frac{R}{r}]^{-1}$, $R = 2M$ which means that $g_{tt} \to g_{\tau\tau} = g_{tt}$, $g_{tr} \to g_{\tau r} = g_{tr} - g_{tt}\ f'$, $g_{rr} \to g_{rr} + g_{tt}[f']^2$. Then, if $g_{tt} = -1 + O(r^{-1}), g_{tr} = O(r^{-1}), g_{rr} = 1 + O(r^{-1})$ we have $g_{\tau\tau} = -1 + O(r^{-1}), g_{\tau r} = O(r^{-1/2}), g_{rr} = 1 + O(r^{-1})$ which means the lapse and shift decay $N = 1 + O(r^{-1}), N^3 = O(r^{-1})$ has changed to $N = 1 + O(r^{-1}), N^3 = O(r^{-1/2})$. Thus, the decay behavior of $m_{\mu\nu}$ in (38) is not affected by the switch between the two time coordinates; however, the changed shift behavior affects the decay behavior of the momenta which will be accounted for below. The fact that only the spherically symmetric part of the shift is affected motivates to change the decay behavior of only the spherically symmetric part of the momenta.

Thus, we first translate the decay behavior of the $x^{\alpha,l,m}$, $y_{\alpha,l,m}$, $X^{\alpha,l,m}$, $Y_{\alpha,l,m}$ unchanged. We could, in principle, choose this individual mode by mode (l,m). But to simplify this, we will write, e.g., for $\alpha \in \{v,h,o\}$

$$x^\alpha = [\sum_{|m|\le l; l/2\in\mathbb{N}} x^{\alpha,l,m} L_{\alpha,l,m}] + [\sum_{|m|\le l;(l+1)/2\in\mathbb{N}} x^{\alpha,l,m} L_{\alpha,l,m}] =: x^\alpha_e + x^\alpha_o \tag{39}$$

and we impose the decay behavior only on the linear combination of all even/odd parity terms rather than individually (for $\alpha = e$ the restrictions on l in the two sums in (39) are switched). Then

$$x^v = \frac{x_e^v}{r} + \frac{x_o^v}{r^2},\ x_A = x_A^e + \frac{x_A^e}{r},\ x^h = x^h\, r + x_o^h,\ X_{AB} = X_{AB}^e\, r + X_{AB}^o$$
$$\frac{y_v}{\omega} = y_v^o + \frac{y_v^e}{r},\ \frac{y^A}{\omega} = \frac{y_o^A}{r} + \frac{y_e^A}{r^2},\ \frac{y_h}{\omega} = \frac{y_h^o}{r^2} + \frac{y_h^e}{r^3},\ \frac{Y^{AB}}{\omega} = \frac{Y_o^{AB}}{r^2} + \frac{Y_e^{AB}}{r^3}, \tag{40}$$

In this way in the integral definining Θ, the leading order terms are of the form

$$\int dr\ (\int_{S^2} d\Omega[y^o\ dx_e])\ \frac{1}{r} = 0 \tag{41}$$

as $[y^o \delta x_e]$ is an odd parity scalar on the sphere. The subleading terms do contribute but decay as r^{-2} and thus converge. Of course in (40) we could also allow for a slower decay of the momenta, we could multiply the right-hand sides of the above equations for y_v, y^A, y_h, Y^{AB} by $r^{1-\epsilon},\ \epsilon > 0$, a freedom to keep in mind when discussing the solutions of the physical equations of motion.

As just motivated, for the spherically symmetric sector we use the vacuum solution as an input and require that

$$q^v = 1 + \frac{k^v}{r^{5/2}},\ q^h = r^2 + \frac{k^h}{r^{1/2}},\ p_v = i_v r^{1/2},\ p_h = i_h\ r^{-3/2} \tag{42}$$

where $k^v,\ k^h,\ i_v,\ i_h$ are functions of r only which approach constants or decay at spatial infinity. Then, $p_v dq^v, p_h dq^h$ decay at least as r^{-2}.

Altogether (40) and (42) provide a consistent set of decay conditions compatible with the vacuum solution in GP coordinates. We take this as the *definition* of the phase space which then may be translated into any other frame.

Next, we consider the constraints. The variation in the spatial diffeomorphism constraint

$$\begin{aligned} d[V_\|[S_\|]] &= \int d^3x\ S^\rho\ d[W^{\mu\nu}\ m_{\mu\nu,\rho} - 2(m_{\rho\mu}\ W^{\mu\nu})_{,\nu}] \\ &= \int d^3x\ \{[dW^{\mu\nu}]\ [\mathcal{L}_S m]_{\mu\nu} - [\mathcal{L}W]^{\mu\nu}\ [dm_{\mu\nu}]\} + \int d\Sigma_\rho \{S^\rho\ W^{\mu\nu}\ dm_{\mu\nu} - 2S^\nu\ d[W^{\rho\mu} m_{\mu\nu}]\} \\ &= \int d^3x\ \{[dW^{\mu\nu}]\ [\mathcal{L}_S m]_{\mu\nu,\rho} - [\mathcal{L}W]^{\mu\nu}\ [dm_{\mu\nu}]\} + \int \frac{d\Omega}{\omega}\ S^3 W^{\mu\nu}\ dm_{\mu\nu} - 2\ d[\int\ d\Omega S^\nu\ W^{3\mu} m_{\mu\nu}] \end{aligned} \tag{43}$$

where $d\Sigma_\rho = \frac{1}{2}\epsilon_{\mu\nu\rho} dz^\mu \wedge dz^\nu = \delta_\rho^3 \frac{d\Omega}{\omega}$ and the surface integral is taken at $r = \infty$ for each asymptotic region. Since by construction $W^{\mu\nu} dm_{\mu\nu}$ to leading order is r^{-2} for the symmetric sector and r^{-1} odd plus r^{-2} even for the nonsymmetric sector, the first boundary term in (43) vanishes if the even part of S^3 grows at most linearly while the odd part approaches a constant. In the decomposition of the previous section this means

$$S^3 = f^h + g^h,\ f^h = O(r),\ g^h = g_e^h\ r + g_o^h \tag{44}$$

where $g_{e/o}^h$ are even/odd functions on the sphere. It follows that

$$H_\|[S_\|] = V_\|[S_\|] + B_\|(S_\|),\ B_\|[S_\|] = 2\int\ d\Omega\ S^\nu\ W^{3\mu} m_{\mu\nu} \tag{45}$$

has well-defined variational derivatives corresponding to the bulk term in (43).

Next, we consider the variation of the Hamiltonian constraint $d[V_\perp[S_\perp]]$. This picks up a boundary term coming purely from the spatial curvature term. Since the decay behavior of the spatial metric is unaffected by the use of GP coordinates, we may take over the standard result that (see, e.g., [100] the second reference in [40–44] and references therein)

$$\begin{aligned} H_\perp[S_\perp] &= V_\perp[S_\perp] + B_\perp[S_\perp] \\ B_\perp[S_\perp] &= -\int \sqrt{\det(m)}\, S^0\, m^{\mu\nu}\, [d\Sigma_\mu\, (\Gamma^\rho_{\rho\nu} - (\Gamma^{\rm ND})^\rho_{\rho\nu}) - d\Sigma_\rho\, (\Gamma^\rho_{\mu\nu} - (\Gamma^{\rm ND})^\rho_{\mu\nu})] \\ &+ \int \sqrt{\det(m)}\, [\nabla_\mu S^0]\, m^{\mu\nu}\, m^{\rho\sigma} (d\Sigma_\nu [m_{\rho\sigma} - m^{\rm ND}_{\rho\sigma}] - d\Sigma_\rho [m_{\nu\sigma} - m^{\rm ND}_{\nu\sigma}]) \end{aligned} \tag{46}$$

where $m^{\rm ND}$ is the non-dynamical part of $m_{\mu\nu}$ which in the present case is just $\delta_{\mu\nu}$ in the Cartesian frame and ∇ is the covariant differential compatible with m. Also, $\Gamma^{\rm ND}$ is the Christoffel symbol of the non-dynamical part. This term is missing in the usual treatment in which one implicitly assumes a flat Cartesian frame at infinity. However, the GPG is not a Cartesian frame and the Christoffel symbol is not a tensor, hence subtraction of that term is necessary, in general, (in the derivation of the boundary term [100] or second reference of [40] = [44] only the variation $d\Gamma$ enters which *is* a tensor). As in (43), in order for $dV_\perp[S_\perp]$ to be written as $d\, H_\perp[S_\perp] - dB_\perp[S_\perp]$ we must assume that

$$S^0 = f^v + g^v,\ f^v = O(1),\ g^v = g^v_e + g^v_o\, r \tag{47}$$

4.3. Installation of the GPG

As usual, we consider those $S_\|, S_\perp$, respectively, for the boundary terms $B_\|[S_\|], B_\perp[S_\perp]$ that vanish a gauge transformation, and for those that do not vanish a symmetry transformation. We must show that it is possible to install the exact GPG by picking suitable $S_\|, S_\perp$ corresponding to gauge transformations.

Having made sure that the functionals $H_\|, H_\perp$ have well-defined variational derivatives they generate the following transformations on the 3-metric

$$\begin{aligned} \delta m_{\mu\nu}(z) &= \{H_\|[S_\|] + H_\perp[S_\perp], m_{\mu\nu}(z)\} \\ &= [\mathcal{L}_{\vec S} m]_{\mu\nu} + S^0\, (2W_{\mu\nu} - m_{\mu\nu}\, W)(x);\ \ P_{\mu\nu} := (m_{\mu\rho}\, m_{\nu\sigma})\, W^{\rho\sigma},\ \ W := m_{\mu\nu}\, W^{\mu\nu} \end{aligned} \tag{48}$$

where $\mathcal{L}$ denotes the Lie derivative. Given arbitrary values of $q_3 = q^v + y^v, q_A = y_A$, $q_0 = q^h + y^h$ consistent with the imposed decay behavior of the previous subsection we want to show that we can find S^3, S^A, S^0 corresponding to a gauge transformation such that $G_\mu + \delta G_\mu = G_\mu + \delta q_\mu = 0$ for $\mu = 3, A, 0$ where $G_\mu = q_\mu - q^{\rm GPG}_\mu$. Decomposing with respect to the tensorial structure on S^2 we find explicitly

$$\begin{aligned} \delta q_3 &= 2\, [q_3\, (S^3)' + q_A (S^A)'] + [S^3\, q_3' + S^A\, D_A q_3] + S^0\, [2W_{33} - q_3\, W] \\ \delta q_A &= [q_{AB} (S^B)' + q_A (S^3)'] + [S^3\, q_A' + q_3\, D_A S^3 + S^B\, D_B q_A + q_B\, S_A S^B] + S^0\, [2W_{3A} - q_A\, W] \\ \delta q_0 &= \Omega^{AB}\, \{[S^3 q'_{AB} + 2q_{(A}\, D_{B)} S^3 + S^C\, D_C q_{AB} + 2\, q_{C(A}\, D_{B)}\, S^C] + S^0\, [2P_{AB} - q_{AB}\, P]\} \end{aligned} \tag{49}$$

where $q_{AB} = q_0 \Omega_{AB} + X_{AB}$. Assuming that $\Omega^{AB}[2\, W_{AB} - q_{AB}\, W] \neq 0$ (otherwise, conduct another gauge transformation on the system first so that this quantity is nonvanishing to begin with which is always possible as it is not a gauge invariant) we can solve the equation $\delta q_0 + G_0 = 0$ algebraically for S^0 and introduce that solution, which depends linearly on $S^3, D_A S^3, S^A, D_B S^A$, into the equations for $\delta q_3 + G_3 = 0, \delta q_A + G_A = 0$. Due to the Euclidian signature of $m_{\mu\nu}$ we have $q_3 > 0$ and that q_{AB} is non-degenerate and thus the resulting set of three equations can be cast into the form

$$[S^\mu]' + F^\mu_\nu\, S^\nu + K^{\mu A}_\nu D_A S^\nu = -q^{\mu\nu}\, G_\nu \tag{50}$$

for certain coefficient functions $F^\mu_\nu,\ K^{\mu A}_\nu$ and $(.)' = \frac{d}{dr}(.)$. Thus, (50) is an inhomogeneous linear, infinite system of ODEs in the variable r and the unknowns S^α_y with $S^\alpha_y(r) = S^\alpha(r, y)$, $y = (y^1, y^2)$ and thus can be solved by the method of variation of constants. It remains to show that the decay behavior of the solution so obtained indeed corresponds to a gauge transformation. We assume this to be the case by making use of the choice of integration constants when solving the system (50).

4.4. Solution of the Constraints in the GPG

We will only treat the gravitational constraints because other constraints corresponding to the Yang–Mills type of gauge transformations can be treated independently, see next section. Accordingly, we will write the constraints of GR as

$$\begin{aligned} V_\mu &:= -2\,\nabla_\nu\, W^\nu{}_\mu + V^m_\mu, \\ V_0 &:= [m_{\mu\rho}\, m_{\nu\sigma} - \frac{1}{2} m_{\mu\nu}\, m_{\rho\sigma}]\, W^{\mu\nu}\, W^{\rho\sigma} + V_0^{c,m} \end{aligned} \tag{51}$$

Here, V^m_μ denotes the matter contribution to the spatial diffeomorphism constraint and $V_0^{c,m}$ the spatial curvature and matter and contribution to the Hamiltonian constraint multiplied by $\sqrt{\det(q)}$. The precise form of these matter and curvature contributions are displayed in the next section but will not be important for the purposes of the present section. The Levi Civita differential compatible with $m_{\mu\nu}$ is denoted by ∇.

The first step is the decomposition of (51) with respect to the canonical chart (23)–(25)

$$\begin{aligned} V^m_\mu &= 2(m_{\mu\nu}\, W^{\nu\rho})_{,\rho} - m_{\nu\rho,\mu}\, W^{\nu\rho} \\ &= 2(m_{\mu 3}\, P^3)' + (m_{\mu 3}\, P^B)_{,B} + (m_{\mu B}\, P^B)' \\ &\quad +2(m_{\alpha B}\, W^{BC})_{,C} - m_{33,\mu}\, P^3 - m_{B,\mu}\, P^B - m_{BC,\mu}\, P^{BC} \\ V^m_3 &= 2(q_3\, P^3)' + (q_3\, P^B)_{,B} + (q_B\, P^B)' + 2(q_B\, P^{BC})_{,C} \\ &\quad -q_3'\, P^3 - q_B'\, P^B - q_{BC}'\, P^{BC} \\ V^m_A &= 2(q_A\, P^3)' + (q_A\, P^B)_{,B} + (q_{AB}\, P^B)' + 2(q_{AB}\, P^{BC})_{,C} \\ &\quad -q_{3,A}\, P^3 - q_{B,A}\, P^B - q_{BC,A}\, P^{BC} \\ -V_0^{c,m} &= [q_3 P^3]^2 + 2\,[q_3 P^3]\,[q_A\, P^A] + \frac{1}{2}\,[q_A P^A]^2 + \frac{1}{2}\, q_3\, q_{AB}\, P^A\, P^B \\ &\quad +2\, q_A\, q_B\, P^{AB}\, P^3 + 2 q_A\, q_{BC}\, P^C\, P^{AB} + q_{AC}\, q_{BD}\, P^{AB}\, P^{CD} + \\ &\quad -\frac{1}{2}[q_3\, P^3 + q_A\, P^A + q_{AB}\, P^{AB}]^2 \end{aligned} \tag{52}$$

where we have written $(.)' := \frac{\partial}{\partial r}(.)$.

Remarkably, the constraints (52) display the following features:
1. All momenta P^3, P^A, P^0 appear only polynomially in V_0.
2. The momentum P^0 does not enter V_3, V_A with radial derivatives.
3. The momenta P^3, P^A do enter V_3, V_A with radial derivatives.
4. All momenta P^3, P^A, P^0 appear in V_3, V_A with angular derivatives.

This suggests the following solution strategy:

1. We solve V_0 algebraically for P^0. In fact, since V_0 is a quadratic polynomial in P^0 we may write

$$V_0 = g_0(q)\; [P^0 + f^0_+(P^3, P^A; P_\perp; q, V_0^{c,m})]\; [P^T + f^0_-(P^3, P^A; P_\perp; q, V_0^{c,m})] \tag{53}$$

where $g_0(q)$ depends polynomially on $q = (q_3, q_A, q_{AB})$ and $f^0_\pm$ are the two possible real roots which depend algebraically on $P^3, P^A, P^{AB}_\perp$ (i.e., no derivatives enter) and algebraically on q and $V_0^{c,m}$ where the latter depends on the gravitational degrees of freedom algebraically only through q and all its first and second spatial derivatives. The explicit calculation reveals

$$
\begin{aligned}
f^0_\pm &= -\frac{A}{B}\,\{1 \pm \sqrt{1-\frac{B}{A^2}\,V_0^{c,m,\perp}}\} \\
A &= r^2\,P^3 - q^\perp_{AC}\,q^\perp_{BD}\,\Omega^{AB}\,P^{CD}_\perp - r^2\,q^\perp_{AB}\,P^{AB}_\perp \\
B &= q^\perp_{AC}\,q^\perp_{BD}\,\Omega^{AB}\,\Omega^{CD} \\
V_0^{c,m,\perp} &= V_0^{c,m} + \frac{1}{2}\,[P^3 - q^\perp_{AB}P^{AB}_\perp]^2 + \frac{1}{2}\,q_{AB}\,P^A\,P^B - \,[q^\perp_{AB}\,P^{AB}_\perp]^2 \\
&\quad + r^4\,\Omega_{AC}\,\Omega_{BD}\,P^{AB}_\perp\,P^{CD}_\perp + 2r^2 q^\perp_{AC}\,\Omega_{BD}\,P^{AB}_\perp\,P^{CD}_\perp + q^\perp_{AC}\,q^\perp_{BD}\,P^{AB}_\perp\,P^{CD}_\perp
\end{aligned}
\tag{54}
$$

The choice of the sign in (54) is in fact unique if we impose that (54) has a regular limit $B \to 0$ as we approach an exactly spherically symmetric solution which selects the solution $P^0 = -f^0_-$.

2. We write V_3, V_A as

$$
2\,q_3\,[P^3]' + q_A\,[P^A]' + \tilde{f}_3(P^3,P^A,P^0,q) = V^m_3,\; 2\,q_A\,[P^3]' + q_{AB}\;[P^B]' + \tilde{f}_A(P^3,P^C,P^0,q) = V^m_A, \tag{55}
$$

where $\tilde{f}_3, \tilde{f}_A$ depend on P^3, P^A, P^0 only linearly and either with no or at most first angular derivatives while q enters linearly and with at most first radial and angular derivatives. Taking linear combinations these can be decoupled and written as

$$
[P^3]' + f^3(P^3,P^A,P^0,q,V^m) = 0,\;\; [P^A]' + f^A(P^3,P^B,P^0,q,V^m) = 0 \tag{56}
$$

where f^3, f^A are still linear in P^3, P^B, P^0, depending at most on angular derivatives and are non-polynomial with respect to q but linear in V^m_3, V^m_B. That (55) can be written as (56) close to the GPG $q_3 = 1, q_A = 0, q_{AB} = r^2\Omega_{AB} + q^\perp_{AB}$ and for the perturbation $q^\perp_{AB}$ sufficiently small is by inspection.

3. We substitute the root $P^0 = -f^0_-$ of (53) into (56) thereby obtaining the constraints

$$
\begin{aligned}
\tilde{V}^3 &:= [P^3]' + \hat{f}^3(P^3,P^A,P_\perp,q,V^m) = 0,\;\; \tilde{V}^A := [P^A]' + \hat{f}^A(P^3,P^B,P_\perp,q,V^m) = 0, \\
\tilde{V}^0 &:= = P^0 + f^0_-(P^3,P^A,P_\perp,q,V_0^{c,m})
\end{aligned}
\tag{57}
$$

where $\hat{f}^3, \hat{f}^A$ still depend only linearly on angular derivatives of P^3, P^A but no longer linearly on P^3, P^A, in fact they depend non-polynomially on P^3, P^A due to the substitution of the square root.

4. The system (57) can be considered as a coupled (inifinite) system of ODE's in the variable $z = r$ for the unknowns $P^\mu_y(r)$ where ($\mu = 1,2,3;\; y := (y^1, y^2)$) is considered as a compound label for these unknowns. Therefore, formal solutions exist and are unique given initial values. They can be found using the Picard–Lindelöf iteration for any $-\infty \le z < \infty$ (recall that we work with two asymptotic ends and $z = r\theta(z) - \theta(-z)\bar{r}$)

$$
P^\mu_y(z) = P^\mu_y(-\infty) + \int_{-\infty}^{z} ds\;\hat{f}^\mu(P_y(s), q_y(s), V^m(s)) \tag{58}
$$

where $P^\alpha_y(-\infty)$ are integration constants. Note, that the integrand not only depends on $P^\beta_y(s)$ but also on $\partial_y P^\beta_y(s)$ and thus the iteration does not decouple with respect to y. Note, also that Equation (58) is identically satisfied for $z = -\infty$. Thus, there is an up to $3 \times S^2$ worth of degeneracy in the constraints and accordingly as many conjugate variables such as $Q^y_\alpha = \int_{-\infty}^{\infty} dz q_\alpha(z,y)$ cannot be gauge fixed but must be counted as belonging to the set of true degrees of freedom in company with the integration constants $P^\alpha_y(-\infty)$. In Appendix A we demonstrate this phenomenon for a lower-dimensional field theory. The degree of degeneracy is reduced by the boundary conditions at infinity.

Let $-h^\alpha_y(r)$ be the solution so obtained. Then, the constraints can be written in the equivalent form

$$\hat{V}^\mu_y(r) = P^\mu(y,r) + h^\mu_y(r),\ \hat{V}^0_y(r) = P^0(y,r) + h^0_y(r) \tag{59}$$

where $h^0 = [f^0_-]_{P^\mu=-h^\mu}$. The functionals h^3, h^A, h^0 depend on the degrees of freedom q_3, q_A, q_0, the integration constants $P^\alpha_y(-\infty)$, as well as the union R of the collection of true matter degrees of freedom with the collection of the true gravitational degrees of freedom $q^\perp_{AB}, P^{AB}_\perp$. By construction (59) is an identity for $r = -\infty$ and thus the set of constraints (59) for $r > -\infty$ is strictly equivalent to the set of constraints (51) for $r \geq -\infty$. Since the degrees of freedom $P^\mu_y(-\infty)$ are thus left unconstrained and since to gauge fix (59) for $r \neq -\infty$ does not require us to impose the GPG for all $-\infty \leq r \leq \infty$, following [61] we consider the set of canonical pairs $(Q_\mu(y) = \int\ dz\ q - \mu(z, y0,\ P^\mu(r = -\infty, y))$ as part of the true degrees of freedom and adjoin them to R (again the boundary conditions reduce this set). The so extended set of true degrees of freedom is denoted as $\hat{R}$. Note, that by virtue of the Picard–Lindelöf integration involved, the functionals h^3, h^A, h^0 are non-local with respect to r consisting of nested radial integrals.

4.5. Reduced Hamiltonian

We first review the general theory of how to construct a reduced Hamiltonian in the presence of boundaries as introduced in [75] and show that this requires a non-trivial generalization. Indeed, the same authors mention in [101] that beyond the linearized gravity setting a non-trivial generalization of [75] is necessary. In Proposition 1 below we state a sufficient condition which when satisfied allows us to construct the reduced Hamiltonian. In the second part of this subsection we then analyze the details of the gauge stability conditions for the the present system. In the third part of this subsection, we confirm that the sufficient condition stated in the proposition holds for the solution of the stability condition constructed and then provide the reduced Hamiltonian.

4.5.1. Reduced Dynamics in the Presence of Boundaries

As we have seen in Section 4.5, in the presence of boundaries, the constraints $V(S)$ are not automatically functionally differentiable which poses a problem when computing Poisson brackets. The problem is displayed by writing the variation of $V(S)$ with respect to the canonical variables $q_{ab}, p^{ab}, \ldots$ as a sum of a bulk and boundary contribution

$$d\ V(S) = [d\ V(S)]_\sigma + [d\ V(S)]_{\partial\sigma} \tag{60}$$

where the first term is a volume integral over the scalar density $D^{\mu\nu}_S\ [dm_{\mu\nu}] + D^S_{\mu\nu}[dW^{\mu\nu}] + \ldots$ while the second term is a boundary integral over the vector density $J^{\mu\nu\rho}_S[d\ m_{\mu\nu} + D^{S\rho}_{\mu\nu}[d\ W^{ab}] + \ldots$ for certain coefficient tensor densities depending on S. The bulk term yields well-defined functional derivatives (the three-dimensional delta distribution is integrated out), the second does not (a one-dimensional delta distribution is left over). As explicitly shown in the previous subsection, the idea to remove that contribution is to impose fall-off conditions on $S, m, W, \ldots$ such that one can write the boundary contribution as an exact differential $[\delta V(S)]_{\partial\sigma} = -\delta B(S)$ for a suitable boundary functional $B(S)$ and then to define $H(S) := V(S) + B(S)$. Then, by construction

$$\delta H(S) = [\delta V(S)]_\sigma \tag{61}$$

is functionally differentiable.

The constraints are still defined by $V(S) = 0$ for all S such that $H(S) = B(S)$ on the constraint surface which can be non-vanishing if S does not decay sufficiently fast at the boundary. Accordingly, one interprets transformations generated by $H(S)$ with S for which $B(S) = 0$ as gauge transformations while those with $B(S) \neq 0$ are considered as symmetry transformations. We subdivide the degrees of freedom $m_{\mu\nu}, W^{\mu\nu}$ into two subsets of canonical pairs q^α, p_α and Q^A, P_A and impose gauge fixing conditions $G^\alpha = q^\alpha - k^\alpha = 0$ on the q^α where k^α are certain fixed functions on σ independent of the foliation time τ and without dependence on the phase space coordinates. We set $q^\alpha_* := k^\alpha$. We also solve the constraints $V_\alpha = 0$ for p_α when $q^\alpha = q^\alpha_*$ which yields solutions $p_\alpha = p^*_\alpha$.

The gauge $G^\alpha = 0$ is supposed to be reachable from any point within the constraint surface $V_\alpha = 0$ and once it is reached the residual transformations allowed are those that preserve them

$$\{H(S), G^\alpha\}_{q=q_*, p=p^*} = 0 \tag{62}$$

These stability conditions can be solved for $S^\alpha = S^\alpha_*$ in terms of q_*, p^* and in general are symmetry transformations rather than gauge transformations. Consider now a functional F depending on Q, P only. Then, the reduced Hamiltonian E on the reduced phase space coordinated by Q, P, if it exists, is supposed to give the same equations of motion as $H(S)$ when we restrict to the fixed quantities q_*, p^*, S_*, that is,

$$\{E, F\} = \{H(S), F\}_{q=q_*, p=p^*, S=S_*} \tag{63}$$

Now, being the boundary value of a volume integral variation that arises due to one or several integrations by parts, the boundary term has the form

$$B(S) = \int_{\partial\sigma} d\Sigma_\mu \; [S^\alpha \; j^\mu_\alpha + S^\alpha_{,\nu} \; j^{\mu\nu}_\alpha + \ldots] \tag{64}$$

for some "currents" $j^\mu_\alpha, \; j^{\mu\nu}_\alpha$. Using integrations by parts on $\partial\sigma$ and exploiting $\partial^2\sigma = \emptyset$ we can assume w.l.g. that $j^{\mu\nu}_\alpha, \ldots = 0$ by redefining j^μ_α. Similarly, the bulk term has the form

$$V(S) = \int_\sigma d^3x \; S^\alpha \; V_\alpha \tag{65}$$

for some "densities" V_α.

Proposition 1. *Let $d\Sigma_\mu = d^2z \; N_\mu(z)$ where $N_\mu(y) = \frac{1}{2}\epsilon^{AB}\epsilon_{\mu\nu\rho}x^\nu_{,A}x^\rho_{,B}$ is the corresponding co-normal of the embedding $S^2 \; \to \; \partial\sigma; \; y \; \mapsto x$. Suppose that there exists a real-valued functional χ of currents j_α on $\partial\sigma$ such that on $\partial\sigma$ (i.e., the functional derivative is with respect to the coordinate dependence on $\partial\sigma$)*

$$S^\alpha_* = [\frac{\delta\chi}{\delta j_\alpha}]_{j=j^*}, \; j^*_\alpha := N_\mu \; j^{*\mu}_\alpha, \; j^{*\mu}_\alpha := [j^\mu_\alpha]_{q=q_*, p=p^*} \tag{66}$$

Then, $E = \chi[j_*]$.

Proof. We simplify the notation and denote $z = (q, p), z_* = (q_*, p^*)$ Then, on the one hand

$$\{B(S)_{z=z_*}, F\}_{S=S_*} = \int d^2y \; S^\alpha_* \; \{j^*_\alpha, F\} \tag{67}$$

Note, that S is set to S_* only *after* the Poisson bracket has been taken, the Poisson bracket is computed with S treated as being independent of the phase space coordinates. On the other hand using the identity $B(S)_{z=z_*} = H(S)_{z=z_*}$ for all S we have

$$\begin{aligned}
& \{B(S)_{z=z_*}, F\}_{S=S_*} = \{H(S)_{z=z_*}, F\}_{S=S_*} \\
= \; & \{H(S), F\}_{z=z_*, S=S_*} + \int d^3x \; ([\frac{\delta H(S)}{\delta q^\alpha(x)}]_{z=z_*, S=S_*} \; \{q^\alpha_*(x), F\} + [\frac{\delta H(S)}{\delta p_\alpha(x)}]_{z=z_*, S=S_*} \; \{p^*_\alpha(x), F\}) \\
= \; & \{E, F\} + \int d^3x \; \{H(S), G^\alpha(x)\}_{z=z_*, S=S_*} \; \{p^*_\alpha(x), F\} \\
= \; & \{E, F\}
\end{aligned} \tag{68}$$

where in the second step we split the Poisson bracket into a contribution which acts on the explicit dependence of $H(S)$ on P, Q and a contribution on the implicit dependence of $H_*(S)$ on P, Q through q_*^α, p_α^* and used that $H(S)$ is functionally differentiable; in the third we used that q_*^α does not depend on the phase space coordinates and rewrote the second contribution as a Poisson bracket with the gauge fixing condition and in the last we used that by construction of S_* that Poisson bracket vanishes, that is, (62).

Thus,

$$\{E, F\} = \{B(S)_{z=z_*}, F\}_{S=S_*} \tag{69}$$

This is different from the result quoted in [75]. This is because $E \neq B(S_*)_{z=z_*}$ unless S_* evaluated on $\partial\sigma$ does not depend on the coordinates P, Q as it is implicitly assumed in [75]. This will in general not be the case because the solution S_* of the stability condition involves solving differential equations and thus depends non-locally on P, Q via integrals on all of its bulk values; therefore, $\{S_*^\alpha(x), F\} \neq 0$ even if $x \in \partial\sigma$ and F is localized with respect to Q, P in the bulk. Comparing with (67) we see that the only chance to write the right-hand side of (69) as a Poisson bracket is that S_α^* is the functional derivative on $\partial\sigma$ with respect to a functional χ which depends on the current j_α that appears in (67). □

The case that S_*^α is a constant on the phase space such that $E = B(S_*)_{z=z_*}$ as it is considered in [75] is included and corresponds to $\chi[j]$ being a linear functional of j. In order that $\{E, F\}$ is well defined, the dependence of j_* on P, Q should be non-local, i.e., involving radial integrals in order that the Poisson brackets $\{E, F\}$ which use functional derivatives on σ rather than $\partial\sigma$ are well-defined. This is, in fact, conceivable for the gravitational system because the stability conditions involve the p_α explicitly which, in turn, are to be solved for the P, Q using the constraints and for this, we need to perform radial integrations as the constraints depend on radial derivatives. Now j_α corresponds to the ADM energy and momentum currents and these again involve p_α explicitly. Then, to see whether j_α^*, S_*^α satisfy all the requirements critically depends on the fall-off behavior of the fields as these decide which terms in $S_*^\alpha\{j_\alpha^*, F\}$ survive as we take the limit $r \to \infty$. It is only with respect to these limiting surviving terms that the assumptions of Proposition 1 have to hold. Fortunately there is a substantial amount of flexibility in the choice of those fall-off conditions and one may also take advantage of the fact that the solution of the constraints for $p = p^*$ and of the stability conditions for $S = S_*$ both at $q = q_*$ involve "integration constants" in the form of functions on S^2, as we have seen in the previous section, because we have to solve differential equations with respect to the radial coordinates and one can try to use the freedom to choose those free functions on the sphere in order to meet the conditions of Proposition 1.

4.5.2. Solution of Stability Conditions

We now proceed to construct the gauge fixed values S_*^3, S_*^A, S_*^0. This has two purposes: First, the leading order behavior at spatial infinity dictates the analytic form of the reduced Hamiltonian, i.e., the global mass or energy. Second, the explicit bulk behavior determines the physical lapse and shift, and therefore, contains information about the local mass.

Asymptotics

For a general transformation of $m_{\mu\nu}$ induced by the functionally differentiable version (45) and (46) of the constraints we have

$$[\delta m]_{\mu\nu} = \{H_\|[S_\|] + H_\perp[S_\perp], m_{\mu\nu}\} = [\mathcal{L}_{S_\|} m]_{\mu\nu} + 2\tilde{S}_0\, [W_{\mu\nu} - \frac{1}{2}\, W\, m_{\mu\nu}] \tag{70}$$

where $\tilde{S}^0 = \frac{S^0}{\sqrt{\det(m)}}, W_{\mu\nu} = m_{\mu\rho} m_{\nu\sigma} W^{\rho\sigma},\ W = m_{\mu\nu} W^{\mu\nu}$. The gauge fixed values $S_*^\cdot$ are determined by the stability conditions $\delta G^\cdot = 0$ where $G^3 = m_{33} - 1,\ G^A = m_{3A},$ $G^0 = \Omega^{AB} m_{AB} - 2r^2$. This needs to hold only at $G^3 = V_3 = G^A = V_A = G^0 = V_0 = 0$ i.e., at

$$m_{33} = q^*_3 = 1,\ m_{3A} = q^*_A = 0,\ \Omega^{AB} m_{AB} = q_0 = q^*_0 = 2r^2,\ P^3 = P^3_*,\ P^A = P^A_*, P^0 = P^0_* \tag{71}$$

where we used the notation (23)–(25) and the values $P^\cdot_* = -h^\cdot_*$ are given implicitly by (59) where $h^\cdot_*$ is $h^\cdot$ evaluated at $G^\cdot = 0$.

We find

$$\begin{aligned}
0 &= \delta G^3 = [\mathcal{L}_{S_\|} q]_{33} + 2\tilde{S}^0\ [P_{33} - \frac{1}{2}\ P\ q_{33}] \\
0 &= \delta G^A = [\mathcal{L}_{S_\|} q]_{3A} + 2\tilde{S}^0\ [P_{3A} - \frac{1}{2}\ P\ q_{3A}] \\
0 &= \delta G^0 = \Omega^{AB}\ ([\mathcal{L}_{S_\|} q]_{AB} + 2\tilde{S}^0\ [P_{AB} - \frac{1}{2}\ P\ q_{AB}]
\end{aligned} \tag{72}$$

Using the GPG we have (we suppress the super/subscript $*$ in $q^*_\cdot, P^\cdot_*$ for notational simplicity) using the decomposition $P^3 = W^{33} = p_v + y_v, P^A = y^A = 2W^{3A}, W^{AB} = P^{AB} = [p_h + y_h]\Omega^{AB}/2 + Y^{AB}$ and $\Omega^{AB} X_{AB} = \Omega_{AB} Y^{AB} = 0$

$$\begin{aligned}
P_{33} &= m_{3\mu}\ m_{3\nu} W^{\mu\nu} = P^3 = p_v + y_v \\
P_{3A} &= m_{3\mu}\ m_{A\nu} W^{\mu\nu} = [r^2\Omega_{AB} + X_{AB}]\ P^B/2 = [r^2\Omega_{AB} + X_{AB}]\ y^B/2 \\
P_{AB} &= m_{A\mu}\ m_{B\nu} W^{\mu\nu} [r^2\Omega_{AC} + X_{AC}]\ [r^2\Omega_{BD} + X_{BD}]\ [\frac{1}{2}(p_h + y_h)\Omega^{CD} + Y^{CD}] \\
P &= m_{\mu\nu} W^{\mu\nu} = P^3 + [r^2\Omega_{AB} + X_{AB}] P^{AB} = [p_v + y_v] + r^2\ [p_h + y_h] + X_{AB} Y^{AB}
\end{aligned} \tag{73}$$

Next with $S^3 = f_h + g_h, S^A = g^A, S^0 = f_v + g_v$

$$\begin{aligned}
&[\mathcal{L}_{S_\|} m]_{33} = S^\mu m_{33,\mu} + 2\ m_{\mu 3} S^\mu_{,3} = 2S^3_{,3} = 2(f_h + g_h)' \\
&[\mathcal{L}_{S_\|} m]_{3A} = S^\mu m_{3A,\mu} + m_{\mu 3} S^\mu_{,A} + m_{\mu A} S^\mu_{,3} = S^3_{,A} + q_{AB} S^{B\prime} = g_{h,A} + [r^2\Omega_{AB} + X_{AB}]\ g^{B\prime} \\
&[\mathcal{L}_{S_\|} m]_{AB} = S^\mu m_{AB,\mu} + 2\ m_{\mu(A} S^\mu_{,B)} = S^3 q'_{AB} + S^D q_{AB,C} + 2m_{C(A} S^C_{,B)} = S^3 q'_{AB} + [\mathcal{L}_{S_{\|\perp}} q]_{AB}
\end{aligned} \tag{74}$$

where $S^A_{\|\perp} := S^A$ has only angular non-vanishing components. Thus, we have explicitly

$$\begin{aligned}
0 &= S^{3\prime} + \tilde{S}^0\ [P^3 - \frac{1}{2} P] \\
0 &= S^3_{,A} + q_{AB}\ [S^{B\prime} + \tilde{S}^0 P^B] \\
0 &= \Omega^{AB}\ \{S^3 q'_{AB} + [\mathcal{L}_{S_{\|\perp}} q]_{AB} + 2\tilde{S}^0 [q_{AC} q_{BD} P^{CD} - \frac{1}{2} q_{AB} P]\}
\end{aligned} \tag{75}$$

We now recall the decay conditions derived in Section 4.3

$$\begin{aligned}
&p_v = O(r^{1/2}),\ p_h = O(r^{-3/2}) \\
&y_v = y^o_v + \frac{y^e_v}{r},\ y^A = \frac{y^A_o}{r} + \frac{y^A_e}{r^2},\ y_h = \frac{y^o_h}{r^2} + \frac{y^e_h}{r^3}, \\
&X_{AB} = X^e_{AB}\ r + X^0_{AB},\ Y^{AB} = \frac{Y^{AB}_o}{r^2} + \frac{Y^{AB}_e}{r^3} \\
&S^3 = f_h + g_h,\ f_h = O(r),\ g_h = g^e_h\ r + g^h_o;\ \ S^0 = f_v + g_v,\ f_v = O(1),\ g_v = g^e_v + g^o_h\ r;
\end{aligned} \tag{76}$$

while the decay behavior of $S^A = f^A + g^A,\ f^A \equiv 0$ has not been fixed yet. The various functions displayed have no $l = 0$ modes except for p_v, p_h, f_v, f_h which are pure $l = 0$ modes and e, o refers to their parity behavior, i.e., not the polar/axial character. The power of r with respect to which these functions decay is at most $O(r^0)$ but can be lower. The same applies to f_h, f_v, i.e., $O(r^n)$ means decay with at most power r^n, it can be faster, e.g., $O(r^{-1})$ allows a decay with power $r^{-(1+m)},\ m \geq 0$.

In what follows we content ourselves with solving the stability conditions with respect to the highest non-vanishing order in r and only in as much detail as necessary to construct the reduced Hamiltonian. We also content ourselves with constructing one particular solution S^3, S^A, S^0 and leave it for further investigation whether that solution is unique.

We consider first the second relation in (75)

$$g_{h,A} + q_{AB}\,[g^{B\prime} + \tilde{S}^0 y^B] = 0 \;\;\Leftrightarrow\;\; g^{A\prime} = -[q^{AB} g_{h,B} + \tilde{S}^0 y^A] \tag{77}$$

We assume that

$$g_v = O(1) \tag{78}$$

which can be achieved by assuming that $g_v^o r$ is $O(1)$. Then, $S^0 = O(1)$ and thus $\tilde{S}^0 = O(r^{-2})$ because

$$\det(q) = \det(r^2\Omega + X) = \frac{1}{2}\epsilon^{AC}\epsilon^{BD}[r^2\Omega + X]_{AB}\,[r^2\Omega + X]_{CD} = r^4\omega^2 + r^2\,\omega^2\Omega^{AB}X_{AB} + \det(X) = r^4\omega^2 + \det(X) \tag{79}$$

where we used

$$\epsilon^{AC}\epsilon^{BD}\Omega_{CD} = \omega^2\Omega^{AB},\;\omega^2 = \det(\Omega) \tag{80}$$

and $\Omega^{AB}X_{AB} \equiv 0$ by definition. Since $\det(X) = O(r^2)$ it follows that $\det(q) = r^4\omega^2[1 + O(r^{-2})],\; [\det(q)]^{-1/2} = r^{-2}\omega^{-1}[1 + O(r^{-2})]$. Thus, $\tilde{S}^0 y^A = O(r^{-3})$.

Furthermore, we assume that

$$g_h = O(r^{-1}) \tag{81}$$

which can be achieved by assuming that $g_h^e\, r, g_h^o$ decay as r^{-1}. Then, it follows from (77) that

$$S^A = g^A = O(r^{-2}) \tag{82}$$

It follows that

$$[\mathcal{L}_{S_\parallel\perp} q]_{AB} = r^2\,[\mathcal{L}_{S_\parallel\perp}(\Omega + r^{-2}X)]_{AB} = O(1) \tag{83}$$

in leading order.

The first relation in (75) gives

$$\begin{aligned} 0 &= 2\,S^{3\prime} + 2\,\tilde{S}^0[P^3 - \frac{1}{2}[P^3 + r^2P^0 + X_{AB}Y^{AB}]] = 2\,S^{3\prime} + \tilde{S}^0[P^3 - r^2P^0 - X_{AB}Y^{AB}] \\ &= 2(f_h + g_h)' + \tilde{S}^0\,[p_v - r^2 p_h] - \tilde{S}^0\,[y_v - r^2 y_h - X_{AB}Y^{AB}] \end{aligned} \tag{84}$$

Since $y_v, r^2 y_h = O(1), X_{AB}Y^{AB} = O(r^{-1})$ and $\tilde{S}^0 = O(r^{-2})$ the third term in (84) is $O(r^{-2})$. It can thus be canceled by $2\,g_h'$ which by (81) is also $O(r^{-2})$. The second term in (84) on the other hand is $O(r^{-2})\,O(r^{1/2}) = O(r^{-3/2})$ and then must be canceled by $2f_h'$. Hence,

$$f_h = O(r^{-1/2}) \tag{85}$$

and we must have

$$f_h' + \frac{\tilde{S}^0}{2}[p_v - r^2 p_h] = 0 \tag{86}$$

to order $r^{-3/2}$ i.e., (86) decays at least as r^{-2}.

The third relation in (75) gives

$$\begin{aligned}
0 &= 4\,r\,S^3 + \Omega^{AB}\,[\mathcal{L}_{S_{\|}\perp}q]_{AB} + 2\tilde{S}^0[\Omega^{AB}\,q_{AC}q_{BD}P^{CD} - r^2\,P] \\
&= 4\,r\,S^3 + \Omega^{AB}\,[\mathcal{L}_{S_{\|}\perp}q]_{AB} \\
&\quad +2\tilde{S}^0[(r^4\Omega_{CD} + 2r^2\,X_{CD} + \Omega^{AB}X_{AC}X_{BD})\,(\frac{P^0}{2}\Omega^{CD} + Y^{CD}) - r^2(P^3 + r^2\,P^0 + X_{AB}Y^{AB})] \\
&= 4\,r\,S^3 + \Omega^{AB}\,[\mathcal{L}_{S_{\|}\perp}q]_{AB} + 2\tilde{S}^0\,\{r^4\,P^0 + \frac{1}{2}P^0\Omega^{AB}\Omega^{CD}X_{AC}X_{BD} \\
&\quad +2r^2\,X_{AB}Y^{AB} + \Omega^{AB}X_{AC}X_{BD})\,Y^{CD} - r^2(P^3 + r^2\,P^0 + X_{AB}Y^{AB})\} \\
&= [4\,r\,S^3 - 2r^2\,\tilde{S}^0\,P^3] + [\Omega^{AB}\,[\mathcal{L}_{S_{\|}\perp}q]_{AB}] \\
&\quad +2\tilde{S}^0[\frac{1}{2}P^0\Omega^{AB}\Omega^{CD}X_{AC}X_{BD}\; + r^2\,X_{AB}Y^{AB} + \Omega^{AB}X_{AC}X_{BD})\,Y^{CD}]
\end{aligned} \tag{87}$$

The second square bracket in (87) is $O(1)$ as follows from (83). In the third square bracket of (87) the first term is $O(r^{-3/2})$, the second is $O(r^{-1})$ and the third is $O(r^{-2})$. In the first square bracket of (83) the second term is $O(r^{1/2})$ in leading order, therefore, the order of $r\,S^3$ must not exceed $O(r^{1/2})$ as there is no term to compensate for this. Thus, we conclude again (85) and

$$f_h - \frac{1}{2}r\,\tilde{S}^0\,p_v = 0 \tag{88}$$

to leading order $r^{-1/2}$, i.e., (88) decays at least as $O(r^{-1})$. Together with

$$f_v = O(1) \tag{89}$$

we see that the leading order decay behavior of our solution of the stability condition is now fixed and falls into the allowed class (44) and (47).

Finally, we consider the constraint

$$\begin{aligned}
V_3 - V_3^m &= W^{\mu\nu}m'_{\mu\nu} - 2[W^{\mu\nu}m_{\mu 3}]_{,\nu} = P^{AP}q'_{AB} - 2\,P^A_{,A} - 2\,P^{3\prime} \\
&= (\frac{P^0}{2}\Omega^{AB} + Y^{AB})\,[r^2\Omega_{AB} + X_{AB}]' - 2\,P^A_{,A} - 2\,P^{3\prime} \\
&= 2\,r\,P^0 + Y^{AB}\,X'_{AB} - 2\,P^A_{,A} - 2\,P^{3\prime} \\
&= 2\,[r\,(p_h + y_h) - (p_v + y_v)' - y^A_{,A}] + Y^{AB}\,X'_{AB}
\end{aligned} \tag{90}$$

We have $ry_h = O(r^{-1}), y'_v = O(r^{-2}), y^A_{,A} = O(r^{-1}), X'_{AB}Y^{AB} = O(r^{-2})$ which means that these terms can cancel among each other in (90). On the other hand $rp_h, p'_v = O(r^{-1/2})$ and these are the only terms of this type if we assume that the matter term V_3^m decays faster than this. Therefore,

$$p_h - \frac{1}{r}p'_v = 0 \tag{91}$$

to leading order $r^{-3/2}$ i.e., (91) decays at least as r^{-2}.

Combining (86), (88) and (91) we find

$$\frac{f'_h}{f_h} = -\frac{p_v - r^2 p_h}{r\,p_v} = -\frac{p_v - rp'_v}{r\,p_v} = -\frac{1}{r} + \frac{p'_v}{p_v} \tag{92}$$

to leading order which leads to the solution

$$f_h = \kappa\,\frac{p_v}{r} \tag{93}$$

where κ is an integration constant. This correctly reproduces $f_h = O(r^{-1/2})$ if $p_v = O(r^{1/2})$. Moreover, from (88) to leading order

$$\tilde{S}^0 = \frac{f_v + g_v}{\sqrt{\det(q)}} = 2\frac{f_h}{r\, p_v} = 2\kappa \quad \Rightarrow \quad f_v = 2\kappa \tag{94}$$

as g_v has no $l = 0$ mode. If one wants the lapse to equal unity at infinity then $\kappa = \frac{1}{2}$.

We summarize: The solution $S^\cdot_*$ of the stability conditions constructed displays the decay behavior (78), (81), (82), (85), (89) and the relations (86), (88) and (91) with p_h, p_v, namely to the order displayed

$$\begin{aligned} S^3_* &= f^*_h + g^*_h,\ f^*_h = \kappa\frac{p_v}{r} = O(r^{-1/2}),\ g^*_h = O(r^{-1}) \\ S^A_* &= g^A_* = O(r^{-2}) \\ S^0_* &= f^*_v + g^*_v,\ f^*_v = 2\kappa = O(1), g^*_v = O(1) \\ p_h &= \frac{p'_v}{r} \end{aligned} \tag{95}$$

where the last relation holds when the constraints are used i.e., they should also carry a label $*$ which we dropped for convenience.

Bulk Solution

We note that (75) is a system of four PDE's in four variables S^3, S^A, S^0. One may, therefore, obtain an exact and non-perturbative solution, in principle, as follows: We solve the fourth equation algebraically for S^0 and insert its solution into the first three equations. This remaining system of three PDEs which is linear in S^3, S^A can then be solved for the radial derivatives i.e., it can be written in the form ($\mu, \nu = 1, 2, 3$)

$$S^{\mu\prime}(r,y) = F^\mu_\nu(r,y)\ S^\nu + G^{\mu A}_\nu\ S^\nu_{,A} =: \int d^2y'\ K^\mu_\nu(r;y,y')\ S^\nu(r,y') \tag{96}$$

where the right-hand side is linear S^μ and its angular derivatives which we have written in terms of an integral kernel. Hence, the solution can be written

$$S^\mu_y(r) = [\mathcal{P}(\exp(\int_{-\infty}^r ds K(s)) \cdot \hat{S}(-\infty)]^\mu_y \tag{97}$$

where the path ordering symbol $\mathcal{P}$ orders the highest radial value to the outmost left and $\hat{S}^\mu_y(-\infty)$ are initial values on the sphere $\bar{r} = -z = \infty$ where (μ, y) is considered a compound label in order to write (96) as a matrix equation. This yields, in particular, lapse S^0 and shift S^μ for the GPG and, therefore, an entire spacetime metric. The initial values have to be adjusted to the boundary conditions stated.

Instead of a non-perturbative solution, a perturbative solution of (96) may be obtained as follows: The coefficient functions F^μ_ν, $G^{\mu A}_\nu$ are under perturbative control, i.e., they have known expansions in terms of say X, Y in the GPG thanks to the possibility to solve for $P^3 = p_v + y_v$, $P^A = y^A$, $P^0 = p_h + y_h$ as we will indicate in the next section. By the notation $A(n)$ we mean the n-th order contribution in X, Y in the expansion of a quantity A. The perturbative scheme implies that the $l = 0$ modes p_v, p_h have no first-order contribution, i.e., $p_v(1) = p_h(1) = 0$ while the $l > 0$ modes y_v, y^A, y_h have no zeroth order contribution, i.e., $y_v(0) = y^A(0) = y_h(0) = 0$. We will solve (96) under the same premise for the decomposition $S^3 = f_h + g_h$, $S^A = g^A$, i.e., that the $l = 0$ mode obeys $f_h(1) = 0$ while the $l > 0$ modes obey $g_h(0), g^A(0) = 0$. We now expand all quantities in (96) in powers of X, Y and obtain a hierarchy of equations for the functions $f_h(n);\ 1 \neq n \geq 0,\ g_h(n),\ g^A(n);\ n \geq 1$.

The structure of these equations is given in more detail by

$$\begin{aligned} 0 &= [S^3]' + [\alpha\ S^3 + \beta_A\ S^A + \gamma^B_A\ S^A_{,B}]\ F^3 \\ 0 &= [S^A]' + q^{AB} S^3_{,B} + [\alpha\ S^3 + \beta_A\ S^A + \gamma^B_A\ S^A_{,B}]\ F^A \end{aligned} \tag{98}$$

where all $\alpha, \beta_A, \gamma_A^B, F^3$ have $n = 0$ contributions while $F^A = y^A$ starts at order $n = 1$.

Since $f_{h,A} = 0$ it is easy to see that the second equation of (98) is identically satisfied at order $n = 0$ while the first equation at $n = 0$ gives a first-order ODE in r for $f_h(0)$ whose solution is exactly the asymptotically leading behavior of f_h displayed in (95).

For $n = 1$, because F^A is already of first order and because we have $f_h(1) = 0$, the second equation can be solved explicitly for $g^A(1)$ by decomposing $g_h(1), g^A(1), F^A(1)$ into scalar and vector harmonics, respectively, which yields a first-order linear inhomogeneous ODE in r for $g_{\alpha,l,m}(1),\ \alpha = e, o$ that relates it to $g_{h,l,m}(1), F_{\alpha,l,m}(1)$ and can be solved by quadrature. When inserted into the first equation of (98) at $n = 1$ we obtain an integrodifferential equation for $g_{h,l,m}(1)$ or equivalently a inhomogeneous linear second-order ODE which can be solved by holonomy and variation of constant methods by transforming it into a system of two homogeneous linear first-order equations.

Proceeding inductively, at order $n \geq 2$ we see that the second equation in (98) takes the form

$$0 = [g^A(n)]' + r^{-2}\Omega^{AB}[g_h(n)]_{,B} + J^A(n) \tag{99}$$

where $J^A(n) \propto F^A$ contains at most (n-1)th order contributions of f_h, g_h, g^A and thus (99) can be solved for $g^A(n)$ by quadrature. For the first equation in (98) we note that the $g^A(n)$ contribution to $\beta_A S^A + \gamma_A^B\ S^A_{,B}$ is proportional to $2r^3 D_A g^A(n)$ and hence can be written

$$0 = [f_h(n) + g_h(n)]' + \alpha(0)[f_h(n) + g_h(n)] + K(0)\ D_A g^A(n) + J^3(n) \tag{100}$$

where $J^3(n)$ contains at most (n-1)th order contributions of f_h, g_h, g^A and $K(0)$ is a computable zeroth order function. Thus, dividing by $K(0)$ and taking the radial derivative of (99) we find

$$\{\frac{1}{K(0)}\ ([f_h(n) + g_h(n)]' + \alpha(0)[f_h(n) + g_h(n)] + J^3(n))\}' = D_A\{r^{-2}\Omega^{AB}[g_h(n)]_{,B} + J^A(n)\} \tag{101}$$

We decompose into scalar harmonics and obtain a second-order, linear, inhomogeneous system among the $f_{h,l,m}(n), g_{h,l,m}(n)$ which can be transformed to a first-order system and solved by variation of constant and holonomy methods.

To construct, for instance, S^3 perturbatively has the following significance: For spherically symmetric vacuum GR we have $2M = [S^3]^2\ r$ for any value of r. With matter and perturbations we may *define a local effective mass function*

$$2M_{\rm eff}(x) := [S^3(x)]^2\ r \tag{102}$$

4.5.3. Evaluation of the Boundary Terms at the Solution of the Stability Conditions

The reason why it was sufficient to determine the asymptotic leading decay order of $S^\cdot_*$ is because in the boundary integrals over the asymptotic spheres we take the limit $r \to \infty$. Thus, the only terms that survive this limit are those that display the leading decay behavior, the subleading terms drop out. We now determine the corresponding boundary values $B_\|[S^*_\|],\ B_\perp[S^*_\perp]$.

We have (we consider only one asymptotic end for simplicity)

$$\begin{aligned} B_\|[S^*_\|] &= 2\lim_{r\to\infty} \int d\Sigma_\mu\ S^\rho_*\ W^{\mu\nu}\ m_{\rho\nu} \\ &= 2\lim_{r\to\infty} \int d\Omega\ \omega^{-1}\ [S^3_*\ W^{3\nu}\ m_{3\nu} + S^A_*\ W^{3\nu}\ m_{A\nu}] \\ &= 2\lim_{r\to\infty} \int d\Omega\ [S^3_*\ P^3 + S^A_*\ \frac{1}{2}P^B\ (r^2\Omega_{AB} + X_{AB})] \\ &= 2\lim_{r\to\infty} \int d\Omega\ [(f^*_h + g^*_h)\ (p_v + y_v) + g^A_*\ \frac{1}{2}y^B\ (r^2\Omega_{AB} + X_{AB})] \end{aligned} \tag{103}$$

The term $g^A_* y^B = O(r^{-3})$ while $r^2\Omega_{AB} + X_{AB} = O(r^2)$ hence the second term in (103) drops out. Next, as $g^*_h = O(r^{-1}))$ while $p_v = O(r^{1/2}), y_v = O(1)$ it follows that the term proportional g_h^* vanishes. Finally, as $f_h^* = O(r^{-1/2})$ it follows that the $f_h^* y_v$ term vanishes. Accordingly,

$$B_{||}[S_{||}^*] = 2 \lim_{r\to\infty} \int d\Omega \; f_h^* \; p_v \tag{104}$$

Since $f_h^* = \kappa \frac{p_v}{r}$ we see that

$$B_{||}[S_{||}^*] = 2\,\kappa \lim_{r\to\infty} \int d\Omega \; \frac{p_v}{r} \; p_v =: \int_{\partial\sigma} d^2y \; s_* \; j_* \tag{105}$$

with $j_* = [\frac{p_v}{r^{1/2}}]_{r=\infty}$ and $s_* = 2\kappa \; j_*$. Hence, we can apply proposition 1 with

$$\chi[j] := \kappa \int_{\partial\sigma} d\Omega \; j^2 \tag{106}$$

The contribution to the reduced Hamilton from $B_{||}$ is, therefore, given per asymptotic end by

$$H_{||} = \kappa \lim_{r\to\infty} \int_{S^2} d\Omega \; \frac{p_v(r)^2}{r} \tag{107}$$

Note, that the naive prescription to use $B_{||}[S_{||}^*]$ would have resulted in *twice* $H_{||}$.

Now, we consider $B_\perp[S_\perp^*]$ which only depends on $F := S_*^0 = f_v^* + g_v^* = O(1)$. We have explicitly

$$\begin{aligned}
B_\perp[S_\perp^*] &= -\int \sqrt{\det(m)} \; F \; m^{\mu\nu} \; (d\Sigma_\mu \; [\Gamma^\rho_{\rho\nu} - \Gamma^{\text{ND}\rho}_{\rho\nu}] - d\Sigma_\rho \; [\Gamma^\rho_{\mu\nu} - \Gamma^{\text{ND}\rho}_{\mu\nu}]) \\
&\quad + \int \sqrt{\det(m)} \; [\nabla_\mu F] \; m^{\mu\nu} \; m^{\rho\sigma} (d\Sigma_\nu [m_{\rho\sigma} - m^{\text{ND}}_{\rho\sigma}] - d\Sigma_\rho [m_{\nu\sigma} - m^{\text{ND}}_{\nu\sigma}]) \\
&= -\int \omega^{-1} \sqrt{\det(m)} \; d\Omega \; F \; (m^{3\nu} \; [\Gamma^\rho_{\rho\nu} - \Gamma^{\text{ND}\rho}_{\rho\nu}] - m^{\mu\nu} \; [\Gamma^3_{\mu\nu} - \Gamma^{\text{ND}3}_{\mu\nu}] \\
&\quad + \int \omega^{-1} \; d\Omega \sqrt{\det(m)} \; [\nabla_\mu F] \; (m^{\mu 3} \; m^{\rho\sigma} \; [m_{\rho\sigma} - m^{\text{ND}}_{\rho\sigma}] - m^{\mu\nu} \; m^{3\sigma} \; [m_{\nu\sigma} - m^{\text{ND}}_{\nu\sigma}]) \\
&= -\int \sqrt{\det(q)/\omega^2} \; d\Omega \; F \; ([\Gamma^\rho_{\rho 3} - \Gamma^{\text{ND}\rho}_{\rho 3}] - [\Gamma^3_{33} - \Gamma^{\text{ND}3}_{33}] - q^{AB} \; [\Gamma^3_{AB} - \Gamma^{\text{ND}3}_{AB}]) \\
&\quad + \int d\Omega \sqrt{\det(q)/\omega^2} \; ([\nabla_3 F] \; m^{\rho\sigma} \; [m_{\rho\sigma} - m^{\text{ND}}_{\rho\sigma}] - [\nabla_\mu F] \; m^{\mu\nu} \; [m_{\nu 3} - m^{\text{ND}}_{\nu 3}]) \\
&= -\int \sqrt{\det(q)/\omega^2} \; d\Omega \; F \; ([\Gamma^A_{A3} - \Gamma^{\text{ND}A}_{A3}] - q^{AB} \; [\Gamma^3_{AB} - \Gamma^{\text{ND}3}_{AB}]) \\
&\quad + \int d\Omega \sqrt{\det(q)/\omega^2} \; ([\nabla_3 F] \; q^{AB} \; [q_{AB} - q^{\text{ND}}_{AB}] \\
&= -\int \sqrt{\det(q)/\omega^2} \; d\Omega \; F \; ([\Gamma^A_{A3} - \Gamma^{\text{ND}A}_{A3}] - q^{AB} \; [\Gamma^3_{AB} - \Gamma^{\text{ND}3}_{AB}]) \\
&\quad + \int d\Omega \sqrt{\det(q)/\omega^2} \; ([\nabla_3 F] \; q^{AB} \; [q_{AB} - q^{\text{ND}}_{AB}] \\
&= -\int \sqrt{\det(q)/\omega^2} \; d\Omega \; F \; ([\Gamma^A_{A3} - \Gamma^{\text{ND}A}_{A3}] - q^{AB} \; [\Gamma^3_{AB} - \Gamma^{\text{ND}3}_{AB}]) + \int d\Omega \sqrt{\det(q)/\omega^2} \; F' \; q^{AB} \; X_{AB}
\end{aligned} \tag{108}$$

where we used $d\Sigma_\mu = \omega^{-1} \; d\Omega\delta^3_\mu$ and that $m_{\mu\nu}$ is block diagonal i.e., $m_{33} = 1, m_{3A} = 0, m_{AB} = q_{AB} = r^2\Omega_{AB} + X_{AB}$ in the GPG so that $m^{33} = 1, m^{3A} = 0, m^{AB} = q^{AB}$, $q^{AC}q_{CB} = \delta^A_B$ with $m^{\text{ND}}_{33} = 1$, $m^{\text{ND}}_{3A} = 0$, $m^{\text{ND}}_{AB} = r^2\Omega_{AB}$.

Consider first the second term in the last line of (108) which has integrand

$$\begin{aligned}
&[\frac{\det(q)}{\omega}^2]^{-1/2} \; F' \; \det(q) \; q^{AB} X_{AB} = [\frac{\det(q)}{\omega}^2]^{-1/2} \; F' \; \epsilon^{AC}\epsilon^{BD}[r^2\Omega_{CD} + X_{CD}] \; X_{AB} \\
&= [\frac{\det(q)}{\omega}^2]^{-1/2} \; F' \; [r^2 \det(\Omega)\Omega^{AB} X_{AB} + \det(X)] = [\frac{\det(q)}{\omega}^2]^{-1/2} \; F' \; \det(X)
\end{aligned} \tag{109}$$

Since $F = O(1)$ we have $F' = 0$ at $r = \infty$ since $F = f_v + g_v,\ f_v = c + d\ r^{-n}$, $g_v = C(\Omega) + D(\Omega) r^{-N},\ n, N > 0$. Moreover, $\det(X) = O(r^2)$ while $\det(q)^{-1/2} = O(r^{-2})$. Hence, the second term has a vanishing limit $r \to \infty$.

To evaluate the first term in (108) we require the Christoffel symbols $2\Gamma_{\mu\nu\rho} = 2m_{\mu(\nu,\rho)} - m_{\nu\rho,\mu},\ \Gamma^{\mu}_{\nu\rho} = m^{\mu\sigma}\Gamma_{\sigma\nu\rho}$

$$\begin{aligned}
&\Gamma_{333} = \Gamma_{A33} = \Gamma_{3A3} = 0 \\
&\Gamma_{3AB} = -\frac{1}{2} q'_{AB} = -\Gamma_{A3B} \\
&\Gamma_{ABC} = r^2 \Gamma^{\Omega}_{ABC} + \Gamma^{X}_{ABC} \\
&\Gamma^3_{33} = \Gamma^3_{A3} = \Gamma^A_{33} = 0 \\
&\Gamma^3_{AB} = \Gamma_{3AB}, \Gamma^A_{3B} = q^{AC}\Gamma_{C3B} \\
&\Gamma^A_{BC} = q^{AD}\ \Gamma_{DBC}
\end{aligned} \tag{110}$$

since $q_{3\mu} = \delta^3_\mu$ is constant and we have used block diagonality.

It follows that the non-vanishing symbols have at most one index $\mu = 3$ and Γ_{3AB}, $\Gamma_{A3B} = O(r),\ \Gamma_{ABC} = O(r^2),\ \Gamma^3_{AB} = O(r),\ \Gamma^A_{3B} = O(r^{-1}), \Gamma^A_{BC} = O(1)$. In particular the combination required in (108) is

$$\begin{aligned}
& [\det(q)\omega^{-2}]^{1/2}\ ([\Gamma^A_{A3} - \Gamma^{\mathrm{ND}A}_{A3}] - q^{AB}\ [\Gamma^3_{AB} - \Gamma^{\mathrm{ND}3}_{AB}]) \\
= \ & [\det(q)\omega^2]^{-1/2}\ \det(q)\ (q^{AB}\ [\Gamma_{BA3} - \Gamma_{3AB}] - q^{AB}_{\mathrm{ND}}\ [\Gamma^{\mathrm{ND}}_{BA3} - \Gamma^{\mathrm{ND}}_{3AB}]) \\
= \ & [\det(q)\omega^2]^{-1/2}\ (\epsilon^{AC}\epsilon^{BD}\ [r^2\Omega_{CD} + X_{CD}]\ [2r\Omega_{AB} + X'_{AB}] - \det(q)\ r^{-2}\Omega^{AB}\ [2r\Omega_{AB}]) \\
= \ & [\det(q)\omega^2]^{-1/2}\ ([r^2 \det(\Omega)\ \Omega^{AB} + \epsilon^{AC}\epsilon BDX_{CD}]\ [2r\Omega_{AB} + X'_{AB}] - 4[r^4\omega^2 + \omega^2\Omega^{AB}X_{AB} + \det(X)]\ r^{-1}) \\
= \ & [\det(q)\omega^2]^{-1/2}\ (4\, r^3\omega^2 + [\det(X)]' - 4[r^4\omega^2 + \det(X)]\ r^{-1}) \\
= \ & [\det(q)\omega^2]^{-1/2}\ ([\det(X)]' - 4\det(X)\ r^{-1})
\end{aligned} \tag{111}$$

which is $O(r^{-1})$. Since $F = O(1)$ it follows

$$B_\perp[S^*_\perp] = 0 \tag{112}$$

Altogether, the reduced Hamiltonian is, therefore, given by (taking both asymptotic ends into account)

$$H = \kappa\ [\lim_{r\to\infty} \int_{S_2} d\Omega\ \frac{[P^3_*(r,\Omega)]^2}{r} + \lim_{\bar{r}\to\infty} \int_{S_2} d\Omega\ \frac{[P^3_*(\bar{r},\Omega)]^2}{\bar{r}}] \tag{113}$$

where P^3_* is the value of P^3 obtained by solving all the constraints and by imposing the GPG. Due to the decay, $y_v = O(r^{-1})$ we may replace $P^3 = p_v + y_v$ by p^*_v in (113).

Several remarks are in order:

Remark 1. In the presentation so far we have omitted the prefactor $1/k,\ k = 16\pi G$ of the action where G is Newton's constant and we use units with $c = 1$. That prefactor propagates into the constraints and thus the boundary term, and therefore, into H. We check that $H = M$ for spherically symmetric vacuum GR when (113) is multiplied by $1/k$. To see this we use with $S^0 = N$, the relations $W^{\mu\nu} = \sqrt{\det(m)}[m^{\mu\nu}m^{\rho\sigma} - m^{\mu\rho}m^{\nu\sigma}]K_{\rho\sigma}$ and $K_{\rho\sigma} = \frac{1}{2N}[\dot{m}_{\rho\sigma} - [\mathcal{L}_{\vec{S}}m]_{\rho\sigma}]$ in GPG. This gives with $\omega = \sqrt{\det(\Omega)}$ the identity $p^v = P^{33}/\omega = r^2[K_{33} - m^{ab}K_{ab}] = -\Omega^{AB}K_{AB}$ and $K_{AB} = -\frac{1}{2N}[\mathcal{L}_{\vec{S}}m]_{AB} = -\frac{1}{2N}[2rS^3]\Omega_{AB} = -\frac{rS^3}{N}\Omega_{AB}$, and therefore, $p_v = 2r\frac{S^3}{N}$. If we compare with (93) and use $f_h = S^3, f_v = 2\kappa = N$ we obtain exact match. It follows, performing the angular integral in (113) $H = \frac{4\pi}{k}\ \kappa\ 4r\ [S^3]^2/N^2$. Since $S^3 = \sqrt{2GM/r}$ in GPG it follows $H = 2\kappa M/N^2$ for one asymptotic end which equals M for $N = 1$ i.e., $\kappa = 1/2$. Again, had we wrongly identified H with the value of the boundary term we would have obtained $H = 2M$, i.e., twice the ADM mass. The difference arises because in the Schwarzschild gauge the ADM momentum vanishes exactly and the stabilising lapse is a constant on the phase space; therefore, in this case H is simply the boundary term and yields correctly $H = M$ with the same prefactor $1/k$ (see, e.g., the second reference in [40–44]).

Remark 2. By contrast to the usual computation, the Hamiltonian results from the boundary term of the ADM momentum rather than the ADM Hamiltonian. This can be traced back to the fact that in the GPG the information about the mass is not encoded in the three metrics but rather in the extrinsic curvature while in the Schwarzschild gauge the roles are switched (the extrinsic curvature vanishes in the static presentation of the metric).

Remark 3. In Cartesian coordinates, the Christoffel symbols vanish exactly for the GP background metric (which is flat) so that the ADM energy term vanishes exactly for that background, not only to leading order. The relation between the Schwarzschild and GP coordinates involves a boost (see Appendix C) so that the resulting Hamiltonian becomes now a component of the ADM momentum.

Remark 4. Remarkably, the expression (113) is *positive definite* no matter what the concrete expression for P^3_* is in terms of the true degrees of freedom. For the present model these are gravitational mass M, electric charge Q, gravitational tracefree (wrt Ω) angular perturbations X_{AB}, Y^{AB} (only $l \geq 2$ modes), electromagnetic angular perturbations $A_C,\ E^A$ (only $l \geq 1$ modes) and Klein–Gordon field Φ, Π (all $l \geq 0$ modes are observables but only $l > 0$ modes are perturbations) when we solve the Gauss constraint for E^3.

Remark 5. At exact spherical symmetry in a vacuum, we have $P^3_* = \sqrt{2Mr}$ hence $H = 2\kappa M$ (with prefactor k included). The freedom κ is, therefore, the same that arises in the purely spherically symmetric sector (see Appendix B) or in the Kantowski–Sachs reformulation (see Appendix D).

Remark 6. When expanding P^3_* perturbatively in terms of the perturbations just mentioned we obtain schematically $P^3_* = P^3_*(0) + P^3_*(1) + P^3_*(2) + \ldots$ where the three terms are, respectively, independent, linear and quadratic in the perturbations. Now, $P^3 = p_v + y_v$ and by the general theory [61] $p_v(1) \equiv 0$ while $y_v(n),\ n \geq 1$ decays too fast to be visible in (113). Therefore, to second order in the perturbations for one asymptotic end

$$H = \frac{\kappa}{k} \lim_r \frac{1}{r} \int d\Omega\ \{[p^*_v(0)]^2 + 2\ p^*_v(0)\ p^*_v(2)\} \tag{114}$$

(the angular integral gives just 4π because p_v has only zero modes). As we will confirm in our companion papers, (114) reproduces the Regge–Wheeler and Zerilli Hamiltonian [52–55] in GP coordinates.

Remark 7. The real virtue of (113), however, is that it is a non-perturbative result. It provides a formula for the physical Hamiltonian entirely expressed in terms of the true degrees of freedom and in that sense is gauge invariant to all orders that one may want to expand it into. For instance, we now have access to a non-ambiguous Hamiltonian that includes cubic ("Non-Gaussian") (self-)interactions of the perturbations. In particular, in the absence of scalar matter, the system can be interpreted as a black hole formed due to the collapse of gravitational and/or electromagnetic waves due to self-interactions mediated by gravity.

Remark 8. In the present situation, although (113) has contributions from both asymptotic ends, since $p^*_v(z),\ z = \theta(z)r - \theta(-z)\bar{r}$ is obtained from a differential equation, the value $p^*_v(-\infty) \propto \sqrt{Mr}$ is a non-perturbative (i.e., fixed in all orders of perturbation theory) integration constant at $z = -\infty$. Therefore, the contribution from $\bar{r} = \infty$ in (113) drops out in Poisson brackets and we may delete it from H.

5. Perturbative Structure of the Constraints

While in the previous section, we have derived the non-perturbative definition of the reduced Hamiltonian, it is given only implicitly. To be practically useful, in particular, for quantization, we need an explicit formula. This can be provided at least perturbatively, which will be the task of the present and next section.

In this section, we discuss subsequently the perturbative structure of Gauss, spatial diffeomorphism and Hamiltonian constraint. Since the Gauss and spatial diffeomorphism constraints are first and second order homogeneous polynomials in all fields, we will be able to exhibit all perturbative orders explicitly where we leave the evaluation of integrals of contractions of three spherical tensor harmonics in terms of Clesch–Gordan coefficients for our companion papers. For the the Hamiltonian constraint, which we treat in its polynomial form, we collect the full non-perturbative structure of all sub-polynomials from which it is assembled but then just keep the orders up to two. The explicit computation of the finite number of higher orders (up to ten in vacuum GR) will be subject of our companion papers.

5.1. Reduction of the Gauss Constraint

Since the Gauss constraint Poisson commutes with all other constraints (we replace $V^M_\mu + V^{KG}_\mu$ by $F_{\mu\nu}E^\nu + \Pi^T[D_\mu\Phi]$ by subtracting $A_\mu G = A_\mu(G^M + G^{KG})$ which can be conducted by redefining the S^μ, S_0) we may reduce the theory with respect to the corresponding gauge degrees of freedom before entering the reduction with respect to Hamiltonian and spatial diffeomorphism constraints. In the case of charge, (i.e., a scalar dublett) it is most convenient to use a "unitary gauge" otherwise (i.e., a scalar singlett) a radial "axial" gauge.

5.1.1. Unitary Gauge

As the Gauss constraint generates rotations of $\Phi = (\phi_1, \phi_2)$, a perfect gauge is $\phi_2 = 0$ and we can solve $G = 0$ algebraically for $\pi_2 = J := \phi_1^{-1}\partial_a E^a$ so that no decay properties of the fields come into play. Then, $(\phi = \phi_1,\ \pi = \pi_1),\ (A_\mu, E^\mu),\ \mu = 1,2,3$ are the true degrees of freedom as far as reduction of the Gauss constraint is concerned. Then, the only task to do is to perform the following replacements in the Klein–Gordon contributions to the SDC and HC, respectively,

$$V^{KG}_\mu \ \to\ \pi\phi_{,\mu},\ \ 2\,V^{KG}_0 \ \to\ \frac{\pi^2 + J^2}{\sqrt{\det(m)}} + \sqrt{\det(m)}m^{\mu\nu}[\phi_{,\mu}\phi_{,\nu} + A_\mu A_\nu \phi^2 + 2V(\phi^2)] \quad (115)$$

5.1.2. Axial Gauge

We now assume that there is just one KG field ϕ with conjugate momentum ϕ, hence the term $\Pi^T\epsilon\Phi$ in G is missing and $D_\mu\Phi \to \partial_\mu\phi,\ \Pi \to \pi$ in both V^{KG}_μ, V^{KG}_0.

In view of the subtle difference between gauge and symmetries that arises for constraints that depend on spatial derivatives of the fields exemplified in Appendix A, we need to specify the decay behavior of the fields at the spatial infinities which we take to be r^{-2} in an asymptotic Cartesian frame for both electric and magnetic fields so that the electromagnetic energy density decays as r^{-4}. This allows the vector potential to decay as r^{-1} or faster. In terms of the spherical frame $A_\mu(z) = (\partial x^a/\partial y^\mu)A_a(x),\ E^\mu(z) = |\det(\partial x/\partial z)|\,(\partial z^\mu/\partial x^a)E^a(x)$ this translates into $E^3 = O(1),\ E^C = O(r^{-1}),\ A_3 = O(r^{-2}),$ $A_C = O(r^0)$. However, we must require that the dynamical part of the Maxwell connection decays as $A_3 = O(r^{-2}),\ A_C = O(r^{-1})$. This makes sure that $E^3\ [dA_3],\ E^B\ [dA_B]$ decay as r^{-2} which then makes the symplectic potential converge. The functionally differential form of the Maxwell contribution to the Gauss constraint is (the Klein–Gordon cointribution is functionally differentiable as it is)

$$H[S_0] = G[S_0] + B[S_0] = -\int d^3z\, E^\mu S_{0,\mu},\ B[S_0] = -\int d^2y\ [E^3\ S^0]_{r=-\infty}^{r=\infty} \quad (116)$$

The solution of the constraint $(E^3)' + E^A_{,A} = 0$ is

$$E^3_* = P^M - \int_{-\infty}^r ds\; E^A_{,A} \tag{117}$$

where P^M is any function on S^2. The boundary term becomes such a solution

$$B[S_0] = \int d^2y; \{-P^M\; [S_0(\infty) - S_0(-\infty)] + [\int_{-\infty}^{\infty} dr\; E^A_{,A}]\; S_0(\infty)\} \tag{118}$$

which vanishes for all E^A, p^M iff $S_0(\infty) = S_0(-\infty) = 0$. Such S_0 correspond to a gauge transformation. The general transformation of A_μ is $\delta A_\mu = -S_{0,\mu}$. We cannot gauge A_3 completely to zero because for general A_3 this would require that $S_0 = \int_{-\infty}^r dsA_3(s)$ which does not necessarily vanish at $r = \infty$. Let w be a function of r only with $\int_{-\infty}^{\infty} drw = 1$, $w = O(r^{-2})$, say $w = \frac{1}{\pi\, r_0(1+r^2/r_0^2)}$. Then, we can gauge A_3 to $A_3^* = w\; Q_M,\; Q_M := \int_{-\infty}^{\infty} dr\;\; A_3$ using $S_0 = \int_{-\infty}^r dr\; [A_3 - Q_M\; w]$ which now is a gauge transformation. Under a gauge transformation Q_M is an invariant. The transformations that stabilize the gauge $A_3 - Q_M w$ satisfy $-S_0' + w\; [S_0]_{-\infty}^{\infty} = 0$ i.e., $S_0^* = S_0^*(-\infty) + [\int_{-\infty}^r w]\; K,\; K = [S_0^*]_{-\infty}^{\infty}$. which does not vanish at $r = \infty$ and thus corresponds to a symmetry transformation. The symplectic structure pulled back to E^3_*, A_3^* is given by

$$\begin{aligned}\Theta_M &= \int dr\; d^2y\; \{[P^M - \int_{-\infty}^r ds\; E^B_{,B}(s)]\; w(r)\; [dQ_M] + E^B\; [dA_B]\;\} \\ &= \int d^2y\; P^M\; [dQ_M] + \int dr\; d^2y\; E^B\; [d(A_B + [\int_r^{\infty} ds\; w(s)]\; Q_{M,B}]\end{aligned} \tag{119}$$

and displays the canonical pair (Q_M, P^M) on the sphere and the bulk canonical pair $(E^B, \hat{A}_B = A_B + [\int_r^{\infty} dsw(s)]Q_{M,B})$. Under a symmetry transformation $E^B, \hat{A}_B$ are both invariant. For the magnetic field we have $B^3 = \epsilon^{BC} A_{C,B} = \epsilon^{BC} \hat{A}_{C,B}$ and $B^A = -\epsilon^{AB}[A'_B - Q_{M,B} w) = -\epsilon^{AB}\; \hat{A}'_B$, i.e., it just depends on the invariant $\hat{A}_B$. Thus, neither the magnetic nor the electric field depend explicitly on the Q_M which thus acquire the same invisibility as the momenta Q conjugate to the gravitational mass if we follow the strategy of Appendix C.6. The electric field does depend on P^M of which the $l = 0$ mode is just the electric charge.

We now perform the same analysis more explicitly in terms of spherical harmonics. The corresponding symmetric and non-symmetric Gauss constraints are easily found to be using $((.)' := \frac{d}{dr}(.))$

$$\begin{aligned}G &= \nabla_\mu E^\mu = \omega[p^{M\prime} + \sum_{l>0} [y^{M\prime}_{l,m} L_{l,m} + \sum_{\alpha \in \{o,e\}} Y^M_{\alpha,l,m}\; D_A\; L^A_{\alpha,l,m}] \\ &= \; = \omega[p^{M\prime} + \sum_{l>0} [y^{M\prime}_{l,m} - \sqrt{l(l+1)} Y^M_{e,l,m}]\; L_{l,m}\end{aligned} \tag{120}$$

Thus

$$C_M(r) = C_{M(0)}(r) = p^{M\prime}(r),\; Z_{M,l,m}(r) = Z_{M,l,m(1)}(r) = y^{M\prime}_{l,m} - \sqrt{l(l+1)} Y^M_{e,l,m}(r) \tag{121}$$

with general solution (we relabel $z = \theta(z)r - \theta(-z)\bar{r}$ by r which has no range on the real axis)

$$p^M(r) = p^M(0),\; y^M_{l,m}(r) = p^M_{l,m}(0) + \sqrt{l(l+1)} \int_{-\infty}^r ds\; Y^M_{e,l,m}(s) \tag{122}$$

We plug these into the symplectic structure for the Maxwell field and obtain up to a total phase space differential

$$\begin{aligned}
\Theta_M &= \int_{-\infty}^{\infty} dr\ \{p^M(r)\ dq_M(r) + \sum_{l>0,|m|\le l} [y^M_{l,m}\ dx^{l,m}_M(r) + Y^M_{e,l,m}(r)\ dX^{e,l,m}_M(r) + Y^M_{o,l,m}(r)\ dX^{o,l,m}_M(r)\} \\
&= P^M_h\ d[\int_{-\infty}^{\infty} dr\ q_M(r)] + \sum_{l>0,|m|\le l} Y^M_{h,l,m}\ d[\int_{-\infty}^{\infty} dr\ x^{l,m}_M(r)] + \sum_{l>0,|m|\le l} \int_{-\infty}^{\infty} dr\ \{Y^M_{e,l,m}(r)\ d[X^{e,l,m}_M(r) \\
&+ \sqrt{l(l+1)} \int_r^{\infty} ds\ x^{l,m}_M(s)] + Y^M_{o,l,m}(r)\ dX^{o,l,m}_M(r)\} \\
&=: P^M_h\ dQ^h_M + \sum_{l>0,|m|\le l} Y^M_{h,l,m}\ dX^{h,l,m}_M + \int_{-\infty}^{\infty} dr\ [Y^M_{e,l,m}\ d\tilde{X}^{e,l,m}_M + Y^M_{o,l,m}\ d\tilde{X}^{o,l,m}_M](r)
\end{aligned} \tag{123}$$

where we have set $P^M_h := p^M(0), Y^M_{h,l,m} := p^M_{l,m}(0)$. We see that the reduced symplectic structure only depends on the Dirac observables (with respect to the Gauss constraint) $(P^M_h, Q^h_M), (Y^M_{h,l,m}, X^{h,l,m}_M)$ which which are independent of r (they are the harmonic modes of P^M, Q_M above) and the Dirac observables $(Y^M_{e,l,m}, \tilde{X}^{e,l,m}_M)(Y^M_{o,l,m}, \tilde{X}^{o,l,m}_M)$ which do depend on r (they are the harmonic modes of $E^B, \hat{A}_B$ above).

For the magnetic fields we find

$$\begin{aligned}
B^3 &= \epsilon^{AB}\ D_A A_B = \omega \sum_{l>0,|m|\le l,\alpha\in\{e,o\}} X^{\alpha,l,m}_M\ \eta^{AB}\ D_A L_{B;\alpha,l,m} = \omega \sum_{l>0,|m|\le l} \sqrt{l(l+1)} X^{o,l,m}_M\ L_{l,m} \\
B^A &= -\omega\ \eta^{AB}\ (A'_B - D_B A_3) = -\omega \sum_{l>0,|m|<l} [(X^{e,l,m\prime}_M - \sqrt{l(l+1)} x^{l,m}_M)\ L^A_{o,l,m} - X^{o,l,m\prime}_M\ L^A_{e,l,m}] \\
&= -\omega \sum_{l>0,|m|<l} [\tilde{X}^{e,l,m\prime}\ L^A_{o,l,m} - X^{o,l,m\prime}_M\ L^A_{e,l,m}]
\end{aligned} \tag{124}$$

which of course also only depends on these Dirac observables.

Thus, we can drop A_3, E^3 from the list of independent variables in Θ and denote $\tilde{X}^{e,l,m}_M$ by $X^{e,l,m}_M$ again. We drop the term proportional to G from the Hamiltonian, note that V_0, V_μ then only depend on electric and magnetic fields and write these in terms of the degrees of freedom $P^M_h, P^M_{h,l,m}, X^{\alpha,l,m}_M, Y^M_{\alpha,l,m}$ explicitly

$$\begin{aligned}
E^3 &= \omega\ \{P^M_h + \sum_{l>0,m} [Y^M_{h,l,m} + \sqrt{l(l+1)}\ \int_{-\infty}^{r} ds\ Y^M_{e,l,m}(s)]\ L_{l,m}\} =: P^M_h + \sum_{l>0,m} \tilde{Y}^M_{h,l,m}\ L_{l,m} \\
E^A &= \omega \sum_{l>0,m,\alpha=e,o} Y_{\alpha,l,m}\ L^A_{\alpha,l,m} \\
B^3 &= \omega \sum_{l>0,m} \sqrt{l(l+1)}\ X^{o,l,m}_M\ L_{l,m} =: \sum_{l>0,m} \tilde{X}^{h,l,m}_M\ L_{l,m} \\
B^A &= -\omega \sum_{l>0,m,\alpha,\beta=e,o} \epsilon_{\alpha\beta}\ X^{\alpha,l,m\prime}_M\ L^A_{\beta,l,m}
\end{aligned} \tag{125}$$

where $\tilde{Y}^M_{h,l,m}$, $\tilde{X}^{h,l,m}_M$ are just abbreviations for the above linear functions of $Y^M_{e,l,m}$, $X^{o,l,m}_M$, respectively, and $\epsilon_{\alpha\beta},\ \alpha,\beta = e,o$ is the skew symbol with $\epsilon_{eo} = 1$. Note, that

$$\eta_{AB} L^B_{\alpha,l,m} = -\sum_\beta \epsilon_{\alpha\beta} L_{A;\beta,l,m} \tag{126}$$

In this way, the Hamiltonian H remains polynomial of degree two in these variables. The field components E^3, B^3 have merely the status of an abbreviation for the r.h.s. of the first line and third line of (125).

5.2. General Perturbative Structure of the Spatial Diffeomorphism Constraint

It is simplest to start with the form of the constraint in which its geometric meaning becomes most transparent (dropping the boundary term for the moment)

$$V_\mu[S^\mu] = \int d^3x \; \{W^{\mu\nu} \; [\mathcal{L}_{\vec{S}} m]_{\mu\nu} + E^\mu \; [\mathcal{L}_{\vec{S}} A]_\mu + \pi^T \; [\mathcal{L}_{\vec{S}} \phi]\} \tag{127}$$

The boundary term picked up by a variation has been discussed at length in the previous section as far as the gravitational degrees of freedom are concerned. The boundary term picked up with respect to the matter fields is $\int \; d\Sigma_\mu S^\mu [E^\nu \delta A_\nu + \pi\delta\phi] = \int \; d^2y \; S^3[E^\nu \delta A_\nu + \pi\delta\phi]$ which vanishes identically since by construction the term in the square bracket which enters the symplectic potential is $O(r^{-2})$. For π, ϕ this is achieved if π, ϕ decay as $O(r^{-2})$ in Cartesian coordinates or π as $O(1)$ and ϕ as $O(r{-}2)$ and ϕ as $O(r^{-2})$ in spherical coordinates. The decay of A, E was specified in the previous subsection.

We have explicitly $((.)' = \frac{d}{dr}(.))$

$$\begin{aligned}
&[\mathcal{L}_{\vec{S}} m]_{33} = S^3 \; m'_{33} + S^A \; D_A m_{33} + 2m_{33} \; S^{3\prime} + 2 \; m_{3A} \; S^{A\prime} \\
&[\mathcal{L}_{\vec{S}} m]_{3A} = S^3 \; m'_{3A} + S^B \; D_B m_{3A} + m_{33} \; D_A S^3 + m_{B3} \; D_A S^B + m_{3A} \; S^{3\prime} + m_{BA} \; S^{B\prime} \\
&[\mathcal{L}_{\vec{S}} m]_{AB} = S^3 \; m'_{AB} + S^C \; D_C m_{AB} + 2m_{C(A} D_{B)} S^C + 2 \; m_{3(A} D_{B)} S^3 \\
&[\mathcal{L}_{\vec{S}} A]_3 = S^3 \; A'_3 + S^B \; D_B A_3 + A_3 \; S^{3\prime} + A_B S^{B\prime} \\
&[\mathcal{L}_{\vec{S}} A]_B = S^3 \; A'_B + S^C \; D_C A_B + A_3 \; D_B S^3 + A_C \; D_B S^C \\
&[\mathcal{L}_{\vec{S}} \phi] = S^3 \; \phi' + S^A \; D_A \phi
\end{aligned} \tag{128}$$

Plugging the expansions (14), (15) into (128) we can carry out the covariant differentials and write (128) in terms of contracted quadratic monomials of tensor harmonics. Then, contracting with the momenta in (127) we obtain a sum of contracted cubic monomials of tensor harmonics that are being integrated with $d\Omega$. These integrals can be performed in closed form. Of interest to us in this work is not their explicit form but the qualitative structure. We note that we are interested in the coefficients of the smearing functions f^a, g^j which are immediately available from (128) modulo an integration by parts with respect to the radial variable. These integrations by parts generate radial derivatives of momenta. We see from (128) that both $S^{3\prime}$ and $S^{A\prime}$ occur only in $[\mathcal{L}_{\vec{S}} m]_{33}$, $[\mathcal{L}_{\vec{S}} m]_{3A}$, $[\mathcal{L}_{\vec{S}} A]_3$; therefore, the only radial derivatives of momenta that appear are those of W^{33}, W^{3A}, E^3 (also the Gauss constraint contains only radial derivatives of E^3). Since the Hamiltonian constraint does not contain momentum derivatives, it follows that the only radial derivatives acting on the radial coefficient functions of the tensor harmonics for the momenta that occur are those of $p^E_v, y^E_{v,l,m}, y^E_{\alpha,l,m}, p^M, y^M_{l,m}$ with $l > 0, \alpha \in \{e, o\}$. Since in the construction algorithm we want to solve jointly the constraints C_a for p_a and the constraints Z_j for y_j it follows that we can solve algebraically for $p^E_h, y^E_{h,l,m}$ but have to solve radial differential equations for the other p, y type momenta just listed. Note, that, in particular, the true momenta P_A, Y_J occur without radial derivatives.

Performing integrations by parts explicitly to recover the actual constraint without derivatives on the smearing function we find

$$\begin{aligned}
&V_\mu[S^\mu] = \int \; d^3x \; \{ \\
&S^3 \; [W^{33} \; m'_{33} - 2(W^{33} \; m_{33})' + 2(W^{3A} \; m'_{3A} - 2(W^{3A} \; m_{3A})') + W^{AB} \; m'_{AB} - 2 \; D_A(W^{3A} \; m_{33} + W^{AB} \; m_{3B}) \\
&+\pi \; \phi' + E^3 \; A'_3 - (E^3 A_3)' + E^B \; A'_B - D_B(E^B A_3)] \\
&+S^A \; [W^{33} \; D_A \; m_{33} - 2(W^{33} \; m_{3A})' + 2 \; W^{3B} \; D_A m_{3B} - 2 \; D_A(W^{3B} m_{3B}) - 2(W^{3B} m_{AB})' + W^{BC} \; D_A m_{BC} \\
&-2 \; D_B(W^{BC} m_{CA})] \\
&+\pi \; D_A \phi + E^3 \; D_A A_3 - (E^3 A_A)' + E^B \; D_A A_B - D_B(E^B A_A)]\}
\end{aligned} \tag{129}$$

Using the result of the previous subsection we may in fact exploit that $G = 0$ is identically satisfied so that the contribution from the Maxwell field can be simplified to

$$\begin{aligned} & S^\mu [E^\nu \partial_\mu A_\nu - \partial_\nu (E^\nu A_\mu)] = 2\, S^\mu \partial_{[\mu} A_{\nu]}\, E^\nu = 2\, S^\mu \epsilon_{\mu\nu\rho}\, E^\nu B^\rho \\ = \; & 2\, [S^3\, \epsilon_{BC}\, E^B\, B^C + S^A\, \epsilon_{AC}\, (E^C\, B^3 - E^3\, B^C)] \end{aligned} \tag{130}$$

We extract the coefficients of S^3, S^A with respect to the decomposition (14), see (18) and (19). The symmetric constraint is

$$\begin{aligned} & f^h C_h = f^h \; < 1, V_3/\omega >_{L_2} = f^h \{ [p_v^E\, (q_E^v)' - 2\, (p_v^E\, q_E^v)' + p_h^E\, (q_E^h)' + P^{KG}\, Q'_{KG}] \\ & + \sum_{l>0,m} [(\sum_{\alpha=v,e,o} y^E_{\alpha,l,m}\, (x_E^{\alpha,l,m})' - 2\, (y^E_{\alpha,l,m}\, x_E^{\alpha,l,m})') + y^E_{h,l,m}\, (x_E^{h,l,m})' + Y^{KG}_{l,m}\, (X^{l,m}_{KG})' \\ & + \sum_\alpha \epsilon_{\alpha\beta} Y^M_{\alpha,l,m}\, X^{\beta,l,m\prime}]_M] \} \\ =: \; & f^h \{ C_{h(0)}((p^E, q_E), (P^{KG}, Q_{KG})) + C_{h(2)}((y^E, x_E), (Y^{KG}, X_{KG}), (Y^M, X_M)) \} \end{aligned} \tag{131}$$

The non-symmetric constraints are

$$\begin{aligned} & g^{h,l,m}\, Z_{h,l,m} = g^{h,l,m} < L_{l,m}, V_3/\omega >_{L_2} \\ = \; & g^{h,l,m}\, \{ [y^E_{v,l,m}\, (q_E^v)' + p_v^E\, (x_E^{v,l,m})' - 2(y^E_{v,l,m}\, q_E^v + p_v^E\, x_E^{v,l,m})' \\ & + p_h^E\, (x_E^{h,l,m})' + y^E_{h,l,m}\, (q_E^h)' + \sqrt{l(l+1)}\, y^E_{e,l,m}\, q_E^v + P^{KG}\, (X^{l,m}_{KG})' + Y^{KG}_{l,m}\, (Q_{KG})'] \\ & + \sum_{l',m',\tilde{l},\tilde{m}} [< L_{l,m}, L_{l',m'}\, L_{\tilde{l},\tilde{m}} >_{L_2}\; \{ y^E_{v,l',m'}\, (x_E^{v,\tilde{l},\tilde{m}})' - 2\, (y^E_{v,l',m'}\, x_E^{v,\tilde{l},\tilde{m}})' \} \\ & + \sum_{\alpha,\beta=o,e} < L_{l,m}, L^A_{\alpha,l',m'}\, L_{A;\beta,\tilde{l},\tilde{m}} >_{L_2}\; \{ y^E_{\alpha,l',m'}\, (x_E^{\beta,\tilde{l},\tilde{m}})' - 2\, (y^E_{\alpha,l',m'}\, x_E^{\beta,\tilde{l},\tilde{m}})' \} \\ & + \sum_{\alpha,\beta=o,e} < L_{l,m}, L^{AB}_{\alpha,l',m'}\, L_{AB;\beta,\tilde{l},\tilde{m}} >_{L_2}\; Y^E_{\alpha,l',m'}\, (X_E^{\beta,\tilde{l},\tilde{m}})' \\ & + \sum_{\alpha=o,e} < L_{l,m}, L^{AB}_{\alpha,l',m'}\, L_{AB;h,\tilde{l},\tilde{m}} >_{L_2}\; Y^E_{\alpha,l',m'}\, (x_E^{h,\tilde{l},\tilde{m}})' \\ & + \sum_{\beta=o,e} < L_{l,m}, L^{AB}_{h,l',m'}\, L_{AB;\beta,\tilde{l},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\, (X_E^{\beta,\tilde{l},\tilde{m}})' \\ & + < L_{l,m}, L^{AB}_{h,l',m'}\, L_{AB;h,\tilde{l},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\, (x_E^{h,\tilde{l},\tilde{m}})' \\ & + 2\, \sqrt{l(l+1)} \sum_{\alpha=o,e} < L_{A;e,l,m}, L^A_{\alpha,l',m'}\, L_{\tilde{l},\tilde{m}} >_{L_2^2}\; y^E_{\alpha,l',m'}\, x_E^{v,\tilde{l},\tilde{m}} \\ & + 2\, \sqrt{l(l+1)} \sum_{\alpha,\beta=e,o} < L_{A;e,l,m}, L^{AB}_{\alpha,l',m'}\, L_{B;\beta\tilde{l},\tilde{m}} >_{L_2^2}\; Y^E_{\alpha,l',m'}\, x_E^{\beta,\tilde{l},\tilde{m}} \\ & + 2\, \sqrt{l(l+1)} \sum_{\beta=e,o} < L_{A;e,l,m}, L^{AB}_{h,l',m'}\, L_{B;\beta\tilde{l},\tilde{m}} >_{L_2^2}\; y^E_{h,l',m'}\, x_E^{\beta,\tilde{l},\tilde{m}} + < L_{l,m}, L_{l',m'}\, L_{\tilde{l},\tilde{m}} >_{L_2}\; Y^{KG}_{l',m'}\, (X^{\tilde{l}\tilde{m}})' \\ & + \sum_{\alpha,\beta=e,o} < L_{l,m}, L^A_{\alpha,l',m'}\, L_{A;\beta\tilde{l},\tilde{m}} >_{L_2}\; Y^M_{\alpha,l',m'}\, (X_M^{\beta,\tilde{l},\tilde{m}})' \,] \\ =: \; & g^{h,l,m}\, \{ Z_{h,l,m(1)}((y_v^E, q_E^v), (p_v^E, x_E^v), (y_h^E, q_E^h), (p_h^E, x_E^h), (P^{KG}, X_{KG}), (Y^{KG}, Q_{KG})) \\ & + Z_{h,l,m(2)}((y^E, x_E); (Y^E, X_E), (Y^E, x_E), (y^E, X_E), (Y^{KG}, X_{KG}), (Y^M, X_M)) \} \end{aligned} \tag{132}$$

and

$$
\begin{aligned}
& g^{\alpha,l,m}\; Z_{\alpha,l,m} = g^{\alpha,l,m} \sum_{A=1,2} (< L^A_{\alpha,l,m}, V_A/\omega >_{L_2})_{\alpha=o,e} \\
= \; & g^{\alpha,l,m}\; \{[\sqrt{l(l+1)}\; p^E_v\; \delta^\alpha_e\; x^{v,l,m}_E - 2(p^E_v\; x^{\alpha,l,m}_E)' - 2(y^E_{\alpha,l,m}\; q^h_E)' \\
& +[-2\sqrt{l(l+1)/2}\; y^E_{h,l,m}\; \delta^e_\alpha + \sqrt{(l-1)(l+2)/2} Y_{\alpha,l,m}] q^h_E \\
& +\sqrt{l(l+1)}\; P^{KG}\; \delta^e_\alpha X^{l,m}_{KG} - P^M_h\; (X^{\alpha,l,m}_M)'] \\
& + \sum_{l',m',\tilde{m},\tilde{m}} [\sqrt{l(l+1)}\; < L^A_{\alpha,l,m}, L_{l',m'}\; L_{A;e,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{v,l',m'}\; x^{v,\tilde{l},\tilde{m}}_E \\
& -2 \sum_{\beta=e,o} < L^A_{\alpha,l,m}, L_{l',m'}\; L_{A;\beta,\tilde{m},\tilde{m}} >_{L_2}\; (y^E_{v,l',m'}\; x^{\beta,\tilde{l},\tilde{m}}_E)' \\
& +2 \sum_{\beta,\gamma=e,o} < L^A_{\alpha,l,m}, L^B_{\beta,l',m'}\; D_A L_{B;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{\beta,l',m'}\; x^{\gamma,\tilde{l},\tilde{m}}_E \\
& +2\sqrt{l(l+1)} \sum_{\beta,\gamma=e,o} \delta^e_\alpha\; < L_{l,m}, L^A_{\beta,l',m'}\; L_{A;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{\beta,l',m'}\; x^{\gamma,\tilde{l},\tilde{m}}_E \\
& -2 \sum_{\beta=e,o} < L^A_{\alpha,l,m}, L^B_{\beta,l',m'}\; L_{AB;h,\tilde{m},\tilde{m}} >_{L_2}\; (y^E_{\beta,l',m'}\; x^{h,\tilde{l},\tilde{m}}_E)' \\
& + \sum_{\beta,\gamma=e,o} < L^A_{\alpha,l,m}, L^{BC}_{\beta,l',m'}\; D_A\; L_{BC;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; Y^E_{\beta,l',m'}\; X^{\gamma,\tilde{l},\tilde{m}}_E \\
& + \sum_{\beta=e,o} < L^A_{\alpha,l,m}, L^{BC}_{\beta,l',m'}\; D_A\; L_{BC;h,\tilde{m},\tilde{m}} >_{L_2}\; Y^E_{\beta,l',m'}\; x^{h,\tilde{l},\tilde{m}}_E \\
& + \sum_{\gamma=e,o} < L^A_{\alpha,l,m}, L^{BC}_{h,l',m'}\; D_A\; L_{BC;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\; X^{\gamma,\tilde{l},\tilde{m}}_E \\
& + < L^A_{\alpha,l,m}, L^{BC}_{h,l',m'}\; D_A\; L_{BC;h,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\; x^{h,\tilde{l}\tilde{m}}_E \\
& +2 \sum_{\beta,\gamma=e,o} < D_B\; L^A_{\alpha,l,m}, L^{BC}_{\beta,l',m'}\; L_{CA;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; Y^E_{\beta,l',m'}\; X^{\gamma,\tilde{l},\tilde{m}}_E \\
& +2 \sum_{\beta=e,o} < D_B\; L^A_{\alpha,l,m}, L^{BC}_{\beta,l',m'}\; L_{CA;h,\tilde{m},\tilde{m}} >_{L_2}\; Y^E_{\beta,l',m'}\; x^{h,\tilde{l},\tilde{m}}_E \\
& +2 \sum_{\gamma=e,o} < D_B\; L^A_{\alpha,l,m}, L^{BC}_{h,l',m'}\; L_{CA;\gamma,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\; X^{\gamma,\tilde{l},\tilde{m}}_E \\
& +2\; < D_B\; L^A_{\alpha,l,m}, L^{BC}_{h,l',m'}\; L_{CA;h,\tilde{m},\tilde{m}} >_{L_2}\; y^E_{h,l',m'}\; x^{h,\tilde{l},\tilde{m}}_E \\
& +\sqrt{l(l+1)}\; < L^A_{\alpha,l,m}, L_{l',m'}\; L_{A;e,\tilde{m},\tilde{m}} >_{L_2}\; Y^{KG}_{l',m'}\; X^{\tilde{l},\tilde{m}}_{KG} \\
& + \sum_{\beta,\gamma=e,o} \epsilon_{\beta\gamma} < L^A_{\alpha,l,m}, L_{A;\gamma,l',m'}\; L_{\tilde{m},\tilde{m}} >_{L_2}\; Y^M_{\gamma,l',m'}\; \tilde{X}^{h,\tilde{l},\tilde{m}}_M \\
& - \sum_{\beta=e,o} \epsilon_{\beta\gamma} < L^A_{\alpha,l,m}, L_{l',m'}\; L_{A,\beta,\tilde{m},\tilde{m}} >_{L_2}\; \tilde{Y}^M_{h,l',m'}\; (\tilde{X}^{\beta,\tilde{l},\tilde{m}}_M)'] \} \\
=: \; & g^{\alpha,l,m}\; \{Z_{\alpha,l,m(1)}((p^E_v, x^\alpha_E), (y^E_\alpha, q^v_E), (y^E_h \delta^e_\alpha, q^h_E), (Y^E_\alpha, q^h_E), (P^{KG}, \delta^e_\alpha X_{KG}), (P^M_h, X^\alpha_M)) \\
& +Z_{\alpha,l,m(2)}((y^E, x_E), (Y^E, X_E), (Y^E, x_E), (y^E, X_E), (Y^{KG}, X_{KG}), (Y^M, X_M))\}
\end{aligned} \tag{133}
$$

where we used the identities (10). The notation is that $C_{h(n)},\ Z_{\alpha,l,m(n)};\ \alpha \in \{h,e,o\}$ are the collection of all terms of order $n = 0,1,2$ in the perturbations x, y, X, Y and we displayed the pairs of variables on which the constraints depend (either a pair of two symmetric, or two non-symmetric or mixed degrees of freedom). We see that $C_{h(1)} = Z_{\alpha,l,m(0)} = 0;\ \alpha \in \{h,e,o\}$. We also note that $C_{h(2)} = \sum_{l,m}\ C_{h,l,m(2)}$ and just like $Z_{\alpha,l,m(1)},\ \alpha = h,e,o$ the contribution $C_{h,l,m(2)}$ just depends on perturbation variables labeled by l,m. By contrast, the constraints

$Z_{\alpha,l,m(2)}$, $\alpha = h, e, o$ are "non-local", i.e., depend not only on variables labeled by l, m but, in general, on an infinite number of them because the triangle inequality $|\tilde{l} - l'| \leq l \leq \tilde{l}' + l$ admits an infinite number of solutions $\tilde{l}, l'$ for any given l, e.g., $\tilde{l} = l' + l,\ l' \in \mathbb{N}$. We display the "colour" label v, h, e, o for the pairs of variables that occur for $C_{h(0)},\ C_{h,l,m(2)}, Z_{\alpha,l,m(1)}$ but drop it in $Z_{\alpha,l,m(2)}$ although not all possible pairs occur in order to make the notation not too heavy.

Note, that (130) is the *exact* expression for the spatial diffeomorphism constraint, no terms have been dropped. We have just written it in terms of the split variables. The explicit computation of the coefficients will be carried out in our companion papers [67–69].

5.3. General Perturbative Structure of the Hamiltonian Constraint

As emphasized in Section 2.3 it is of considerable computational advantage to decompose the polynomial constraint $[\det(m)]^{5/2}\ V_0$ displayed in (11) with respect to the perturbations x, y, X, Y which for vanishing potential U is just a polynomial of order ten. This is because it remains a polynomial rather than an infinite series as long as the potential is a polynomial in ϕ. Still, working out all orders explicitly is a tedious task both algebraically and because one needs to perform iterated Clebsch–Gordan decompositions, i.e., we need the general coefficient $\mathrm{Tr}(< \prod_{k=0}^{N} L_k >)$ where N is the top polynomial degree that occurs, each L_k is a spherical harmonic (scalar, vector, tensor) and the trace and expectation value indicate contraction of all spherical tensor indices and integration on the sphere, respectively. We thus, just display the terms of order zero, one and two. In particular, we need

$$f^v\ C_v = f^v\ < 1, [\det(m)]^{5/2}\ V_0\ \omega^{-6} >_{L_2},\quad g^{v,l,m}\ Z_{v,l,m} = g^{v,l,m}\ < L_{l,m}, [\det(m)]^{5/2}\ V_0\ \omega^{-6} >_{L_2} \tag{134}$$

to those orders and it is clear from Section 2 that $C_{v(1)} = Z_{v,l,m(0)} = 0$.

All terms in $[\det(m)]^{5/2}\ V_0$ except for the curvature term contain two or three factors of

$$\begin{aligned} M &:= \det(m) = \frac{1}{3!}\ \epsilon^{\mu\nu\rho}\epsilon^{\mu'\nu'\rho'}\ m_{\mu\mu'}\ m_{\nu\nu'}\ m_{\rho\rho'} \\ &= \frac{1}{2}\epsilon^{AC}\epsilon^{BD}\ [m_{33}\ m_{AB}\ m_{CD}\ - 2\ m_{3A}\ m_{3B}\ m_{CD}] = \omega^2\frac{1}{2}\eta^{AC}\eta^{BD}\ [m_{33}\ m_{AB}\ m_{CD}\ - 2\ m_{3A}\ m_{3B}\ m_{CD}] \end{aligned} \tag{135}$$

We also need

$$\begin{aligned} M^{\mu\mu'} &:= \det(m)\ m^{\mu\mu'} = \frac{1}{2}\ \epsilon^{\mu\nu\rho}\epsilon^{\mu'\nu'\rho'}\ m_{\nu\nu'}\ m_{\rho\rho'} \\ M^{33} &= \frac{1}{2}\epsilon^{AC}\epsilon^{BD}\ m_{AB}\ m_{CD} = \omega^2\frac{1}{2}\eta^{AC}\eta^{BD}\ m_{AB}\ m_{CD} \\ M^{3A} &= -\epsilon^{AC}\ \epsilon^{BD}\ m_{3B}\ m_{CD} = -\omega^2\ \eta^{AC}\ \eta^{BD}\ m_{3B}\ m_{CD} \\ M^{AB} &= \epsilon^{AC}\epsilon^{BD}\ [m_{33}\ m_{CD} - m_{3C}\ m_{3D}] = \omega^2\eta^{AC}\eta^{BD}\ [m_{33}\ m_{CD} - m_{3C}\ m_{3D}] \end{aligned} \tag{136}$$

Next, we compute $[\det(m)]^3$ times the Ricci scalar

$$R = 2\ m^{\mu\rho}\ [-\partial_{[\mu}\ \Gamma^{\nu}_{\nu]\rho} + \Gamma^{\lambda}_{\rho[\mu}\ \Gamma^{\nu}_{\nu]\lambda}] \tag{137}$$

which after some algebra yields

$$\begin{aligned} U^E &:= M^3\ R \\ &= M^{\mu\rho}\ m_{\lambda\mu,\rho}\ [M\ M^{\nu\lambda}_{,\nu} - \frac{1}{2}\ M_{,\nu}\ M^{\nu\lambda}] - \frac{1}{2}\ M\ M^{\mu\nu}\ M_{,\mu\nu} + \frac{3}{4}\ M^{\mu\nu}\ M_{,\mu}\ M_{,\nu} - \frac{1}{2}\ M\ M^{\mu\nu}_{,\nu}\ M_{,\mu} \\ &\quad - M^{\mu\rho}\ M^{\nu\lambda}\ M^{\sigma\tau}\ \Gamma_{\nu\mu\sigma}\ \Gamma_{\tau\rho\lambda} \end{aligned} \tag{138}$$

which is manifestly a homogeneous polynomial of order eight. We refrain from computing its low-order expression explicitly as they do not involve momenta and just denote them as

$$\omega^6\ [U^E_{(0)}(q^v_E, q^h_E) + U^E_{(1)}(q^v_E, q^h_E, x_E, X_E) + U^E_{(2)}(q^v_E, q^h_E, x_E, X_E)] \tag{139}$$

where all three terms are scalars of density weight zero with respect to S^2.

We discuss the expansion to order two of the various other terms separately denoting by $[.]_{(n)}$ the homogeneous n-th order contribution of [.] and dropping terms of order three or higher

$$\begin{aligned} & [M^2]\ [m_{\mu\rho}\ m_{\nu\sigma} - \frac{1}{2}\ m_{\mu\nu} m_{\rho\sigma}]\ [W^{\mu\nu}\ W^{\rho\sigma}] \\ = & \sum_{r,s,n\geq 0, r+s+n\leq 2} [M^2]_{(r)}\ [m_{\mu\rho}\ m_{\nu\sigma} - \frac{1}{2}\ m_{\mu\nu} m_{\rho\sigma}]_{(s)}\ [W^{\mu\nu}\ W^{\rho\sigma}]_{(n)} \end{aligned} \tag{140}$$

We have

$$\begin{aligned} M_{(0)} &= q^v_E\ (q^h_E)^2\ \omega^2 \\ M_{(1)} &= [m_{33(1)}\ (q^h_E)^2 + q^v_E\ q^h_E\ \Omega^{AB}\ m_{AB(1)}]\ \omega^2 \\ M_{(2)} &= [m_{33(1)}\ q^h_E\ \Omega^{AB}\ m_{AB(1)} + + \frac{1}{2}\ m_{33(0)}\ \eta^{AC}\ \eta^{BD}\ m_{AB(1)}\ m_{CD(1)}\ - q^h_E\ \Omega^{AB}\ m_{3A(1)}\ m_{3B(1)}]\ \omega^2 \end{aligned} \tag{141}$$

and thus

$$[M^2]_{(0)} = [M_{(0)}]^2,\ [M^2]_{(1)} = 2\ [M_{(0)}]\ [M_{(1)}],\ [M^2]_{(2)} = [M_{(1)}]^2 + 2\ [M_{(0)}]\ [M_{(2)}], \tag{142}$$

Likewise exactly

$$\begin{aligned} M^{33} &= \omega^2 \frac{1}{2}[2\ (q^h_E)^2 + 2\ (q^h_E)\ \Omega^{AB}\ m_{AB(1)} + \eta^{AC}\eta^{BD}\ m_{AB(1)}\ m_{CD(1)}] \\ M^{3A} &= -\omega^2\ [q^h_E\ \Omega^{AB}\ m_{3B(1)} + \eta^{AC}\ \eta^{BD}\ m_{3B(1)}\ m_{CD(1)}] \\ M^{AB} &= \omega^2\ \{\Omega^{AB}\ (q^v_E)\ (q^h_E) + [\Omega^{AB}\ m_{33(1)}\ (q^h_E) + +\eta^{AC}\eta^{BD}\ (q^v_E)\ m_{CD(1)}] \\ & \quad +\eta^{AC}\eta^{BD}\ [m_{33(1)}\ m_{CD(1)} - m_{3C(1)}\ m_{3D(1)}]\} \end{aligned} \tag{143}$$

Next we have the exact result

$$\begin{aligned} W &:= m_{\mu\nu}\ W^{\mu\nu} = m_{33} W^{33} + 2\ m_{3A}\ W^{3A} + m_{AB}\ W^{AB} \\ &= [q^v_E\ p^v_E + q^h_E\ p^E_h]\ \omega + [m_{33(1)}\ p^v_E\ \omega + q^v_E\ W^{33}_{(1)} + + q^h_E\ \Omega_{AB}\ W^{AB}_{(1)} + + \frac{1}{2}\ m_{AB(1)}\ \Omega^{AB}\ p^E_h\ \omega] \\ & \quad +[m_{33(1)}\ W^{33}_{(1)} + 2\ m_{3A(1)}\ W^{3A}_{(1)} + m_{AB(1)}\ W^{AB}_{(1)}] =: W_{(0)} + W_{(1)} + W_{(2)} \end{aligned} \tag{144}$$

and thus up to the second order

$$W^2 = [W_{(0)}]^2 + [2\ W_{(0)}\ W_{(1)}] + [W^2_{(1)} + 2\ W_{(0)}\ W_{(2)}] \tag{145}$$

Next, we have the exact expression

$$\begin{aligned} T^E &:= m_{\mu\rho}\ m_{\nu\sigma}\ W^{\mu\nu}\ W^{\rho\sigma} \\ &= [m_{33}\ W^{33}]^2 + 4\ [m_{33}\ W^{33}]\ [m_{3A}\ W^{3A}] + 2\ [m_{3A}\ W^{3A}]^2 \\ & \quad +2\ m_{33}\ [m_{AB}\ W^{3A}\ W^{3B}] + 2\ W^{33}\ [W^{AB}\ m_{3A}\ m_{3B}] \\ & \quad +4\ m_{3A}\ P^{AB}\ m_{BC}\ W^{3C} + m_{AC}\ m_{BD}\ W^{AB}\ W^{CD} \end{aligned} \tag{146}$$

It follows to second order

$$
\begin{aligned}
T^E_{(0)} &= \omega^2([q^v_E\; p^E_v]^2 + \frac{1}{2}[q^h_E\; p^E_h]^2) \qquad (147)\\
T^E_{(1)} &= \omega\; [2\; (q^v_E\; p^E_v)\; (q^v_e\; W^{33}_{(1)} + m_{33(1)}\; p^E_v) + 2\; \omega\; \Omega^{AB}\; m_{AB(1)}\; (p^E_h)^2 + 2\; \Omega_{AB}\; W^{AB}_{(1)}\; (q^h_E E)^2]\\
T^E_{(2)} &= 2\; \omega (q^v_E\; p^E_v)\; m_{33(1)}\; W^{33}_{(1)} + (q^v_e\; W^{33}_{(1)} + \omega\; m_{33(1)}\; p^E_v)^2\\
&\quad +4\; \omega\; [q^v_E\; p^E_v]\; [m_{3A(1)}\; W^{3A}_{(1)}] + 2\; [q^v_E\; q^h_E]\; \Omega_{AB}\; W^{3A}_{(1)}\; W^{3B}_{(1)} + 2\; \omega^2\; [p^E_v\; p^E_h]\; \Omega^{AB}\; m_{3A(1)}\; m_{3B(1)}\\
&\quad +4\; \omega\; [q^h_E\; p^E_h]\; m_{3A(1)}\; W^{3C}_{(1)}\\
&\quad +\omega^2\; (p^E_h)^2\; m_{AC(1)}\; m_{BD(1)}\; \Omega^{AB}\; \Omega^{CD} + (q^h_E)^2\; \Omega_{AC}\; \Omega_{BD}\; W^{AB}_{(1)}\; W^{CD}_{(1)} + 4\omega\; q^h_E\; p^E_h\; m_{AB(1)}\; W^{AB}_{(1)}
\end{aligned}
$$

As far as the matter contributions are concerned we note that these are up to second order (we consider for concreteness only the uncharged case, the charged case can be treated analogously)

$$
\begin{aligned}
&\quad 2\; M^2\; T^{KG} = M^2\; \pi^2\\
&= [\omega^2\; [M^2]_{(0)}\; (P^{KG})^2] + 2\; \omega\; [M^2]_{(0)}\; P^{KG}\; \pi_{(1)} + \omega^2\; [M^2]_{(1)}\; (P^{KG})^2]\\
&\quad +[+\omega^2\; [M^2]_{(2)}\; (P^{KG})^2 + +\omega\; [M^2]_{(1)}\; P^{KG}\; \pi_{(1)} + [M^2]_{(0)}\; (\pi_{(1)})^2]\\
&\quad 2\; U^{KG} := M^{\mu\nu}\; \phi_{,\mu}\; \phi_{,\nu} = M^{33}\; (\phi')^2 + 2\; M^{3A}\; \phi'\; (D_A\phi) + M^{AB}\; (D_A\phi)\; (D_B\phi)\\
&= [M^{33}_{(0)}\; (Q'_{KG})^2] + [M^{33}_{(1)}\; (Q'_{KG})^2 + 2M^{33}_{(0)}\; (Q'_{KG})\; (\phi'_{(1)})]\\
&\quad +[M_{33(2)}\; (Q'_{KG})^2 + M_{33(0)}\; (\phi'_{(1)})^2 + +2\; M_{33(1)}\; (Q'_{KG})\; (\phi'_{(1)}) + 2\; M^{3A}_{(1)}\; (Q'_{KG}\; (D_A\phi_{(1)})\\
&\quad +M^{AB}_{(0)}\; (D_A\phi_{(1)})\; (D_B\phi_{(1)})]\\
&\quad M^2\; U^{KG} = \sum_{r+s\le 2} [M^2]_{(r)}\; A_{(s)}\\
&\quad V(\phi) = V(Q_{KG}) + V'(Q_{KG})\; \phi_{(1)} + \frac{1}{2}V''(Q_{KG})\; (\phi_{(1)})^2\\
&\quad 4\; T^M = m_{\mu\nu}\; E^\mu\; E^\nu\\
&= m_{33}\; (E^3)^2 + 2\; m_{3A}\; E^3\; E^A + m_{AB}\; E^A\; E^B\\
&= [q^v_E\; (P^M_h)^2] + [m_{33(1)}\; (P^M_h)^2 + 2\; (q^v_E)\; (P^h_M)\; (E^3_{(1)})]\\
&\quad +[m_{33(0)}\; (E^3_{(1)})^2 + 2\; m_{33(1)}\; (P^M_h)\; E^3_{(1)} + 2m_{3A(1)}\; (P^M_h)\; E^A_{(1)} + (q^h_E)\; \Omega_{AB}\; E^A_{(0)}\; E^B_{(1)}]\\
&\quad 4\; U^M = m_{\mu\nu}\; B^\mu\; B^\nu\\
&= q^v_E\; (B^3_{(1)})^2 + q^h_E\; \Omega_{AB}\; B^A_{(1)}\; B^B_{(1)} \qquad (148)
\end{aligned}
$$

It remains to compute zeroth, first and second order of $\tilde{V}_0 := [\det m]^{5/2}\; V_0$ where for the purposes of this paper it will be sufficient to consider

$$
C_v :=< 1, \tilde{V}_0/\omega^6 >_{L_2} = C_{v(0)} + C_{v(2)} + \ldots\;,\quad Z_{v,l,m} :=< L_{l,m}, \tilde{v}_0/\omega^6 >_{L_2} = Z_{v,l,m(1)} + \ldots \qquad (149)
$$

because we wish to compute the reduced Hamiltonian only up to second order for which the solution of C_a to second order and of Z_j to first order is required. Accordingly,

$$
\begin{aligned}
C_{v(0)} &= C^E_{v(0)} + C^{KG}_{v(0)} + C^M_{v(0)}\\
C_{v(2)} &= C^E_{v(2)} + C^{KG}_{v(2)} + C^M_{v(2)}\\
Z_{v,l,m(1)} &= Z^E_{v,l,m(1)} + C^{KG}_{v,l,m(1)} + C^M_{v,l,m(1)} \qquad (150)
\end{aligned}
$$

and we find to zeroth order

$$
\begin{aligned}
C^E_{v(0)}\ \omega^6 &= [M^2]_{(0)}\ [T^E_{(0)} - \frac{1}{2}\ [W^2]_{(0)}] - U^E_{(0)} \\
&= \omega^6\ [q^E_v\ (q^h_E)^2]^2\ \{[q^v_E\ p^E_v]^2 + \frac{1}{2}[q^h_E\ p^E_h]^2) - \frac{1}{2}[q^v_E\ p^v_E + q^h_E\ p^E_h]^2\} - \omega^6\ U^E_{(0)} \\
2\ C^{KG}_{v(0)}\ \omega^6 &= [M^2]_{(0)}\ [\pi^2]_{(0)} + [M^2]_{(0)}\ U^{KG}_{(0)} + 2\ [M^3]_{(0)}\ V_{(0)} \\
&= \omega^6\ [q^E_v\ (q^h_E)^2]^2\ \{(P^{KG})^2 + (q^h_E)^2\ (Q'_{KG})^2 + 2[q^E_v\ (q^h_E)^2]\ V(Q_{KG})\} \\
4C^M_{v(0)}\ \omega^6 &= [M^2]_{(0)}\ T^M_{(0)} = \omega^6\ [q^E_v\ (q^h_E)^2]^2\ q^v_E\ (P^M_h)^2
\end{aligned} \tag{151}
$$

The higher orders will be worked out in our companion papers.

6. Perturbative Construction of the Reduced Hamiltonian

We first provide the general strategy and then display the details for the zeroth, first and second order.

6.1. Overview

We follow the general procedure of [61]: Adapted to the present situation, it consists the following steps:

1. We denote by $(.)_{(n)}$ the homogenous n-th order contribution of $(.)$ with respect to an expansion into the perturbations (which are considered of first order):
   a. $x_E^{\alpha,l,m},\ y^E_{\alpha,l,m};\ \alpha = v,h,e,o;\ l \geq 1$
   b. $X_E^{\alpha,l,m},\ Y^E_{\alpha,l,m};\ \alpha = e,o;\ l \geq 2$
   c. $X^{l,m}_{KG},\ Y^{KG}_{l,m};\ l \geq 1$
   d. $X_M^{\alpha,l,m},\ Y^M_{\alpha,l,m};\ \alpha = e,o;\ l \geq 1$.
2. Suppose that one solves the constraints $C_v, C_h, Z_{\alpha,l,m}; \alpha = v,h,e,o$ exactly for p^E_v, p^E_h, $y^E_{\alpha,lm}$, then that solution $\hat{p}^E_v, \hat{p}^E_h, \hat{y}^E_{\alpha,lm}$ can itself be expanded into the contributions b.-d. above. We write those expansions as $\hat{p}^E_\alpha = p^E_\alpha(0) + p^E_\alpha(2) + p^E_\alpha(3) + \ldots\ ;\ \alpha = v,h$ and $\hat{y}^E_{\alpha,l,m} = y^E_{\alpha,l,m}(1) + y^E_{\alpha,l,m}(2) + \ldots\ ;\ \alpha = v,h,e,o$, respectively, where $(.)_{(n)}$ means the homogeneous n-th order contribution of $(.)$ with respect to X, Y in b.-d.
3. Expand the constraints $C_v, C_h, Z_{\alpha,l,m}$ first with respect to all variables a.-d. for general $p^E_\alpha, y^E_{\alpha,l,m}$ and then in addition with respect to the decomposition of the solution $p^E_\alpha = \hat{p}^E_\alpha,\ y^E_{\alpha,l,m} = \hat{y}^E_{\alpha,l,m}$. Denote the n-th order homogeneous contribution with respect to that combined expansion by $C_{\alpha(n)},\ Z_{\alpha,l,m(n)}$ where by construction $C_{\alpha(1)} = Z_{\alpha,l,m(0)} = 0$ due to spherical symmetry.
4. Solve the symmetric, zeroth order constraints $C_{v(0)} = 0, C_{h(0)} = 0$ exactly for $p^E_v(0), p^E_h(0)$. The symmetric, first order constraints $C_{v(1)} \equiv 0, C_{h(1)} \equiv 0$ are equivalent to the statement that $p^E_v(1) = p^E_h(1) = 0$.
5. Solve the unsymmetric first order constraints $Z_{\alpha,l,m(1)} = 0,\ \alpha = v,h,e,o; l \geq 1, |m| \leq l$ for $y^E_{\alpha,l,m}(1)$ at $p^E_v = p_v(0),\ p^E_h = p^E_h(0)$.
6. Proceeding iteratively, by construction [61], for $n \geq 2$ the constraint contribution $C_{\alpha(n)}$ depends linearly on the $p^E_\beta(n)$ and polynomially on the $p^E_\beta(k),\ y^E_{\beta,l,m}(k)\ k \leq n-1$ while the constraint contribution $Z_{\alpha,l,m(n)}$ depends linearly on the $y^E_{\beta,l',m'}(n)$ and polynomially on the $p^E_\beta(k),\ y^E_{\beta,l',m'}(k)\ k \leq n-1$. Therefore, one can successively solve $C_{\alpha(n)}$ for $p^E_\beta(n)$ and $Z_{\alpha,l,m(n)}$ for $y^E_{\beta,l',m'(n)}$.
7. In this way, one perturbatively determines the Abelianised form of the constraints

$$\begin{aligned} \hat{C}_\alpha &= p^E_\alpha + h_\alpha, \;\; h_\alpha = -\sum_{1\neq n=0}^{\infty} p^E_\alpha(n), \;\; \alpha = v,h \\ \hat{Z}_{\alpha,l,m} &= y^E_{\alpha,l,m} + h_{\alpha,l,m}, \;\; h_{\alpha,l,m} = -\sum_{n=1}^{\infty} y^E_{\alpha,l,m}(n), \;\; \alpha = v,h,e,o \end{aligned} \tag{152}$$

8. For the reduced Hamiltonian we are supposed to evaluate (152) in the GPG $q^v = q_{33} = 1, \; q^h = \Omega^{AB} q_{AB}/2 = r^2, q^A = q_{3A} = 0$. Therefore, we may solve (152) already with GPG installed.
9. The reduced Hamiltonian is then given for each asymptotic end by (113) (we drop constant pre-factors)

$$H_{\rm red} = \lim_{r\to\infty} \frac{1}{r} \, [h_v(r)^2 + \sum_{l>0,\,|m|\le l} h_{v,l,m}(r)^2] \tag{153}$$

which follows from $P^3 = p_v + \sum_{l,m} y_{v,l,m} L_{l,m}$. Using the expansion of $h_v, h_{v,l,m}$ into the $p_v(n), \; y_{v,l,m}(n)$ one can compute $H_{\rm red}$ to any desired order of accuracy. The decay condition on the y^E_α stated in Section 4 in fact implies that the $h_{v,l,m}$ contributions in (153) vanish as $r \to \infty$.

6.2. Zeroth Order

At zeroth order, we just need to solve the zeroth order of the symmetric parts of the constraints for the zeroth orders $p^E_h(0), \; p^E_v(0)$ which are (we drop the label "0" for p^E_h, p^E_v and evaluate at GPG)

$$\begin{aligned} C_{h(0)} &= -2(q_{33(0)} P^{33})' - P^{33} \, q'_{33(0)} + q'_{AB(0)} \, P^{AB} + \pi_{0)} \, \phi'_{(0)} \\ &= -2(p^E_v \, q^v_E)' - p^E_v \, (q^v_E)' + p^h) E \, (q^h_E)' + P^{KG} \, Q'_{KG} \\ &= -2(p^E_v)' + 2r \, p^h_E + P^{KG} \, Q'_{KG} \\ C_{v(0)} &= \frac{1}{\sqrt{\det(q)_{(0)}}} [(q_{33(0)} \, P^{33})^2 + q_{AC(0)} q_{BD(0)} \, P^{AB} \, P^{CD} - \frac{1}{2} (q_{33(0)} P^{33} + q_{AB(0)} P^{AB})^2] \sqrt{\det(q)_{(0)}} \, R[q]_{(0)} \\ &+ \frac{1}{2} [\frac{\pi^2_{(0)}}{\sqrt{\det(q)}_{(0)}} + \sqrt{\det(q)_{(0)}} \, (q^{33}_{(0)} \, (\phi'_{(0)})^2 + 2 \, V(\phi_{(0)})] + \frac{1}{2} \sqrt{\det(q)_{(0)}} \, q_{33(0)} \, (E^3_{(0)})^2 \\ &= \frac{1}{\sqrt{q^v_E (q^h_E)^2}} \, [(q^v_E \, p^v_E)^2 + \frac{1}{2} \, (q^h_E)^2 \, (p^E_h)^2 - \frac{1}{2} (q^v_E \, p^E_v + q^h_E \, p^E_h)^2] \sqrt{\det(q)_{(0)}} \, R[q]_{(0)} \\ &+ \frac{1}{2} [\frac{(P^{KG})^2}{\sqrt{q^v_E \, (q^h_E)^2}} + \sqrt{q^v_E \, (q^h_E)^2} \, (q^E_v \, (Q'_{KG})^2 + 2 \, V(Q_{KG})] + \frac{1}{2\sqrt{q^v_E \, (q^h_E)^2}} \, q^v_E \, (P^M)^2 \\ &= \frac{1}{r^2} \, [(p^v_E)^2 + \frac{1}{2} \, r^4 \, (p^E_h)^2 - \frac{1}{2} (p^E_v + r^2 \, p^E_h)^2] \\ &+ \frac{1}{2} [\frac{(P^{KG})^2}{r^2} + r^2 \, (q^E_v \, (Q'_{KG})^2 + 2 \, V(Q_{KG})] + \frac{1}{2 \, r^2} \, (P^M)^2 \\ &= \frac{1}{2 \, r^2} [(p^v_E)^2 - 2 \, r^2 \, p^E_h \, p^E_v] \\ &+ \frac{1}{2} [\frac{(P^{KG})^2}{r^2} + r^2 \, (Q'_{KG})^2 + 2 \, V(Q_{KG})] + \frac{1}{2 \, r^2} \, (P^M)^2 \end{aligned} \tag{154}$$

We solve $C_{h(0)}$ for p^E_h

$$p^E_h = \frac{1}{r^2} \, [2 \, (p^E_v)' - I_{KG}]; \; I^{KG}_{(0)} := P^{KG} \, Q'_{KG} \tag{155}$$

and insert this into $C_{v(0)}$

$$\begin{aligned} C_{v(0)} &= \frac{1}{2\,r^2}[(p_E^v)^2 - 2\,r^2\,p_v^E\,[2\,(p_v^E)' - I_{(0)}^{KG}]) \\ &\quad + \frac{1}{2\,r^2}[(P^{KG})^2 + r^4\,(Q'_{KG})^2 + 2\,V(Q_{KG})] + \frac{1}{2\,r^2}\,(P^M)^2 \\ &= \frac{1}{2\,r^2}[\{(p_E^v)^2 - 2\,r^2\,[(p_v^E)^2]'\} + p_v^E\,I_{(0)}^{KG}] \\ &\quad + \frac{1}{2\,r^2}\{(P^{KG})^2 + r^4\,(Q'_{KG})^2 + 2\,V(Q_{KG}) + (P^M)^2\} \\ &=: -\frac{1}{2}\,[\frac{(p_v^E)^2}{r}]' + p_v^E\,I_{(0)}^{KG} + E_{(0)}^{KG} + E_{(0)}^M \end{aligned} \tag{156}$$

where $I_{(0)}^{KG}$ is the symmetric part of the Klein–Gordon momentum density and $E_{(0)}^{KG}$, $E_{(0)}^M$ the symmetric part of the Klein–Gordon and Maxwell energy density, respectively.

The equation $C_{v(0)} = 0$ is solvable in closed form if there is no scalar "hair" (exploiting that P^M is a spatial constant)

$$\frac{(p_v^E)^2}{2r} = \hat{M} - \frac{(P^M)^2}{r} \tag{157}$$

where $\hat{M}$ is the mass of the black hole and $\sqrt{2}\,P^M$ its electric charge. Indeed in GPG one can easily check that the information about mass and charge resides in the extrinsic curvature part of the initial data.

In the presence of scalar hair, we solve (156) by the Picard–Lindelöf method. Let us introduce the abbreviations

$$z := \frac{p_v^E}{\sqrt{r}},\ a := I_{(0)}^{KG}\,\sqrt{r},\ b := E_{(0)}^{KG} + E_{(0)}^M \tag{158}$$

to cast (156) into the ODE

$$z' = a + \frac{b}{z} \tag{159}$$

or equivalently into the integral equation

$$z(r) = z_0 + \int_{r_0}^r ds\,[a(s) + \frac{b(s)}{z(s)}] \tag{160}$$

(with $z(r_0) = z_0$ an integration constant) which can be iterated. To solve that iteration we expand (essentially an inverse square root of core mass $\hat{M}$ expansion)

$$z(r) = z_0 + \sum_{N=0}^{\infty} C_N(r)\,z_0^{-N} \tag{161}$$

and compare coefficients. Introducing the abbreviations

$$A(r) := \int_{r_0}^r ds\,a(s),\ B(r) := \int_{r_0}^r ds\,b(s) \tag{162}$$

one finds by expanding the geometric sums

$$z(r) = A(r) + \frac{B(r)}{z_0} + \frac{1}{z_0}\sum_{M=1}^{\infty}(-1)^M \sum_{n_1,\ldots,n_M=1}^{\infty} z_0^{-[n_1+\ldots+n_M]} \int_{r_0}^r ds\,b(s)\prod_{k=1}^{M} C_{n_k-1}(s) \tag{163}$$

i.e., for $N \geq 2$

$$C_0 = A,\ C_1 = B,\ C_N = \sum_{M=1}^{\infty} (-1)^M \sum_{n_1,\ldots,n_M=1}^{\infty} \delta_{N-1,n_1+\ldots+n_M}\, \zeta_{n_1,\ldots,n_M}$$

$$\zeta_{n_1,\ldots,n_M} = \int_{r_0}^{r} ds\, b(s) \prod_{k=1}^{M} C_{n_k-1}(s) \tag{164}$$

where $\zeta_{n_1,\ldots,n_M}$ is completely symmetric.

The hierarchy can be solved iteratively: For each N we have $M \leq N-1$ since $n_k \geq 1$, hence at most finitely many terms survive in (165). At the same time, even for $M = 1$ we have $n_1 = N-1$ and thus at most C_{N-2} appears on the right-hand side of (165). The first few terms are

$$\begin{aligned} C_2 &= -\zeta_1 = -\int_{r_0}^{r} ds\, b(s)\, A(s) \\ C_3 &= -\zeta_2 + \zeta_{1,1} = \int_{r_0}^{r} ds\, b(s)\, [A(s)^2 - B(s)] \\ C_4 &= -\zeta_3 + 2\,\zeta_{1,2} - \zeta_{1,1,1} = \int_{r_0}^{r} ds\, b(s)\, [-C_2(s) + 2\, A(s)\, B(s) - A(s)^3] \end{aligned} \tag{165}$$

We see that the coefficients C_n are polynomials in P^{KG}, Q_{KG}, P^M which appear in nested integrals with respect to the radial coordinate. Note, that for a discharged black hole z_0 is simply $\sqrt{\hat{M}}$ which is a constant of motion when the metric does not depend on the momentum conjugate to $\hat{M}$. This means that for large $\hat{M}$ the inverse core mass expansion remains a good approximation also during time evolution as one expects the perturbation contributions to the nested energy integrals to be much smaller than $\hat{M}$.

6.3. First Order

We now consider $p_v^E(0), p_h^E(0)$ to be explicitly known via (158), (160) and (163) and insert these as well as $p_v^E(1) := 0,\ p_h^E(1) := 0$ into the first-order expansions $Z_{\alpha,l,m(1)}$; $\alpha = v, h, e, o$. Dropping the labels $_{(0)}$ and $_{(1)}$ for $p_\alpha^E(0), y_{\alpha,lm,}^E(1)$ we find in the GPG with $\alpha = e, o$

$$\begin{aligned} Z_{h,l,m(1)} &= -(2(q_E^v\, y_{v,l,m}^E)' + (q_E^v)'\, y_{v,l,m}^E) + \sqrt{2}\, (q_E^h)'\, y_{h,l,m}^E + \sqrt{l(l+1)}\, q_E^v\, y_{e,l,m}^E + Z_{h,l,m(1)}^R \\ &= -2(y_{v,l,m}^E)' + 2\, r\, \sqrt{2}\, y_{h,l,m}^E + \sqrt{l(l+1)}\, y_{e,l,m}^E + Z_{h,l,m(1)}^R \\ Z_{\alpha,l,m(1)} &= -(q_E^h\, y_{\alpha,l,m}^E)' + \sqrt{2l(l+1)}\, q_E^h\, \delta_\alpha^e\, y_{h,l,m}^E + Z_{\alpha,l,m(1)}^R \\ &= -(r^2\, y_{\alpha,l,m}^E)' + \sqrt{2l(l+1)}\, r^2\, \delta_\alpha^e\, y_{h,l,m}^E + Z_{\alpha,l,m(1)}^R \\ Z_{v,l,m(1)} &= [q_E^v q_E^h]^2\, \{2(q_E^v)^2\, p_v^E\, y_{v,l,m}^E + \frac{1}{\sqrt{2}}(q_E^h)^2\, p_h^E\, y_{h,l,m}^E \\ &\quad +(q_E^v\, p_v^E\ + q_E^h\, p_h^E)\ + (q_E^v\, y_{v,l,m}^E\ + \frac{1}{\sqrt{2}}\, q_E^h\, y_{h,l,m}^E)\} + Z_{v,l,m(1)}^R \\ &= r^8\, \{\{2p_v^E\, y_{v,l,m}^E + \frac{1}{\sqrt{2}} r^4\ \ p_h^E\, y_{h,l,m}^E \\ &\quad -(p_v^E + r^2 p_h^E)\ + (y_{v,l,m}^E\ + \frac{r^2}{\sqrt{2}}\, y_{h,l,m}^E)\} + Z_{v,l,m(1)}^R \end{aligned} \tag{166}$$

Here, the remainder $Z_{\alpha,l,m(1)}^R$ depends on q_E^v, q_E^h polynomially, on $p_v^E(0), p_h^E(0)$ quadratically, on P^{KG}, Q_{KG}, P^M quadratically, on $x_E^{\alpha,l,m}$; $\alpha = v, h, e, o$ linearly (but is set to zero in GPG), on $Y_{\alpha,l,m}^E$, $X_E^{\alpha,l,m}$; $\alpha = e, o$; $l \geq 2$ linearly and on $Y_{\alpha,l,m}^M$, $X_m^{\alpha,l,m}$; $\alpha = e, o$; $l \geq 1$ linearly.

The system (166) does not contain derivatives of $y^E_{h,l,m}$ and $y^E_{o,l,m}$ decouples from the system. We can, therefore, directly integrate

$$r^2\, y^E_{o,l,m} = Y^E_{o,l,m} + \int_0^r ds\; Z^R_{\alpha,l,m(1)}(s) \tag{167}$$

and solve $Z_{v,l,m(1)} = 0$ algebraically for $y^E_{h,l,m}$

$$\frac{r^2}{\sqrt{2}}\, p^E_h\, y^E_{h,l,m} = (p^E_v - r^2\, p^E_h)\, y^E_{v,l,m} + \frac{Z^R_{v,l,m(1)}}{r^8} \tag{168}$$

When inserted into the equations $Z_{h,l,m(1)} = Z_{e,l,m(1)} = 0$ we can cast the remaining system of ODE's into the form

$$\begin{bmatrix} y^E_{v,l,m} \\ y^E_{e,l,m} \end{bmatrix}' = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \cdot \begin{bmatrix} y^E_{v,l,m} \\ y^E_{e,l,m} \end{bmatrix} - \begin{bmatrix} Z^R_{v,l,m(1)} \\ Z^R_{e,l,m(1)} \end{bmatrix} \tag{169}$$

for certain known functions a, b, c, d that one can find from (166). The inhomogeneous linear system (169) which we write as $z' = A \cdot z + B$ is easily integrated in terms of the holonomy of the matrix valued function A

$$\mathrm{Hol}(r) = \mathcal{P}(e^{\int_0^r ds\; A(s)}) \tag{170}$$

where the path ordering symbol $\mathcal{P}$ orders the radial dependence of polynomials of $A(r)$ with the highst radius to the left. Then,

$$z(r) = \mathrm{Hol}(r)\; [\tilde{z}_0 + \int_0^r ds\; \mathrm{Hol}^{-1}(s)\; B(s)]\;\; \tilde{z}_0 = \begin{bmatrix} Y^E_{v,l,m} \\ Y^E_{e,l,m} \end{bmatrix} \tag{171}$$

Here, $Y^E_{\alpha,l,m},\ \alpha = v, e, o$ are integration constants. One may be worried that solving (168) introduces inverse powers of p^h_E and thus p^v_E. However, these inverse powers can again be expanded in terms of powers of the inverse core mass times polynomials in Q_{KG}, P^{KG}, P^M. We will show in our companion papers that these differential equations can be solved explicitly.

6.4. Second Order

We now consider $y_{\alpha,l,m}(1)$ to be explicitly known via (167), (168), (171) and insert the expansion $p^E_\alpha = p_\alpha(0) + p^E_\alpha(2);\ \alpha = e, o$ and $y^E_{\alpha,l,m} = y^E_{\alpha,l,m}(1) + y^E_{\alpha,l,m}(2)$ into $C_{\alpha(2)} = 0$ and $Z_{\alpha,l,m(2)} = 0$. In fact, since we just need to second-order $p^E_v =< 1, P^{33} >= p^E_v(0) + p^E_v(2)$ and thus $[p^E_v]^2 = [p^E_v(0)]^2 + 2\; p - v^E(0)\; p^E_v(2)$ it is sufficient to compute the linear order $y_{\alpha,l,m}(1)$ and insert it into $C_{v(2)}, C_{h(2)}$ which already allows to extract $p^E_v(2)$. We find in the GPG

$$\begin{aligned} C_{h(2)} &= -2\;(p^E_v(2)\; q^v_E)' - p^E_v(2)(q^v_E)' + p^E_h(2)\;(q^h_E)' + \tilde{C}_{h(2)} \\ &= -2\;(p^E_v(2)\; q^v_E)' + 2\; r\; p^E_h(2)\; + \tilde{C}_{h(2)} \\ C_{v(2)} &= [q^v_E(q^h_E)^2]^2\; [(q^v_E\; p^E_v(0))\; (\frac{1}{2}\; q^v_E\; p^E_v(2) - q^h_E\; p^h_E(2)) + q^v_E\; p^E_v(2))\; (\frac{1}{2}\; q^v_E\; p^E_v(0) - q^h_E\; p^h_E(0))] + \tilde{C}_{v(2)} \\ &= r^8\; [p^E_v(2)(p^E_v(0) - r^2\; p^E_h(0)) - r^2\; p^E_h(2)\; p^E_v(0)] + \tilde{C}_{v(2)} \end{aligned} \tag{172}$$

Here, $\tilde{C}_{v(2)}, \tilde{C}_{h(2)}$ depend quadratically on $y^E_{\alpha,l,m(1)},\ x^{\alpha,l,m}_E;\ \alpha = v, h, e, o$, on $Y^E_{\alpha,l,m},\ X^{\alpha,l,m}_E;$ $\alpha = e, o$, on $Y^{KG},\ X_{KG}$, on $Y^M_{\alpha,l,m},\ X^{\alpha,l,m}_M;\ \alpha = e, o$, on Q_{KG}, P^{KG}, P^M and polynomially on $q^\alpha_E,\ \alpha = v, h, e, o$ but we assume their gauge fixed values and set $x^{\alpha,l,m}_E = 0$. Similar to the zeroth order we solve the first equation in (172) algebraically for $p_{h(2)}$ and insert into the second. The result is a single linear inhomogeneous ODE for $p^E_v(2)$ which can be solved by standard methods. One has to divide by $p^E_v(0)$ in an intermediate step which upon an inverse mass expansion can be written again in terms of just polynomial fields to arbitrary precision. The details are contained in our companion papers [67–69].

7. Perturbative Structure of the Irreducible Mass

In this section, we show that the same perturbative scheme that one applies to the reduced Hamiltonian can be employed in order to compute the irreducible mass perturbatively whose dynamics we consider as a measure for mass loss due to Hawking radiation as we argued in Section 3. In the first subsection, we recall some of the notions associated with horizons and the irreducible mass, see [17] and references therein for the rather extensive literature on the subject. In the second we compute the irreducible mass perturbatively. This is based partly on [79] but here we conduct this directly in the Hamiltonian framework.

7.1. Horizons, Expansions and Irreducible Mass

We begin with some elementary definitions.

Consider a globally hyperbolic spacetime (M, g) and a Cauchy surface Σ in it. Let n be the future-oriented timelike unit normal of Σ. Let $S \subset \Sigma$ be a closed, oriented 2-surface in Σ without boundary $\partial S = \emptyset$ and s be the spacelike unit normal of S pointing outward from S and tangential to Σ. Hence, $g(n, s) = 0$ at S. We note that if we are just given Σ, S, then n, s are known only at Σ, S, respectively, and thus the covariant derivatives of n, s with respect to ∇, the torsion-free covariant differential compatible with g, are only computable in directions tangential to Σ, S, respectively. The tensor $q = g + n \otimes n$ on Σ has the property $q(n, u) = 0$ for every tangent vector u of Σ and the tensor $h = q - s \otimes s$ on S has the property $h(n, v) = h(s, v) = 0$ for every tangent vector v of S.

On S we can define the future (from Σ) and outward, respectively, inward (from S) oriented null vectors $l_+ = n + s$, $l_- = n - s$. We can now construct the affinely parametrized null geodesics starting from S with initial tangent $l_\pm$, respectively. This defines two null geodesic congruences $C^\pm_S$ and thus three-manifolds in M. Such a geodesic carries parameters s, y^A, $A = 1, 2$ where s is the affine parameter and y are coordinates on S. Thus, $C^\pm_S$ is an embedded three-manifold with local coordinates $(s, y) \mapsto c^\pm_y(s)$ where $c^\pm_y(s)$ is the geodesic with initial data $c^\pm_y(0) = Y(y)$, $\dot{c}^\pm_y(0) = l_\pm(Y(y))$ and $Y : U \subset \mathbb{R}^2 \to S$ is an embedding of S. The tangential vectors to $C^\pm_S$ are $\partial^\pm_A = \frac{\partial c^\mu_y(s)}{\partial y^A}\, \partial_\mu =: e^\mu_{A\pm}\partial_\mu$ and $\partial^\pm_s = \frac{\partial c^\mu_y(s)}{\partial y^A}\, \partial_\mu =: l_\pm$. Note, that by definition $\nabla_{l_\pm} l_\pm = 0$ by definition of an affinely parametrized geodesic, i.e., $l_\pm$ at $C^\pm_S$ is just the parallel transport of the initial $l_\pm$ at S.

Since these vector fields are known on all of $C^\pm_S$ we can take covariant derivatives of those in directions of $C^\pm_S$. Thus, we have access to $\nabla_u v$ on $C^\pm_S$ where u, v are in the span of $e_{A\pm}, l_\pm$. We note that $\nabla_{l_\pm}\, g(l_\pm, l_\pm) = 2g(l_\pm, \nabla_{l_\pm} l_\pm) = 0$ i.e., the quantity $g(l_\pm, l_\pm)$ is constant along every geodesic and since it is zero initially it follows $g(l_\pm, l_\pm) = 0$ on all of $C^\pm_S$. Then

$$\nabla_{l_\pm}\, g(e_{A,\pm}, l_\pm) = g(\nabla_{l_\pm} e_{A\pm}, l_\pm) = g(\nabla_{e_{A\pm}} l_\pm, l_\pm) = \frac{1}{2}\nabla_{e_{A\pm}}\, g(l_\pm, l_\pm) = 0 \tag{173}$$

as $[\partial^\pm_A, \partial^\pm_s] = 0$. Thus, also $g(e_{A,\pm}, l_\pm)$ is constant along every geodesic and since it vanishes initially ($e_{A,\pm}$ is tangential to S initially and $l_\pm$ is normal to S initially) whe have $g(e_{A\pm}, l_\pm) = 0$ everywhere on $C^\pm_S$.

The vectors $e_{A\pm}$ are geodesic deviation vectors, i.e., they carry information about the deviation of nearby geodesics as we move infinitesimally in the direction of y^A within the congruence. The vector $\nabla_{l_\pm} e_{A\pm} = \nabla_{e_{A\pm}} l_\pm$ thus contains the information on how the deviation vectors expand, shear and rotate along the "fluid" with fluid tangent $l_\pm$. It has no components in the direction of $l_\pm$ by (173) hence the full information about the geodesic deviation is contained in the quantity

$$\kappa^\pm_{AB} := g(e_{A\pm}, \nabla_{e_{B\pm}} l_\pm) \tag{174}$$

We also define on $C_S^{\pm}$ the objects

$$h_{AB}^{\pm} := g(e_{A\pm}, e_{B,\pm}),\ h_{\pm}^{AC}\ h_{CB}^{\pm} = \delta_B^A \tag{175}$$

Then

$$\theta_{\pm} := h_{\pm}^{AB}\ \kappa_{AB}^{\pm},\ \sigma_{AB}^{\pm} := \kappa_{(AB)}^{\pm},\ \omega_{AB}^{\pm} := \kappa_{[AB]}^{\pm}, \tag{176}$$

are, respectively, called expansion, shear and rotation of the congruence (rotation vanishes because $l_{\pm}$ is also normal to $C_S^{\pm}$ and $l_{\pm}$ is explicitly hypersurface orthogonal with $C_S^{\pm}$ as the integral manifold so $\nabla_{[\mu} l_{\pm\nu]} = \alpha_{[\mu}\ l_{\pm\nu]}$ by the Frobenius theorem). Using the definition of the Riemann tensor one can compute $\nabla_{l_{\pm}}\theta_{\pm}$ which leads to Raychaudhuri's equation [14].

We note that $\theta^{\pm}$ evaluated at S only requires information available at S, i.e., we need not know anything about the actual geodesic congruence $C_S^{\pm}$ away from S. Nevertheless the above theory is useful as it equips us with a geometric interpretation of $\theta_{\pm}$ familiar from hydrodynamics: If $\theta^{\pm} > 0/ < 0$ then a volume element that flows with the fluid (here: a light ray) starting from S expands/contracts along the flow lines. In flat space always $\theta^{+} > 0,\ \theta^{-} < 0$ for a sphere S (light leaves the sphere outwards/inwards). In a general spacetime one can have both $\theta_{-},\ \theta_{+} \leq 0$.

Definition 1. *Consider a globally hyperbolic spacetime (M, g) and a Cauchy surface Σ in it.*

i. *A closed, orientable 2-surface in Σ $S \subset \Sigma$ without boundary $\partial_\Sigma S = \emptyset$ is called trapped if $\theta_{+} = 0$.*

ii. *A trapped region in Σ is a closed subset $T \subset \Sigma$ such that $S := \partial_\Sigma T$ is trapped.*

iii. *The trapped surface in Σ defined by the total trapped region (closure of union of all trapped regions) is called the apparent horizon A_Σ of Σ.*

Definition 2. *Consider a globally hyperbolic spacetime (M, g) and a foliation $\mathcal{F} = \cup_{\tau\in\mathbb{R}} \Sigma_\tau$ of M by Cauchy surfaces Σ_τ.*

i. *If $\tau \mapsto S_\tau \subset \Sigma_\tau$ is a one-parameter family of trapped surfaces then $\mathcal{S} := \cup_\tau S_\tau$ is called a trapping horizon.*

ii. *Let $A_\tau := A_{\Sigma_\tau}$ be the apparent horizon of Σ_τ. Then, $\mathcal{A}_{\mathcal{F}} := \cup_\tau\ A_\tau$ is called the apparent horizon of $\mathcal{F}$.*

If M is asymptotically flat then by definition it has a conformal completion $\hat{M}$ which, in particular, is equipped with future null infinity $\mathcal{S}_{+}$. The manifold M is embedded into $\hat{M}$ via some $\varphi : M \to \hat{M}$ and $B := \varphi^{-1}(\varphi(M) \cap [\hat{M} - J_{-}(\mathcal{S}_{+})])$ is called the black hole region. Its boundary $\mathcal{H} := \partial_M B$ is called the event horizon of M. If Σ is a Cauchy surface then $H_\Sigma := \mathcal{H} \cap \Sigma$ is called the event horizon of Σ. Given a foliation $\mathcal{F}$ with corresponding Cauchy leaves Σ_τ, the classical black hole area theorem states that for all $\tau_1 \leq \tau_2$ we have $\mathrm{Ar}[H_{\Sigma_{\tau_1}}] \leq \mathrm{Ar}[H_{\Sigma_{\tau_2}}]$ when the Einstein equations and suitable matter conditions (inequalities for the energy momentum tensor) hold. One also shows that every trapped region lies in B, and therefore, every trapped surface in any Σ, in particular, the apparent horizon in Σ, lies in B. This means that with respect to a foliation, while the area of the event horizon can only grow within classical GR, the area of the apparent horizon can both shrink (e.g., radiation emission) and grow (e.g., radiation absorption).

Definition 3. *A (part of a) trapping horizon $\mathcal{S}$ is called a dynamical horizon, trapped tube or isolated horizon, respectively, if $\mathcal{S}$ is a spacelike, timelike and null three-manifold, respectively.*

The advantage of the various notions of trapping and apparent horizons over the event horizon is that they are by construction local in nature both spatially and temporally while the event horizon is a so-called "teleological" construct requiring us to know the entire future development of a spacetime which is neither practical nor operational: after all an astronomer detects a black hole as the limited region of space from which no light can escape and within her limited lifetime. Furthermore, an astronomer will measure the time development of that region with respect to a certain notion of time, i.e., a certain foliation. This makes the apparent horizon the ideal and physically motivated notion of a black hole. It is often objected that an apparent horizon is foliation-dependent while the event horizon is an absolute notion; however, when viewed as a necessary part of the definition of an observer, the foliation dependence is actually physically well-motivated.

Definition 4. *Given a foliation $\mathcal{F}$ of a globally hyperbolic (M, g) by Cauchy surfaces Σ_τ the irreducible mass at time τ is defined as*

$$[M_{\mathsf{irr}}(\tau)]^2 := \mathsf{Ar}[A_\tau] \tag{177}$$

i.e., the square root of the apparent horizon.

We slightly abuse here the terminology as the irreducible mass squared is usually defined as the area of the event horizon rather than the apparent horizon.

We now have to provide a concrete formula for $\theta_+(\tau)$ and $M_{\mathsf{irr}}(\tau)$. Given a foliation $\mathcal{F}$ we introduce ADM coordinates $\tau, x^a;\; a = 1,2,3$. We restrict attention to trapped surfaces of spherical topology and thus have embeddings $Y_\tau :\; S^2 \to \sigma_\tau \subset \sigma,\; y \mapsto Y_\tau(y)$ and $E_\tau :\;\; S^2 \to S_\tau \subset M = \mathbb{R} \times \sigma;\; y \mapsto (\tau, Y_\tau(y))$. The future oriented timelike unit normal to Σ_τ has components $n^\tau = \frac{1}{N},\; n^a = -\frac{N^a}{N}$ where the usual metric components are $g_{\tau\tau} = -N^2 + q_{ab}N^a N^b,\; g_{\tau a} = q_{ab}N^b,\; g_{ab} = q_{ab}$ with $a, b, c = 1,2,3$. The vectors $T_A := \frac{\partial E}{\partial y^A}$ are tangential to S_τ, therefore, (in this section $\mu, \nu, \ldots = 0,1,2,3$ while $a, b, c, \ldots = 1,2,3$)

$$\tilde{s}_\mu := -\frac{1}{2}\epsilon_{\mu\nu\rho\sigma} n^\nu\; T^\nu_A\; T^\nu_B\; \epsilon^{AB} \tag{178}$$

is co-normal to and outgoing fom S_τ and normal to n. Therefore, up to normalization $\tilde{s}^\mu = g^{\mu\nu}\tilde{s}_\nu$ is the spacelike unit normal to S_τ. Explicitly with $\epsilon_{\tau abc} = \epsilon_{abc}$ and $Y(\tau, y) := Y_\tau(y)$ and not displaying the τ dependence

$$\tilde{s}_a = \frac{1}{N}\; \hat{s}_a, \tilde{s}_\tau = \frac{1}{N}\hat{s}_\tau, \hat{s}_a := \frac{1}{2}\epsilon_{abc}\; \epsilon^{AB} Y^b_{,A} Y^c_{,B},\; \hat{s}_\tau := N^a \hat{s}_a \tag{179}$$

Thus,

$$\hat{s}^\tau = \frac{1}{N^2}[-\hat{s}_\tau + N^a\hat{s}_a] = 0,\; \hat{s}^a = \frac{1}{N^2}[N^a\hat{s}_\tau - N^a N^b \hat{s}_b] + q^{ab}\hat{s}_b = q^{ab}\hat{s}_b \tag{180}$$

It follows $g(\hat{s}, \hat{s}) = q_{ab}\hat{s}^a\hat{s}^b = q^{ab}\hat{s}_a\hat{s}_b$ thus

$$s_a = \frac{\hat{s}_a}{\sqrt{q^{cd}\hat{s}_c\hat{s}_d}},\; s_\tau = N^a\hat{s}_a \tag{181}$$

is the properly normalized ouward oriented outgoing spacelike unit co-normal from S_τ. It follows for the corresponding outgoing future oriented null normal $l := l_+$

$$l^\tau = n^\tau = \frac{1}{N},\; l^a = n^a + s^a = -\frac{N^a}{N} + q^{ab}\; s_b \tag{182}$$

Next, the pull-back metric on S^2 is given by (recall $h = g + n \otimes n - s \otimes s$)

$$h_{AB}(\tau; y) := [Y^*_\tau g]_{AB}(y) = Y^\mu_{\tau,A}\; Y^\nu_{\tau,B}\; g_{\mu\nu}(Y_\tau(y)) \tag{183}$$

and thus

$$\mathsf{Ar}[A_\tau] = \int_{S^2}\; d^2y\; \sqrt{\det(h(\tau; y))} \tag{184}$$

Note the identity

$$h^{\mu\nu} = g^{\mu\nu} + n^\mu n^\nu - s^\mu s^\nu = h^{AB} Y^\mu_{,A} Y^\nu_{,B} \tag{185}$$

as one can quickly show by contacting with the co-basis $n_\mu, s_\mu, g_{\mu\nu} Y^\nu_{,A}$. Thus, by definition

$$\begin{aligned} \theta_\pm &= h^{\mu\nu}\,\nabla_\mu l_{\pm\nu} = h^{AB}\,Y^\mu_{,A}\,Y^\nu_{,B}[\nabla_\mu l_{\pm\nu}] \\ &= h^{AB}\,Y^\mu_{,A}\,Y^\nu_{,B}[(\nabla_\mu n_\nu) \pm (\nabla_\mu s_\nu)] \\ &= h^{AB}\,[Y^\mu_{,A}\,Y^\nu_{,B} K_{\mu\nu} \pm Y^\mu_{,A}\,Y^\nu_{,B}\,(D_\mu s_\nu)] \end{aligned} \tag{186}$$

where we have used the spatial–spatial projection of $\nabla_\mu n_\nu$ is the extrinsic curvature $K_{\mu\nu}$ of Σ_τ and D is the torsion-free covariant derivative compatible with $q = g + n \otimes n$ acting on spatial tensors (i.e., whose contraction of any index vanishes). Now, $n_\tau = g_{\tau\mu} n^\mu = -N,\ n_a = g_{a\mu} n^\mu = 0$ and thus $n_\mu Y^\mu_{,a} = -N Y^\tau_{,A} = 0$ compatible with $Y^\tau = \tau$. It follows

$$\theta_\pm = h^{AB}\,[Y^a_{,A}\,Y^b_{,B} K_{ab} \pm Y^a_{,A}\,Y^b_{,B}\,(\nabla s)_{ab}] \tag{187}$$

By working out these expressions explicitly in ADM coordinates and using (180) and (181) one finds

$$K_{ab} = \frac{1}{2N}\,[\partial_\tau q_{ab} - [\mathcal{L}_{\vec{N}} q]_{ab}],\ [\nabla s]_{ab} = [Ds]_{ab} = \partial_a s_b - \Gamma^c_{ab}(q) s_c \tag{188}$$

where $\Gamma(q)$ is constructed from $q_{ab},\ q^{ab},\ q^{ac} q_{cb} = \delta^a_b$. Thus,

$$\theta_\pm = h^{AB}\,[Y^a_{,A}\,Y^b_{,B} K_{ab} \mp Y^a_{,A}\,s_b\,D_a\,Y^b_{,B}] \tag{189}$$

where we exploited $Y^a_{,A} s_a = 0$. Next, one verifies that

$$h^{AB} Y^a_{,A} Y^b_{,B} = q^{ab} - s^a s^b \tag{190}$$

by checking with the co-basis $s_a, q_{ab} Y^b_{,A}$. Therefore,

$$h^{AB} Y^a_{,A} Y^b_{,B} K_{ab} = [q^{ab} - s^a s^b]\,K_{ab} = -s_c\,s_d\,[q^{ac} q^{bd} - q^{ab} q^{cd}]\,K_{ab} = -s_a s_b \frac{p^{ab}}{\sqrt{\det(q)}} \tag{191}$$

where we used normalization $q^{ab} s_a s_b = 1$ and the definition of the ADm momentum p^{ab} conjugate to q_{ab}. Accordingly the final formula reads

$$\theta_\pm = -s_a s_b \frac{p^{ab}}{\sqrt{\det(q)}} \mp Y^a_{,A}\,s_b\,D_a\,Y^b_{,B} \tag{192}$$

which expresses the expansion explicitly in terms of ADM data (q, p) and the embedding function Y with $s_a = s_a(Y, q)$ via (180), (181) considered as also defined by these.

The time derivative of $\mathrm{Ar}[S_\tau]$ is given by

$$\frac{d}{d\tau}\,\mathrm{Ar}[A_\tau] = \frac{1}{2}\int_{S^2} d^2y\,\sqrt{\det(h(\tau;y))}\,h^{AB}\,[\frac{d}{d\tau} h_{AB}] \tag{193}$$

and with the vector fields $\xi(Y_\tau(y)) := \frac{\partial Y(\tau,y)}{\partial\tau},\ T_A(Y_\tau(y)) := \frac{\partial Y(\tau,y)}{\partial y^A}$ tangential to the apparent horizon $\mathcal{A}_\mathcal{F}$

$$[\frac{d}{d\tau} h_{AB}] = \xi^\mu\,\partial_\mu g(T_A, T_B) \circ Y = 2\xi^\mu\,g(T_{(A}, \nabla_\mu T_{B)}) = 2\,g(Y_{(A}, \nabla_\xi T_{B)}) = 2\,g(T_{(A}, \nabla_{T_{B)}} \xi) \tag{194}$$

whence

$$\frac{d}{d\tau}\,\mathrm{Ar}[A_\tau] = \int_{S^2} d^2y\,\sqrt{\det(h(\tau;y))}\,\theta_\xi,\ \theta_\xi = h^{AB}\,Y^\mu_{,A} Y^\nu_{,B}[\nabla_\mu \xi_\nu] \tag{195}$$

This would vanish for Y the embedding of the apparent horizon if we had $\xi \propto l_+$ but generically it is not because ξ is generically not even null.

The extreme cases are that $\xi \propto n, s, l_+$ which means that the apparent horizon is a timelike, spacelike or null surface (trapped tube, dynamical horizon, isolated horizon). Now $\theta_\pm = \theta_n \pm \theta_s$ and if $\theta_- < 0$ as one usually assumes, from $\theta_+ = 0$ we obtain $\theta_s = -\theta_n > 0$. Then, either $\theta_\xi \propto \theta_n < 0$, $\theta_\xi \propto \theta_s > 0$ or $\theta_\xi \propto \theta_{l_+} = 0$.

7.2. Constructing the Apparent Horizon in GPG

To construct the apparent horizon in GPG we proceed as in [79] and assume that it has spherical topology. Then, the embedding function takes the explicit form

$$Y^\tau(\tau, y) = \tau,\ Y^3(\tau, y) = \rho(\tau, y), Y^A(\tau, y) = y^A \tag{196}$$

The function ρ is called the *radial profile*. Then,

$$\hat{s}_a = \frac{1}{2}\epsilon_{abc}\epsilon^{BC} Y^b_{,B} Y^c_{,C} = \begin{cases} -\rho_{,A} & a = A = 1,2 \\ 1 & a = 3 \end{cases} \tag{197}$$

Hence, $\hat{s}_3 > 0$ correctly implements outward orientation. The normalized components are

$$s_a = f\ \hat{s}_a,\ f = \frac{1}{\sqrt{q^{ab}\hat{s}_a\hat{s}_b}} = \frac{1}{\sqrt{1 + q^{AB}\rho_{,A}\rho_{,B}}}, \tag{198}$$

where we used the GPG $q_{33} = q^{33} = 1,\ q_{3A} = q^{3A} = 0,\ q_{AB} = r^2\Omega_{AB} + X_{AB},\ q^{AC}q_{CB} = \delta^A_B$. Thus, s_a is determined entirely by ρ. The profile function ρ must then solve the *trapping equation*

$$-\theta_+ = \frac{P^{ab}}{\sqrt{\det(q)}} s_a s_b + h^{AB} s_a\ D_{Y_{,A}} Y^a_{,B} = 0 \tag{199}$$

where

$$\begin{aligned} h_{AB} &= q_{ab} Y^a_{,A} Y^b_{,B} = \rho_{,A}\ \rho_{,B} + q_{AB},\ \det(h) h^{AB} = \epsilon^{AC}\epsilon^{BD} h_{CD},\ = \rho^A\rho^B + \det(q) q^{AB},\ \rho^A = \epsilon^{AB}\ \rho_{,B} \\ \det(h) &= \frac{1}{2}\epsilon^{AC}\epsilon^{BD} h_{AB} h_{CD} = \det(q)\ f^{-2} \end{aligned} \tag{200}$$

and $P^{33} = P^3, P^{3A} = \frac{1}{2}P^A,\ P^{AB} = \frac{1}{2}P^0\Omega^{AB} + Y^{AB}$ where P^3, P^A, P^0 are themselves functions of X_{AB}, Y^{AB} and the physical matter fields upon solving the constraints. Then, the trapping condition reads

$$-\theta_+ = \frac{p^{ab}}{\sqrt{\det(q)}} s_a s_b + h^{AB} s_a\ [Y^a_{,AB} + \Gamma^a_{bc}(q) Y^b_{,A} Y^c_{,B}] = 0 \tag{201}$$

where $Y^a_{,AB} = \delta^a_3 \rho_{,AB}$. It is a non-linear second order PDE for the profile function on the sphere.

To solve it exactly for general X, Y is too complicated. However, since also p^{ab} is only known perturbatively, it is well motivated to compute the profile function also only perturbatively. Thus, we consider

$$\rho = \sum_{n=0} \rho_n \tag{202}$$

where ρ_n is a monomial in X, Y and matter perturbations of order n. Then, one inserts (202) into (201) and expands all $p, q, s, Y_{,A}$ in terms of the perturbations X_{AB}, Y^{AB}, etc., extracts the terms of order n and aims for a hierarchy of equations that one can iteratively solve in closed-form.

We begin with the zeroth order and consider all X, Y dependence vanishing. Thus, $(R = 2M,\ \kappa = 1/2)$

$$\begin{array}{rcl} q_{ab} &=& \delta^3_a\delta^3_b + r^2\,\Omega_{AB}\,\delta^A_a\delta^B_b \\ \frac{P^{ab}}{\omega} &=& 2\sqrt{R\,r}\delta^a_3\delta^b_3 + \frac{1}{2}\sqrt{R/r^3}\,\Omega^{AB}\,\delta^a_A\delta^b_B \\ s_a &=& f\,\hat{s}_a,\ \hat{s}_a = \delta^3_a - \rho_{,A}\delta^A_a,\ f = [1 + r^{-2}\Omega^{AB}\rho_{,A}\rho_{,B}]^{-1/2} \\ h_{AB} &=& \rho_{,A}\rho_{,B} + r^2\Omega_{AB},\ \det(h) = r^4\,\omega^2\,f^2,\ \det(h)\,h^{AB} = \rho^A\rho^B + r^2\omega^2\Omega^{AB},\ \rho^A = \epsilon^{AB}\,\rho_{,A} \end{array} \tag{203}$$

The Christoffel symbols in the GPG at $X = 0$ were already computed in Section 4

$$\Gamma^3_{33} = \Gamma^3_{3A} = \Gamma^A_{33} = 0,\ \Gamma^A_{B3} = \frac{1}{r}\delta^A_B,\ \Gamma^3_{AB} = -r\Omega_{AB},\ \Gamma^A_{BC} = \Gamma^A_{BC}(\Omega) \tag{204}$$

Then

$$\begin{array}{rl} & h^{AB}\,s_c\,[Y^c_{,AB} + \Gamma^c_{ab}Y^a_{,A}Y^b_{,B}] = f\,h^{AB}\,[\rho_{,AB} + \Gamma^3_{ab}Y^a_{,A}Y^b_{,B} - \rho_{,C}\,\Gamma^C_{ab}Y^a_{,A}Y^b_{,B}] \\ = & f\,h^{AB}\,[\rho_{,AB} + \Gamma^3_{CD}Y^C_{,A}Y^D_{,B} - \rho_{,C}\,(2\Gamma^C_{3D}Y^3_{,(A}Y^D_{,B)} + \Gamma^C_{DE}Y^D_{,A}Y^E_{,B})] \\ = & f\,h^{AB}\,[\rho_{,AB} + \Gamma^3_{AB} - \rho_{,C}\,(2\Gamma^C_{3(A}\,\rho_{,B)} + \Gamma^C_{AB})] \\ & P^{ab}s_a s_b = \omega\,f^2\,[2(Rr)^{1/2} + \frac{1}{4}\,(R/r^3)^{1/2}\,\Omega^{AB}\,\rho_{,A}\,\rho_{,B}] \end{array} \tag{205}$$

We make the Ansatz $\rho = \rho_0 =$ const. then $f = 1, h_{AB} = q_{AB} = r^2\Omega_{AB},\ s_a = \delta^3_a$ and

$$-\theta_+ = [\frac{P^{33}}{\sqrt{\det(q)}} + q^{AB}\Gamma^3_{AB}]_{r=\rho_0} = \frac{2}{r^2}[\sqrt{Rr} - r]_{r=\rho_0} = 0 \tag{206}$$

has a unique solution

$$\rho_0 = R \tag{207}$$

as expected.

We will assume inductively that $\rho_0,\ \rho_1,\ \ldots,\rho_{n-1},\ n \geq 1$ have been already computed. We write the unperturbed trapping equation in the form (recall $\det(q) = \omega^2 r^4 + \det(X)$ and all quantities are evaluated at $r = \rho$)

$$\begin{array}{rcl} 0 &=& [P^{33} - 2P^{3A}\rho_{,A} + P^{AB}\rho_{,A}\rho_{,B}]\ [1 + q^{AB}\,\rho_{,A}\,\rho_{,B}]^{1/2}\ [\rho^2\omega]\ [1 + \frac{\det(X)}{\rho^4\omega^2}]^{1/2} \\ && +[\rho^A\rho^B + \det(q)q^{AB}]\ [\rho_{,AB} + \Gamma^3_{AB} - \rho_{,C}(\Gamma^C_{AB} + 2\Gamma^C_{3(A}\rho_{,B)})] \end{array} \tag{208}$$

To capture the full n-th order dependence of this expression, all quantities that depend on ρ need to be Taylor expanded up to the n-th order in $\Delta = \rho - \rho_0$ around $\rho = \rho_0 = R$, for example, $P^{33}(\rho) = P^{33}(\rho_0) + P^{33\prime}(\rho_0)\ \Delta + \frac{1}{2}P^{33\prime\prime}(\rho_0)\ \Delta^2 + \ldots$ and the second order contribution in Δ^2 is given by $\rho_1^2 + 2\rho_0\rho_2$, etc.

Let us denote the four factors in the first term of (208) by A, B, C, D from left to right and the two factors in the second term of (208) by E, F from left to right. We isolate all terms of order n by expanding each factor to order n. In the resulting sum of terms, which is now a monomial of order n, we want to isolate all terms that contain ρ_n. These are contained in the following contribution

$$A_n B_0 C_0 D_0 + A_0 B_n C_0 D_0 + A_0 B_0 C_n D_0 + A_0 B_0 C_0 D_n + E_n F_0 + E_0 F_n \tag{209}$$

where A_n, A_0 is the n-th and 0-th order contribution, respectively, of A, etc. We now consider the individual terms $A_n, \ldots, F_n$ and isolate the terms that contain ρ_n:

$$A = P^{33} - 2P^{3A}\rho_{,A} + P^{AB}\rho_{,A}\rho_{,B} \tag{210}$$

Since $\rho_{,A} = \rho_{1,A} + \ldots$ is already of first order and P^{rA} has no zeroth order perturbation, the only term in A_n that contains ρ_n is $P_0^{33\prime}(\rho_0)\,\rho_n$ and $A_0 = P_0^{33}(\rho_0)$ where the subscript 0 of P_0^{33} means that we first expand P^{33} in terms of the perturbations X, Y and then take the zeroth order term of that. The resulting function is still to be expanded in terms of $\rho - \rho_0$ and we note the corresponding derivatives by a prime.

$$B = [1 + q^{AB}\,\rho_{,A}\,\rho_{,B}]^{1/2} \tag{211}$$

For the same reason this term has no ρ_n contribution in B_n and $B_0 = 1$.

$$C = \rho^2\omega \tag{212}$$

The ρ_n contribution to C_n is $2\rho_0\rho_n\omega$ and $C_0 = \rho_0^2\omega$.

$$D = [1 + \frac{\det(X)}{\rho^4\omega^2}]^{1/2} \tag{213}$$

There is no ρ_n contribution to D_n because $\det(X)$ is a second order perturbation and thus $D_0 = 1$.

$$E = \rho^A\rho^B + \epsilon^{AC}\epsilon^{BD}[\rho^2\Omega_{CD} + X_{CD}(\rho)] \tag{214}$$

As X_{CD} is already of first order, the ρ_n contribution to E_n is $2\rho_0\rho_n\omega^2\Omega^{AB}$ and $E_0 = \rho_0^2\omega^2\Omega^{AB}$.

$$F = \rho_{,AB} + \Gamma^3_{AB} - \rho_{,C}(\Gamma^C_{AB} + 2\Gamma^C_{3(A}\rho_{,B)}) \tag{215}$$

The ρ_n contribution to F_n is $\rho_{n,AB} + \Gamma^{3\prime}_{0;AB}(\rho_0)\,\rho_n - \rho_{n,C}\Gamma^C_{0;AB}(\rho_0)$ and $F_0 = \Gamma^3_{AB}(\rho_0)$.

It follows that the n-th order perturbation equation can be written in the form

$$\begin{aligned} G_n &= [P_0^{33\prime}(\rho_0)\rho_0^2\omega + P_0^{33}(\rho_0)2\rho_0\omega + 2\omega^2\Omega^{AB}\rho_0\Gamma^3_{0;AB}(\rho_0) + \omega^2\rho_0^2\Gamma^{3\prime}_{0;AB}(\rho_0)]\,\rho_n \\ &\quad +\omega^2\rho_0^2\Omega^{AB}(\rho_{n,AB} - \Gamma^C_{0;AB}(\rho_0)\rho_{,C}) \\ &= [P_0^{33}(r)r^2\omega + \omega^2\Omega^{AB}r^2\Gamma^3_{0;AB}(r)]'_{r=\rho_0}\,\rho_n \\ &\quad +\omega^2\rho_0^2\Omega^{AB}(\rho_{n,AB} - \Gamma^C_{0;AB}(\rho_0)\rho_{,C}) \\ &= \omega^2\,\rho_0^2[\Omega^{AB}\,D_A\,D_B - 1]\rho_n = \omega^2\,\rho_0^2[\Delta_{S_2} - 1]\,\rho_n \end{aligned} \tag{216}$$

where we used (206) and that $\Gamma^C_{0,AB} = \Gamma^C_{AB}(\Omega)$ is the Christoffel symbol of the sphere metric independent of $r = \rho_0$ to write the last relation in terms of the sphere Laplacian. The term G_n is the complete n-th oder contribution to (208) except for the terms that contain ρ_n. It thus contains the $\rho_m,\ m \le m-1$ and their derivatives polynomially which already have been solved for. It remains to expand

$$G_n = \sum_{l\ge|m|} G_n^{l,m}\,L_{l,m},\ \rho_n = \sum_{l\ge|m|} \rho_n^{l,m}\,L_{l,m},\ \Rightarrow\ \rho_n^{l,m} = -\frac{G_n^{l,m}}{l(l+1)+1} \tag{217}$$

This proves that the radial profile ρ of the apparent horizon can be solved for the arbitrary order in the perturbations in closed-form.

7.3. Expansion of the Irreducible Mass Squared

Having computed the radial profile ρ of the apparent horizon we can compute the irreducible mass squared perturbatively as follows. The non-perturbative expression is

$$\begin{aligned} \mathsf{Ar} &= \int d^2y\,\sqrt{\det(h)} = \int d^2y\,\sqrt{\det(q)}\,\sqrt{1 + q^{AB}\,\rho_{,A}\,\rho_{,B}} \\ &= \int d\Omega\,\rho^2\,\sqrt{1 + \frac{\det(X)}{\rho^4\omega^2}}\,\sqrt{1 + q^{AB}\,\rho_{,A}\,\rho_{,B}} \end{aligned} \tag{218}$$

This expression can be systematically expanded to any order in the perturbations. To second order

$$\begin{aligned}\mathsf{Ar} &= \int d\Omega\,[\rho_0^2+2\rho_0\rho_1+\rho_1^2+2\rho_0\rho_2]\,[1+\frac{1}{2}(\frac{\det(X)(\rho_0)}{\rho_0^4\omega^2}+q^{AB}(\rho_0)\,\rho_{1,A}\,\rho_{1,B})]\\ &= \int d\Omega\,\{[\rho_0^2]+[\rho_1^2+2\rho_0\rho_2+\frac{\rho_0^2}{2}(\frac{\det(X)(\rho_0)}{\rho_0^4\omega^2}+q^{AB}(\rho_0)\,\rho_{1,A}\,\rho_{1,B})]\}\\ &=: \mathsf{Ar}_0+\mathsf{Ar}_2 \end{aligned} \tag{219}$$

where the linear term has dropped out because it contains no $l=0$ mode. Thus, the mass itself to second order is

$$M_{\rm irr}=\mathsf{Ar}_0^{1/2}\,[1+\frac{1}{2}\frac{\mathsf{Ar}_2}{\mathsf{Ar}_0}] \tag{220}$$

which to the zeroth order just reproduces M while to the second order is a functional quadratic in X,Y. In a Fock representation of X,Y we expect quantum fluctuations in the irreducible mass, non-trivial dynamics and even violations of positivity inequalities [80].

8. Quantum Fields in a BHWHT Spacetime

We consider free quantum fields on the spherically symmetric BHWHT spacetime (M,g) with mass parameter M or Schwarzschild radius $R=2M$. The line element is given by

$$ds^2=-(1-\frac{R}{|z|})\,d\tau^2+2\sqrt{\frac{R}{|z|}}\,d\tau\,dz+dz^2+z^2\,d\Omega^2 \tag{221}$$

and $M=\mathbb{R}^4\cup\mathbb{R}^4$ with coordinates $\tau\in\mathbb{R},\ \Omega=(y^1,y^2)\in\mathbb{S}^2,\ z\in\mathbb{R}$ and radial coordinates $r=z,\ z>0;\ \bar{r}=-z,\ z<0$. Hence, (221) is the Schwarzschild solution in ingoing/outgoing Gullstrand–Painlevé coordinates for $z>0/{<}0$. The singularity is at $r=\bar{r}=0$. However, causal geodesics can be continued across it and this spacetime is foliated by $\tau=$ const. spacelike hypersurfaces which are Cauchy surfaces and define the simultaneity of proper time surfaces of free-falling timelike observers that fall all the way from past timelike infinity in a past universe towards future timelike infinity in a future universe. Those Cauchy surfaces extend all the way from the spatial infinity of the past universe to the spatial infinity of the future universe. Together both universes, therefore, define a globally hyperbolic spacetime if one allows singularity crossing. That spacetime is the common domain of dependence of all those hypersurfaces. Global hyperbolicity is very important for constructing quantum field theories and sticking to only one universe the free-falling synchronous hypersurfaces form a foliation but none of its leaves is a Cauchy surface as they stop at the singularity. If needed, we can consider two regular spacetimes glued at the cylinder surface $r=\bar{r}=l\ll R$ and with the solid cylinder cut out as a regularization step for what follows. More details are given in Appendix C.

The spacetime metric (221) naturally appears in our perturbative scheme to compute the reduced Hamiltonian and the black hole apparent horizon at second order and enters the Regge–Wheeler and Zerilli equations. It, therefore, motivates a natural class of Fock representations, and therefore, plays a fundamental role also for higher order contributions to the reduced Hamiltonian which we will treat by standard methods of perturbative QFT. In the first subsection, we give a brief introduction to QFT in general CST. Then, we specialize to CST equipped with a Killing vector field which is not necessarily everywhere timelike but such that the constant Killing time hypersurfaces are everywhere spacelike so that the time dependence of the wave equation obeyed by the quantum field can be separated. After that, we specialize even further in CST with spherical symmetry so that even the angular dependence can be separated off and the wave equation reduces from a PDE to an ODE of second order. In this case, one can gain important information on the modes of the quantum field using the Wronskian identities and without explicitly solving the wave equation. Finally, we discuss some of the details of the wave equation for the concrete CST given by (221) and outline the applications that we have in mind with regard to particle production and Hawking radiation.

8.1. Elements of QFT in CST

Consider a bosonic Quantum Field Theory (QFT) in globally hyperbolic Curved Spacetime (CST) (M, g). The classical, real valued, free spacetime fields are subject to a linear wave equation of the form

$$\Box\Phi = U\Phi,\ \Box = g^{\mu\nu}\nabla_\mu\ \nabla_\nu \tag{222}$$

where U is a real valued potential function (e.g., a position dependent mass term, it does not depend on Φ). This equation is either an Euler–Lagrange equation derived from some Lagrangian or from the correponding Hamiltonian formulation.

Let V be the vector space of real valued solutions of (222) that vanish sufficiently fast at spatial infinity. Given a Cauchy surface Σ in M consider the anti-symmetric bilinear form on V defined by

$$B(u, v) := \int_\Sigma d\Sigma_\mu\ \{u\ [\nabla^\mu v] - [\nabla^\mu u]\ v\} \tag{223}$$

where $d\Sigma_\mu = \frac{1}{3!}|\det(g)|^{1/2}\epsilon_{\mu\nu\rho\sigma} dX^\nu \wedge dX^\rho \wedge dX^\sigma$ is the volume element defined by g. It is not difficult to see that the three-form defined by the integrand of (223) is closed which is why B is independent of the choice of Σ.

Next, we consider the complexification $V_\mathbb{C}$ of linear combinations $w = u + iv,\ u, v \in V$ and consider the sesqui-linear form on $V_\mathbb{C}$ defined by

$$< w, w' >:= -i\ B(\overline{w}, w') = -i\ \int_\Sigma d\Sigma_\mu\ \{\overline{w}\ [\nabla^\mu w'] - \overline{[\nabla^\mu w]}\ w'\} \tag{224}$$

Decomposing w, w' into real and imaginary parts one sees that the sesqui-linear form is still independent of Σ; however, it is not positive semi-definite and does not equip all of $V_\mathbb{C}$ with a Hilbert space structure.

Suppose that we find a subspace $V_+ \subset V_\mathbb{C}$ such that $< ., . >$ restricted to V_+ is positive semi-definite. Then, automatically $< ., >$ restricted to $\overline{V_+}$ is negative semi-definite because

$$< \overline{w}, \overline{w}' >= -i\ B(w, \overline{w}') = i\ B(\overline{w}', w) = -< w', w > \tag{225}$$

If, moreover, $V_+, V_- := \overline{V}_+$ are orthogonal with respect to $< ., . >$ and $V_+ \oplus V_- = V_\mathbb{C}$ then $(V_\mathbb{C}, < ., . >)$ carries a *Krein structure*, i.e., an orthogonal decomposition

$$V_\mathbb{C} = V_+ \oplus V_- \tag{226}$$

such that $< ., \ldots >$ restricted to V_+, V_- is, respectively, positive semi-definite and negative semi-definite, respectively, (we refrain from the usual separate treatment of zero norm vectors for convenience. Then, $(V_\pm,\ \pm\ < ., . >)$ is a pre-Hilbert space whose completion (after moding by null vectors) is a Hilbert space $\mathcal{H}_\pm$. Equivalently, $(V_\mathbb{C},\ (., .))$ is a pre Hilbert space with an inner product

$$((w_+, w_-), (w'_+, w'_-)) =< w_+, w'_+ > - < w_-, w'_- > \tag{227}$$

with completion $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ Then, $\mathcal{H}_\pm$ are orthogonal subspaces of $\mathcal{H}$ with corresponding self-adjoint projections $P_\pm$ i.e., $P_+ + P_- = 1_\mathcal{H},\ P_\pm^2 = P_\pm = P_\pm^*,\ P_+ P_- = 0$ where the adjoint is with respect to $(., .)$.

Consider the anti-self adjoint operator

$$J := -i(P_+ - P_-),\ J^* = -J,\ J^2 = -1_\mathcal{H},\ P_\pm = \frac{1}{2}(1_\mathcal{H} \mp\ i\ J) \tag{228}$$

It preserves the real vector space V: By assumption we have $\overline{P_+ V_\mathbb{C}} = P_- V_\mathbb{C}$ whence $\overline{P_- V_\mathbb{C}} = P_+ V_\mathbb{C}$. Therefore, for $w, w' \in V_\mathbb{C}$ we have using $< w, w' >= - < \overline{w'}, \overline{w} >$

$$\begin{aligned} & (w, \overline{P_+ w'}) = (P_- w, \overline{P_+ w'}) = - < P_- w, \overline{P_+ w'} >=< P_+ w', \overline{P_- w} >= (P_+ w', \overline{P_- w}) \\ = \; & (w', P_+ \overline{P_- w}) =< w', \overline{P_- w} >= - < P_- w, \overline{w'} >= (P_- w, \overline{w'}) = (w, P_- \overline{w'}) \end{aligned} \tag{229}$$

i.e., $\overline{P_\pm w} = P_\mp \overline{w}$. Thus, for $u \in V$

$$\overline{J u} = i(\overline{P_+ u} - \overline{P_- u}) = -i(P_+ - P_-)\, \bar{u} = J\, u \tag{230}$$

Moreover $i J P_\pm = \pm\, P_\pm$ i.e., $\mathcal{H}_\pm$ are eigenspaces of iJ with eigenvalues ± 1. Finally,

$$B(u, J\, v) = -i[B(u, P_+ v) - B(u, P_- u)] =< u, P_+ v > - < u, P_- v >= (u, P_+ v) + (u, P_- v) = (u, v) \tag{231}$$

is positive semidefinite definite on V and for $u, v \in V$

$$\begin{aligned} & B(J\, u, J\, v) = (J\, u, P_+ v) + (J\, u, P_- v) = -(u, J\, P_+ v) + (u, J\, P_- v) \\ = \; & i(u, P_+ v) - i(u, P_- v) = B(u, P_+ v) + B(u, P_- v) = B(u, v) \end{aligned} \tag{232}$$

One calls B a symplectic structure, $J : V \to V, J^2 = -1_V$ a complex structure, a Kaehler structure if $B(J.,J.) = B(.,.)$, a positive Kaehler structure if $B(.,J.)$ is positive semidefinite. One can reverse the argument and start from a complex structure on V which is positive Kaehler with respect to B and then arrives at a Krein structure on $V_\mathbb{C}$ such that $V_- = \overline{V_+}$ and $(w, w') =< w, (P_+ - P_-) w' >= B(\overline{w}, J w')$.

The classical, real-valued field ϕ is an element of V and thus

$$\phi = [P_+ \phi] + [P_- \phi] =: A + A^* \tag{233}$$

is a decomposition into annihilation and creation parts. If $w \in V_+$ set

$$A(w) :=< w, A >= -i B(\overline{w}, \Phi) \tag{234}$$

Consider a foliation of M with corresponding lapse and shift functions such that Σ is one of its leaves, i.e., a $\tau =$ const. hypersurface. Then, recalling that $g^{\tau\mu} = -\frac{1}{N^2}[\delta^\mu_\tau - N^a \delta^\mu_a] = -\frac{1}{N} n^\mu$, $\epsilon_{\tau abc} = -\epsilon_{abc}$

$$\begin{aligned} A(w) \; &= \; = i \int_\sigma d^3x\; N\, \sqrt{\det(q)}\; g^{\tau\mu} [\bar{w}\, \Phi_{,\mu} - \bar{w}_{,\mu}\, \Phi] \\ &= \; -i \int_\sigma d^3x\, \sqrt{\det(q)}\; [\bar{w}\;\; [\nabla_n \Phi] - \overline{\nabla_n w}; \Phi] = -i \int_\sigma d^3x\; [\bar{w}\, \pi - \sqrt{\det(q)} \overline{\nabla_n w}\; \phi] \end{aligned} \tag{235}$$

where $\pi = \sqrt{\det(q)}\; [\nabla_n; \Phi]_{|\Sigma}$ is the momentum conjugate to $\phi = \Phi_{|\Sigma}$. It follows with $Q = [\det(q)]^{1/2}$

$$\begin{aligned} & \{A(w), [A(w')]^*\} = \int d^3x \int d^3y\; \{[\bar{w}\pi - Q[\overline{\nabla_n w}]\phi](x), [w'\pi - Q[\nabla_n w']\phi](y)\} \\ = \; & - \int d^3x\; Q\; [\bar{w}\; [\nabla_n w'] - \overline{\nabla_n w}\; w'] \\ = \; & = -i < w, w' > \end{aligned} \tag{236}$$

so that the canonical commutation relations (CCR) are

$$[A(w), [A(w')]^*] =< w, w' >\;\; 1 \tag{237}$$

confirming the roles of A, A^* as annihilation and creation operator valued distributions in potential Fock representations.

8.2. CST with Spacelike Killing Time Hypersurfaces

The question is, of course, given B, how to obtain either the Krein or complex structure with the additional properties mentioned, and how much freedom there is in choosing them. In the case that is of interest here, namely that there is a Killing vector field ∂_τ such that the $\tau =$ const. surfaces are spacelike Cauchy surfaces, the following construction may be applied. Note, that this is more general than the stationary case in which the Killing vector field is supposed to be everywhere timelike. In fact, this does not hold for our ∂_τ where the GPG time τ defines the free-falling foliation with synchronous $\tau =$ const. surfaces. We consider the Hamiltonian

$$H = \int_\sigma d^3x \, [\frac{N}{2}(\frac{\pi^2}{Q} + Q \, [q^{ab}\phi_{,a}\phi_{,b} + U\phi^2]) + \pi N^a \phi_{,a}] \tag{238}$$

where N, N^a, q_{ab} are not explicitly τ dependent. The Hamiltonian equations of motion

$$\dot{\phi} = \{H, \phi\} = N \, \frac{\pi}{Q} + N^a \phi_{,a}, \;\; \dot{\pi} = \{H, \pi\} = (N \, Q \, q^{ab} \, \phi_{,a})_{,b} - NQU\phi + (N^a \pi)_{,a} \tag{239}$$

reproduce the Euler Lagrange Equations (222) since from the first relation in (239) $\pi = Q\nabla_n \phi$ thus

$$\begin{aligned} U \, \phi = \Box\phi &= |\det(g)|^{-1/2} \, [g^{\mu\nu} \, |\det(g)|^{1/2} \phi_{,\mu}]_{,\nu} \\ &= [N \, Q]^{-1} \, \{[g^{\mu\tau} \, N \, Q\phi_{,\mu}]_{,\tau} + [g^{\mu a} \, N \, Q\phi_{,\mu}]_{,a}]\} \\ &= [N \, Q]^{-1} \, \{-[Q \, \nabla_n \phi]_{,\tau} + [QN^a \, \nabla_n \phi]_{,a}] + [NQq^{ab}\phi_{,a}]_{,b}\} \\ &= [N \, Q]^{-1} \, \{-\dot{\pi} + [\pi N^a]_{,a}] + [NQq^{ab}\phi_{,a}]_{,b}\} \end{aligned} \tag{240}$$

The idea is now to construct a system of complex solutions of (222) whose normalizable span defines the space V_+ of the Krein structure, i.e., $V_+, <.,.>$ is a pre-Hilbert space such that $V_- = \overline{V_+}$ and $V_+ \perp V_-$. To conduct this we write out the d'Alembertian explicitly

$$\Box W = \frac{1}{N \, Q} \, \{-[Q \, \nabla_n W]_{,\tau} + [QN^a \, \nabla_n W]_{,a}] + [NQq^{ab} W_{,a}]_{,b}\}; \;\; \nabla_n = N^{-1}(\partial_\tau - N^a \partial_a) \tag{241}$$

which is still the general expression. Now, we exploit that N, N^a, q_{ab} do not depend on τ and thus can separate off the τ dependence in w

$$W_\omega(\tau, x) := e^{i\omega\tau} \, w_\omega(x), \; \omega \in \mathbb{C} \tag{242}$$

For $\omega \in \mathbb{R}$ the corresponding solutions are called *modes*, for $\Im(\omega) \in \mathbb{R}_+ - \{0\}$ ring down or *quasi-normal modes*. It follows

$$0 = \frac{1}{NQ} \, [\omega^2 \, \frac{Q}{N} \, w_\omega + i\omega \, (\frac{Q}{N} N^a \partial_a + \partial_a \frac{Q}{N} N^a) w_\omega + \partial_a (NQ(q^{ab} - \frac{N^a N^b}{N^2}) \partial_b w_\omega - N \, Q \, U \, w_\omega] \tag{243}$$

This suggests to introduce the operators

$$E := \frac{Q}{N} \, 1, \;\; A := \partial_a \, N^a \, E + E \, N^a \, \partial_a, \;\; B := -\partial_a (NQ(q^{ab} - \frac{N^a N^b}{N^2}) \partial_b + N \, Q \, U \, 1 \tag{244}$$

where E, B and A are formally symmetric and anti-symmetric, respectively, on the auxiliary Hilbert space $\mathfrak{H} = L_2(\sigma, d^3x)$. Formally, each of them maps scalars into scalar densities of weight one on σ because Q carries density weight one and N, N^a are scalars and vectors, respectively, of density weight zero. Accordingly,

$$[\omega^2 \, E + i\omega \, A - B] \, w_\omega = 0 \tag{245}$$

We focus on real ω. Taking the complex conjugate of (245) we see that w^*_ω solves the same equation as a solution $w'_{-\omega}$ would. Next, we compute the $\mathfrak{H}$ inner product of (245) with $w'_{\omega'}$

$$
\begin{aligned}
& < w_\omega,\ B\ w'_{\omega'} >_{\mathfrak{H}} = < w_\omega, [(\omega')^2\ E + i\omega'\ A]\ w'_{\omega'} >_{\mathfrak{H}} = \\
= \quad & < B\ w_\omega,\ w'_{\omega'} >_{\mathfrak{H}} = < [(\omega)^2\ E + i(\omega)\ A] w_\omega,\ w'_{\omega'} >_{\mathfrak{H}}
\end{aligned} \tag{246}
$$

where we used the symmetry of B. It follows from the symmetry of $E, i\ A$ that

$$
(\omega - \omega')\ [(\omega + \omega')\ \ < w_\omega,\ E\ w'_{\omega'} >_{\mathfrak{H}} + i\ \ < w_\omega,\ A\ w'_{\omega'} >_{\mathfrak{H}}] = 0 \tag{247}
$$

Now we compute on the other hand the inner product with respect to the sesqui-linear form (224)

$$
\begin{aligned}
< W_\omega, W'_{\omega'} > \quad &= \quad -i \int_\sigma \ d^3x\ Q\ [\overline{W_\omega}\ (\nabla_n W'_{\omega'}) - \overline{\nabla_n W_\omega}\ W'_{\omega'}] \\
&= \quad -i\ e^{i(\omega'-\omega)\tau} \int_\sigma \ d^3x\ E\ [\overline{w_\omega}\ ((i\omega' - N^a\partial_a) w'_{\omega'}) - \overline{(i\omega - N^a\partial_a) w_\omega}\ w'_{\omega'} \\
&= \quad e^{i(\omega'-\omega)\tau} \int_\sigma \ d^3x\ \overline{w_\omega}\ [(\omega+\omega')E + i(E\ N^a\ \partial_a + \partial_a\ N^a\ E)]\ w'_{\omega'} \\
&= \quad e^{i(\omega'-\omega)\tau}\ [(\omega+\omega')\ \ < w_\omega,\ E\ w'_{\omega'} >_{\mathfrak{H}} + i\ \ < w_\omega,\ A\ w'_{\omega'} >_{\mathfrak{H}}] = 0
\end{aligned} \tag{248}
$$

which coincides up to the τ dependent phase with the square bracket in (247). Thus, we obtain from (247) and (248) that

$$
< W_\omega, W'_{\omega'} > \propto \delta^{(1)}(\omega, \omega') \tag{249}
$$

i.e., the solutions are orthonormal with respect to the inner product (224) and the label ω in the sense of delta distributions. If the sign of the proportionality factor in (249) is positive or negative, respectively, then the solution lies in V_+ or V_-, respectively. When V_+ coincides with the subspace of solutions corresponding to $\omega \in \mathbb{R}_+$ one calls V_+ the positive frequency subspace but, in general, V_+ can also contain negative frequency (e.g., for the potential barrier underlying the Klein paradox [102]) and thus, should better be called the positive inner product subspace. In particular, if $W_\omega \in V_+$ then $W^*_\omega = W'_{-\omega},\ w'_{-\omega} = w^*_\omega$, hence $V_+ \perp \overline{V_+}$ and since by the properties of the scalar product $< .,. >$ we have $< \bar{W}, \bar{W}' > = - < W', W >$ it follows that $V_- = \overline{V_+}$.

8.3. Further Reduction of PDE to ODE in Sperically Symmetric CST

Accordingly we have found a possible Krein structure in the present situation once we know the space of solutions of (245). In general, this is a complicated second order PDE. However, in the presence of further symmetries as is the case for our spherically symmetric background or an axisymmetric background (rotating black hole), a further separation of variables is possible which then turns (245) into a second order ODE in just the radial variable z. Namely, in the case of spherical symmetry we have the general structure $q_{ab} = \gamma^2(z)\delta^3_a\delta^3_b + \rho(z)^2\Omega_{AB}\delta^A_a\delta^B_b,\ Q = \gamma\ \rho^2\sqrt{\det(\Omega)},\ N = N(z), N^a = N^3(z)\ \delta^a_3$

$$
\begin{aligned}
E &= \sqrt{\det(\Omega)}\ e,\ e = \frac{\gamma\rho^2}{N},\ A = \sqrt{\det(\Omega)}\ a,\ a = (e\ N^3\ \partial_z + \partial_z\ N^3\ e), \\
B &= \sqrt{\det(\Omega)}\ [b + c\ \Delta + N\gamma\rho^2\ U],\ b = -\partial_z\ N\ \gamma\rho^2[\gamma^{-2} - [\frac{N^3}{N}]^2]\ \partial_z,\ c = -N\gamma
\end{aligned} \tag{250}
$$

where Δ is the Laplacian on the sphere. Then, the separation Ansatz $w_\omega(z,y) = w_{\omega,l,m}(z)\ L_{l,m}(y)$ yields the ODE

$$
[\omega^2\ e + i\omega\ a - b_l]\ w_{\omega,l,m} = 0,\ b_l = b - l(l+1)\ c + N\gamma\rho^2 U \tag{251}
$$

and we have with $\mathfrak{h} = L_2(\mathbb{R},\ dz)$

$$< W_{\omega,l,m},\ W'_{\omega',l',m'} >= e^{i(\omega'-\omega)\tau}\ \delta_{l,l'}\ \delta_{m,m'}\ [(\omega+\omega')\ < w_{\omega,l,m},\ e\ w'_{\omega',l,m} >_{\mathfrak{h}} +i\ < w_{\omega,l,m},\ a\ w'_{\omega',l,m} >_{\mathfrak{h}}] \tag{252}$$

and

$$(\omega-\omega')\ [(\omega+\omega')\ < w_{\omega,l,m},\ e\ w'_{\omega',l,m} >_{\mathfrak{h}} +i\ < w_{\omega,l,m},\ a\ w'_{\omega',l,m} >_{\mathfrak{h}}] = 0 \tag{253}$$

One can find out more about the normalization of those solutions without actually computing them explicitly. These follow from the *Wronskian identities*. Let us abbreviate

$$g(z) = e\ N^3,\ f(z) = N\ \gamma\rho^2[\gamma^{-2} - [\frac{N^3}{N}]^2],\ u_l = -l(l+1)\ c + N\gamma\rho^2 U,$$
$$[\omega^2\ e + i\omega\ (g\ \partial_z + \partial_z\ g) + \partial_z\ f\ \partial_z - u_l]\ w_{\omega,l,m} = 0 \tag{254}$$

In the previous section and in (252) and (253) we have implicitly assumed that ia, $a = g\partial_z + \partial_z g,\ b = \partial_z f \partial_z$ are symmetric operators on $\mathfrak{h} = L_2(\mathbb{R}, dz)$, i.e., that no boundary terms are picked up when integrating by parts. In what follows we will drop this assumption, i.e., no assumptions about boundary terms will be needed. The inner product between two solutions is defined by (we drop the labels l, m as the solutions are rigorously orthogonal for $l \neq \tilde{l}, m \neq \tilde{m}$)

$$< W_\omega, \tilde{W}_{\tilde{\omega}} >= e^{i(\tilde{\omega}-\omega)\tau} \int dz\ \{[\overline{w_\omega}\ [(e\ \tilde{\omega} + i\ g\partial_z)\ \tilde{w}_{\tilde{\omega}}] + \overline{[(e\ \omega + i\ g\partial_z)\ w_\omega]}\ \tilde{w}_{\tilde{\omega}}\} \tag{255}$$

By construction, (254) is time-independent, therefore, taking the time derivative of (254) we find

$$0 = (\tilde{\omega}-\omega)\ \int dz\ \{[\overline{w_\omega}\ [(e\ \tilde{\omega} + i\ g\partial_z)\ \tilde{w}_{\tilde{\omega}}] + \overline{[(e\ \omega + i\ g\partial_z)\ w_\omega]}\ \tilde{w}_{\tilde{\omega}}\} \tag{256}$$

which means that the integral in (254) must be proportional to $\delta^{(1)}(\tilde{\omega}, \omega)$. On the other hand we have the *Green identity*, using that e, f, g are real-valued

$$\begin{aligned}
& \overline{w_\omega}\ [b\ \tilde{w}_{\tilde{\omega}}] - \overline{b\ w_\omega}\ \tilde{w}_{\tilde{\omega}} = \{\overline{w_\omega}\ f\ \tilde{w}'_{\tilde{\omega}} - \overline{w_\omega}'\ f\ \tilde{w}_{\tilde{\omega}}\}' \\
= & -\overline{w_\omega}\ [(\tilde{\omega}^2\ e\ + i\tilde{\omega}\ a - u_l)\ \tilde{w}_{\tilde{\omega}}] + \overline{[(\omega^2\ e\ + i\omega\ a - u_l)\ w_\omega]}\ \tilde{w}_{\tilde{\omega}}] \\
= & (\omega-\tilde{\omega})\ (\omega+\tilde{\omega})\ \overline{w_\omega}\ e\ \tilde{w}_{\tilde{\omega}} - i\ (\omega\ [a\ \overline{w_\omega}]\ \tilde{w}_{\tilde{\omega}} + \tilde{\omega}\ \overline{w_\omega}]\ [a\ \tilde{w}_{\tilde{\omega}}]) \\
= & (\omega-\tilde{\omega})\ [I - i\ g\ (\overline{w_\omega}\ \tilde{w}'_{\tilde{\omega}} - \overline{w_\omega}'\ \tilde{w}_{\tilde{\omega}}) - i\ (\omega\ [a\ \overline{w_\omega}]\ \tilde{w}_{\tilde{\omega}} + \tilde{\omega}\ \overline{w_\omega}]\ [a\ \tilde{w}_{\tilde{\omega}}]) \\
= & (\omega-\tilde{\omega})\ I - i\{\omega\ [(2g\ \overline{w_\omega}' + g'\ \overline{w_\omega})\ \tilde{w}_{\tilde{\omega}} + g(\overline{w_\omega}\ \tilde{w}'_{\tilde{\omega}} - \overline{w_\omega}'\ \tilde{w}_{\tilde{\omega}})] + \tilde{\omega}\ [\overline{w_\omega}\ (2g\ \tilde{w}'_{\tilde{\omega}} + g'\ \tilde{w}_{\tilde{\omega}}) - g(\overline{w_\omega}\ \tilde{w}'_{\tilde{\omega}} - \overline{w_\omega}'\ \tilde{w}_{\tilde{\omega}})]\} \\
= & (\omega-\tilde{\omega})\ I - i\{\omega\ [g\ (\overline{w_\omega}'\ \tilde{w}_{\tilde{\omega}} + \overline{w_\omega}\ \tilde{w}'_{\tilde{\omega}})g'\ \overline{w_\omega})\ \tilde{w}_{\tilde{\omega}}] + \tilde{\omega}\ [g\ (\overline{w_\omega}\ \tilde{w}'_{\tilde{\omega}} + \overline{w_\omega}'\ \tilde{w}_{\tilde{\omega}}) + g'\ \overline{w_\omega}\ \tilde{w}_{\tilde{\omega}}]\} \\
= & (\omega-\tilde{\omega})\ I - i\{(\omega+\tilde{\omega})\ g\ \overline{w_\omega}\ \tilde{w}_{\tilde{\omega}}\}'
\end{aligned} \tag{257}$$

where I is the integarnd of the integral in (254). We obtain the *Wronskian identity*

$$W'(w_\omega, \tilde{w}_{\tilde{\omega}}) := \frac{d}{dz}\ [\overline{w_\omega}\ f\ \tilde{w}'_{\tilde{\omega}} - \overline{w_\omega}'\ f\ \tilde{w}_{\tilde{\omega}} + i\ (\omega+\tilde{\omega})\ g\ \overline{w_\omega}\ \tilde{w}_{\tilde{\omega}}] = (\omega-\tilde{\omega})\ I \tag{258}$$

which holds for arbitrary solutions $w_\omega,\ \tilde{w}_{\tilde{\omega}}$ with the same l, m labels and frequencies $\omega, \tilde{\omega}$, respectively. The term in the square bracket on the left-hand side is the (generalized) Wronskian of the two solutions.

Formula (258) has two applications:

1. If we integrate (258) over $\mathbb{R}$ we find

$$< W_\omega,\ \tilde{W}_{\tilde{\omega}} >= e^{i(\tilde{\omega}-\omega)\ \tau}\frac{1}{\omega-\tilde{\omega}} \int dz\ W'(w_\omega, \tilde{w}_{\tilde{\omega}}) \tag{259}$$

In the present application of this formula, we anticipate singular behavior of the solution at $z = 0, \pm R$ hence, we interpret the r.h.s. of (259) as the *principal value*

$$\int dz\, W'(w_\omega, \tilde{w}_{\tilde{\omega}}) := \lim_{l\to 0+} [\int_{-\infty}^{-R-l} + \int_{-R+l}^{-l} + \int_{l}^{R-l} + \int_{R+l}^{\infty}]\, dz\, W'(w_\omega, \tilde{w}_{\tilde{\omega}})$$
$$= [W(w_\omega, \tilde{w}_{\tilde{\omega}})]_{-\infty}^{\infty} + \lim_{l\to 0+} ([W(w_\omega, \tilde{w}_{\tilde{\omega}})]_{-R-l}^{-R+l} + [W(w_\omega, \tilde{w}_{\tilde{\omega}})]_{-l}^{+l} + [W(w_\omega, \tilde{w}_{\tilde{\omega}})]_{R-l}^{R+l}) \quad (260)$$

Thus, the inner product between two solutions can be expressed in terms of their values and first derivatives at both spatial infinities plus a term that is exactly given by the *discontinuities* of the Wronskian at $z = 0, \pm R$. Indeed, as the coefficients of the second order ODE have singularities, we expect singularities of the second derivatives compatible with discontinuities of the first derivative.
Since the right-hand side of (259) does not vanish and becomes singular for $\omega = \tilde{\omega}$ we conclude that the solutions are not normalizable in the strict sense but in the generalized sense, i.e., the inner product will be proportional to $\delta^{(1)}(\omega, \tilde{\omega})$.
To read off the normalization constant $\kappa_{\omega,l,m}$ suppose that the discontinuity vanishes. Then, note that far out at infinity the solutions obey the flat space wave equations and thus will display a radial dependence corresponding to radial plane waves $e^{i\,\pm\omega z}/|z|$ while e, f grow as z^2. Then, we make use of the distributional identity

$$\lim_{z\to\infty} \frac{\sin(z(\omega - \tilde{\omega}))}{\pi(\omega - \tilde{\omega})} = \lim_{z\to\infty} \int_{-z}^{z} \frac{dz'}{2\pi}\, e^{iz'(\omega-\tilde{\omega})} = \delta(\omega, \tilde{\omega}) \quad (261)$$

The positive solution subspace is then selected to be the span of the $W_{\omega,l,m}$, $\kappa_{\omega,l,m} > 0$. To actually compute $\kappa_{\omega,l,m}$ we must of course gain sufficient knowledge on the solution and its first derivative near $z = -\infty$ once we specify those data near $z = \infty$ or vice-versa, paying attention to the singularities. This is a non-trivial task as one has to compute the influence of the curvature and its singularity at $z = 0$ as we follow the solution from $z = \infty$ to $z = -\infty$. We expect that methods from the theory of Heun functions [87] and the rich literature on the solutions of singular second order linear ODE's [103] can be employed.

2. For $\omega = \tilde{\omega}$ we see that the Wronskian is a constant. This leads to *Wronskian relations* between the solutions and their first derivatives at the two spatial infinities. Moreover, for $w_\omega = \tilde{w}_\omega$ we find the constant

$$f(\bar{w}_\omega\, w'_\omega - \bar{w}_\omega\, w'_\omega) + 2i\omega|w_\omega|^2 =: 2ic_\omega \quad (262)$$

Using the WKB decomposition $w_\omega = m_\omega\, e^{i\alpha_\omega}$ into modulus and phase we obtain

$$m_\omega^2\, [f\, \alpha' + \omega\, g] = c_\omega \quad (263)$$

which allows us to determine the phase exactly in terms of the modulus. The differential equation for w_ω can be split into real and imaginary parts and vanishing of the imaginary part is equivalent to (263). For the real part we find, using (262) and using the abbreviation $A := m_\omega^2$

$$[e\omega^2 - u_l]\, A^2 + \frac{1}{2}\, f'\, A\, A' - \frac{1}{f}(c_\omega^2 - \omega^2\, g^2\, A^2) + f(\frac{1}{2}A\, A'' - \frac{1}{4}(A')^2) = 0 \quad (264)$$

Unsurprisingly, this equation has a similar structure as the one for the modulus of the wave function in cosmology (both are obtained from the WKB Ansatz) whose iterative solution leads to the adiabatic vacua [90]. For $c_\omega = 0$ one can transform this into a first-order Riccati equation for $B = A'/A$.

8.4. Details for the GPG Background

We discuss some of the details of the required steps where we keep a close analogy with the treatment of the potential barrier problem of QED and the resolution of the Klein paradox (Schwinger effect, superradiant scattering) discussed in [102]. The analogy is only very rough: In contrast to (221) the external electric field of the potential barrier problem is finite everywhere and has at most jump discontinuities. However, both problems share the feature that the external potential is asymmetric under reflection of $z \to -z$ because in the past Kruskal universe the metric is given by ingoing GP coordinates while in the future universe, it is given by outgoing ones.

In what follows, we define past (P) and future (F) by GP time τ and forget about the past and future labels attached to the Kruskal universes: Every synchronous $\tau = \text{const.}$ surface crosses both Kruskal universes and has a "left" end (L) at spacelike infinity of the future Kruskal universe and a "right" end (R) in the past Kruskal universe. Thus, the P, L labels have very different meaning. Thus, in what follows:

P means $\tau \to -\infty$,
F means $\tau \to +\infty$,
L means $z \to -\infty \quad \Rightarrow \quad \bar{r} \to +\infty$,
R means $z \to +\infty \quad \Rightarrow \quad r \to +\infty$.

An observer in the infinite past P located a L can emit spherical waves into the spacetime which, therefore, must travel towards smaller values of $\bar{r}$ or larger values of z. Such a mode is described by $\frac{e^{-ikz}}{|z|}, k > 0$ (we define the radial momentum operator by $p = i\frac{x^a}{r}\,\partial_a = i\frac{d}{dz}$ so that $[p, z] = i$ and $p\ e^{-ikz} = k\ e^{ikz}$). Since at (P, L) the spacetime metric is flat and the potential U vanishes we have for a temporal dependence $e^{i\omega\tau}$ the dispersion relation $k^2 = \omega^2$, hence $k = |\omega|$. That wave will be transmitted and reflected by the curvature and will at F reach both ends L, R. The transmitted part travels to R at $z = \infty$ and is described by ${}^{-ikz}$, the reflected part travels to L and is described by e^{ikz}. Thus, we define the modes

$$W^{P,L}_{\omega,l,m} := N^{P,L}_{\omega,l,m}\,\frac{e^{i\omega\tau}}{|z|}\begin{cases} e^{-i|\omega|z} + R^{P,L}_{\omega,l,m}\,e^{i|\omega|z} & z \to -\infty \\ T^{P,L}_{\omega,l,m}\,e^{-i|\omega|z} & z \to \infty \end{cases} \tag{265}$$

where N, R, T are called normalization, reflection and transmission coefficients.

In complete analogy, we can consider emission from (P, R) of waves traveling towards smaller r, i.e., smaller z described by modes $e^{i|\omega|z}$. Now, the transmitted mode travels towards L and the reflected towards R again. Thus, we define the modes

$$W^{P,R}_{\omega,l,m} := N^{P,R}_{\omega,l,m}\,\frac{e^{i\omega\tau}}{|z|}\begin{cases} T^{P,R}_{\omega,l,m}\,e^{i|\omega|z} & z \to -\infty \\ e^{i|\omega|z} + R^{P,R}_{\omega,l,m}\,e^{-i|\omega|z} & z \to \infty \end{cases} \tag{266}$$

An observer in the infinite future F located at L can receive waves that travel to larger values of $\bar{r}$, i.e., smaller values of z. Those waves are the result of a superposition of two waves coming from (P,L) and (P,R), respectively. The wave from (P,R) looks like a a wave transmitted from (F,L) if we travel to the past while the wave from (P,L) looks like a wave reflected from (F,L) if we travel to the past. This gives the modes

$$W^{F,L}_{\omega,l,m} := N^{F,L}_{\omega,l,m}\,\frac{e^{i\omega\tau}}{|z|}\begin{cases} e^{i|\omega|z} + R^{F,L}_{\omega,l,m}\,e^{-i|\omega|z} & z \to -\infty \\ T^{F,L}_{\omega,l,m}\,e^{i|\omega|z} & z \to \infty \end{cases} \tag{267}$$

In complete analogy, an observer in F located at R can receive waves traveling towards increasing r, i.e., larger values of z and is described by $e^{-i|\omega|z}$ which is the result of a superposition of waves from P from both ends where the wave from L and R looks as transmitted and reflected, respectively, from (F,R) when followed towards the past. Thus, we define the modes

$$W^{F,R}_{\omega,l,m} := N^{F,R}_{\omega,l,m}\,\frac{e^{i\omega\tau}}{|z|}\begin{cases} T^{F,R}_{\omega,l,m}\,e^{-i|\omega|z} & z \to -\infty \\ e^{-i|\omega|z} + R^{F,R}_{\omega,l,m}\,e^{i|\omega|z} & z \to \infty \end{cases} \tag{268}$$

For both choices of P, F, the modes labeled by $* \in \{L, R\}$, $\omega \in \mathbb{R}$, $0 \leq |m| \leq l \in \mathbb{N}_0$ are complete generalized orthonormal bases of the Krein–Hilbert space but given $*, l, m$ only for $\omega \in \Delta^{P/F}_{+,*,l,m}$ correspond to positive norm solutions with respect to the 1-particle inner product (224) which selects the annihilation operators $A^{P/F,*}_{\omega,l,m} =< W^{P/F,*}_{\omega,l,m}, \Phi >$, $\omega \in \Delta^{P/F}_{+,*,l,m}$. Thus, there will be particle production in the sense that the observers at P,F do not agree on what the zero particle (vacuum state) is when the sets $\Delta^{P/F}_{+,l,m} := \Delta^{P/F}_{+,L,l,m} \cup \Delta^{P/F}_{+,R,l,m}$ do not coincide.

These sets will be in bijection with $\mathbb{R}_+$, i.e., we have bijections $b^{P/F}_{l,m} : \mathbb{R}_+ \to \Delta^{P/F}_{+,l,m}$. Given $\omega \in \mathbb{R}_+, l, m$ we define the Fock space $\mathcal{H}^{P/F}$ as the excitations by the modes $b^{P/F}_{l,m}(\omega), l, m$ of the Fock vacuum $\Omega^{P/L}$. If these Fock spaces are the same, that is, when Ω^F constructed as the excitation by particle pairs of Ω^P is normalizable in $\mathcal{H}^P$, then the unitary S-matrix S defined by the matrix elements

$$< \psi^F_\alpha, \psi^P_\beta >=:< \psi^F_\alpha, S\psi^F_\beta >=< \psi^P_\alpha, S\psi^P_\beta > \tag{269}$$

will be non-trivial.

We note that the four sets of modes $W^{P/F,L/R}_{\omega,l,m}$ with asymptotics given in (265)–(268) allow us to compute their inner products via (259) and (260) in terms of the twelve complex numbers $N^{P/F,L/R}_{\omega,l,m}$, $R^{P/F,L/R}_{\omega,l,m}$, $T^{P/F,L/R}_{\omega,l,m}$. The modulus $|N^{P/F,L,R}_{\omega,l,m}|$ will be fixed by the condition that the corresponding $\kappa^{P/F,L/R}_{\omega,l,m}$ equals ± 1.

Further analysis has to take the concrete details of (221) and the potential into account. One finds explicitly

$$\begin{aligned} &N = 1,\ N^3 = \sqrt{\frac{R}{|z|}},\ e = z^2,\ g = eN^3,\ f = e(1 - [N^3]^2), U = \frac{(1 - s^2)\ R}{|z|\ z^2}, \\ &u_l = e\left(\frac{l(l+1)}{z^2} + U\right) = l(l+1) + (1 - s^2)\ (N^3)^2 \end{aligned} \tag{270}$$

where $s = 0, 1, 2$ is the spin of the field (scalar, vector, tensor).

We see that f grows as z^2 while g only as $|z|^{3/2}$ and thus its contribution to the Wronskian vanishes at infinity since by (265)–(268) the solutions decay as $|z|^{-1}$. It follows (drop labels l, m)

$$\lim_{z \to \pm\infty} W(w_\omega, \tilde{w}_{\tilde{\omega}})(z) = \lim_{z \to \pm\infty} [\overline{|z|\ w_\omega}\ (|z|\tilde{w}_{\tilde{\omega}})' - (\overline{|z|\ w_\omega})'\ (|z|\tilde{w}_{\tilde{\omega}})] \tag{271}$$

It is not difficult to see that equality of (271), which holds in the absence of discontinuities, at $z = \pm\infty$ for $\omega = \tilde{\omega}$, $w_\omega = \tilde{w}_\omega = w^{P/L,L/}_{\omega,l,m}$ gives the continuity equations

$$1 = |R^{P/L,L/R}_{\omega,l,m}|^2 + |T^{P/L,L/R}_{\omega,l,m}|^2 \tag{272}$$

8.5. Particle Production and Hawking Radiation in BHWHT Spacetime

Assuming that these interesting challenges can be met, one then would have access to QFT on a BHWHT spacetime, i.e., the quantum field is given by

$$\Phi = \sum_{l,m} \int_{\Delta_{+,l,m}} d\omega\ \{A_{\omega,l,m}\ W_{\omega,l,m} + c.c.\};\ \ \Delta_{+,l,m} = \{\omega \in \mathbb{R};\ \kappa_{\omega,l,m} > 0\} \tag{273}$$

This has several aspects. One may construct modes that look like those of Minkowski space for $z = r \to \infty, \tau \to -\infty$ in the past universe or for $z = -\bar{r} \to -\infty, \tau \to +\infty$ in the future universe. This selects the corresponding Fock vacua Ω_P, Ω_F and particle number operators $N_P = A^*_P A_P, A_P\Omega_P = 0$ and $N_F = A^*_F A_F, A_f\Omega_F = 0$ and one may study the particle content of F particles in the P state $< \Omega_P, N_F\Omega_P >$ or vice versa which may be interpreted as particle creation effect due to curvature and singularity. Or one may consider only the

SS portion of the past universe (or the MSS portion of the future universe) and construct a Fock representation with respect to the Schwarzschild time t foliation in the SS (or MSS) portion. One can expand the spacetime field Φ in SS with respect to both sets of mode systems and compute A_{SS} in terms of A_P, A_P^* (Bogol'ubov coefficients). This would be the analog of the Unruh effect with the free-falling GP observer and stationary SS observer, respectively, playing the role of the inertial and accelerated observer. As usual, the selection of say, the P vacuum is not unique and may wonder whether there exists a choice for which the two-point function $< \Omega_P, \Phi(\tau, x)\ \Phi(\tau', x')\Omega_P >$ has the short-distance singularity structure of Minkowski space (Hadamard state [90]) which has an elegant reformulation in terms of the wave front set of this two point function [104].

9. Quantization and Backreaction

In this section, we discuss further challenges of quantum black hole perturbation theory without going into much detail.

Let us summarize: The concrete expression for the physical or reduced Hamiltonian which depends only on the true X, Y, P, Q degrees of freedom cannot be provided in closed form but can be approximated in terms of two distinct perturbative hierarchies: First, the deviation from spherical symmetry as parametrized by the perturbations X, Y which are considered as of first order. Second, an inverse core mass expansion. The first expansion arises from the split of the degrees of freedom into spherically symmetric and spherically non-symmetric sets and is a simple canonical transformation on the phase space. This step is, in principle, non-perturbative and can be performed exactly in closed form if one uses an equivalent polynomial form of the constraints. The expansions come into play upon the solution of the constraints for the momenta: First, as the constraints depend non-linearly on the momenta, we obtain an infinite set of non-linear constraints which are challenging to solve non-perturbatively as is known already from finite-dimensional algebraic geometry [105]. However, exploiting the first perturbative hierarchy this becomes feasible as shown in [61] provided one can solve the zeroth order equations of that scheme. It is this assumption that triggers the second perturbative hierarchy: The zeroth order constraints (one for each value of the radius) are still nonlinear in the symmetric momenta but almost decoupled. The coupling is via the fact that the constraints depend on radial derivatives. There would be no second hierarchy necessary if one could solve that ODE system exactly. However, unless there is no scalar hair, this is not the case and thus we must release the inverse core mass expansion as a second approximation scheme of the Picard–Lindelöf type. Here, the core mass is identified as an integration constant in that system of zeroth order differential equations which reduce to the Schwarzschild mass in the absence of scalar hair (in which case the core mass equals the ADM mass). From here on at each order in the first perturbative scheme, one just has to solve linear ODE systems for which uniqueness and existence results as well as efficient approximation schemes are available. The inverse mass expansion continues to play an important role also in those higher orders.

At any order with respect to both expansions, the approximate expression for $H_{\rm red}$ depends non-polynomially on the core mass $\hat{M}$ and polynomially on the fields Q, P, X, Y in terms of nested radial integrals and multiple sums over the harmonic labels l, m. Its quantization is, therefore, challenging in two aspects: First, it is not clear that the operators $\hat{M}^n,\ n \in \mathbb{Z}$ can be densely defined. This question has been answered affirmatively in [96,106]. Second, consider the energy density $e_{KG}(r)$ of the symmetric Klein–Gordon field which is a quadratic function of P^{KG} and a polynomial function of Q_{KG} (that polynomial has degree two unless the scalar field is self-interacting). Then, one can envisage a Fock quantization of the total Klein–Gordon Energy $E_{KG} = \int_0^\infty\ ds\ e_{KG}(s)$. However, the physical Hamiltonian depends on the nested radial integrals of the form

$$\int_0^\infty\ ds\ e_{KG}(s)\ \int_0^s\ dt\ e_{KG}(t) \tag{274}$$

and not on polynomials of E_{KG}. The energy density integral with a sharp radial cut-off could be problematic in QFT and perhaps must be regularized by smoothening the cut-off. Upon removal of the regulator, the result could retain a regulator dependence which must be controlled.

Next, we come to the question of backreaction beyond the backreaction on the spacetime causal structure discussed in Section 3. To avoid misunderstanding, the notion of backreaction used in this work is *not* that of the semiclassical Einstein equations $G(g) :=< T(g) >_g$ where $G(g)$ is the classical Einstein tensor, $T(g)$ the quadratic form corresponding to the matter energy-momentum tensor and $< . >_g$ is a positive linear functional on the Weyl algebra $\mathfrak{A}_g$ of the (free) spacetime matter fields which are supposed to solve the (free) Heisenberg equations generated by (the quadratic part of) the matter Lagrangian in the background metric g. The reasons are manifold: First of all, the semiclassical Einstein equations treat g as a classical field rather than a quantum field. Second, they are supposed to be diffeomorphism covariant rather than singling out a preferred gauge condition and thus do not distinguish between true and gauge degrees of freedom. This has the following consequences: Not only is it a complicated task to find a self-consistent metric that solves these equations because the state $< . >_g$ depends on g as well, it also is inconsistent with the Bianchi identity $\nabla_g \cdot G \equiv 0$ if one does not carefully supplements the chosen (normal) ordering by suitable counter terms which, for example, is responsible for the trace anomaly in conformally invariant theories [18]. By contrast, our notion of backreaction is in the context of quantum gravity in which we quantize the metric as well after reducing the phase space so that only the true degrees of freedom are quantized, the issue of gauge invariance has been solved from the outset and no Bianchi identities have to be obeyed. In fact, it is not even a priori clear what one would mean by a "quantum Bianchi identity". A possible interpretation of this term would be to try to construct a quadratic form corresponding to the classical objects $\nabla_g, G(g)$ where g is to be replaced by the quantum metric and then to consider $\nabla_g \cdot G(g)$. Due to the non-commutativity of operator-valued distributions involved, this is unlikely to vanish identically as a quadratic form, at best we expect it to vanish to zeroth order in $\hbar$ when computing the expectation value of the quadratic form with respect to semiclassical (low fluctuation) states.

Having clarified this, consider first the classical theory. Given the Hamiltonian $H = H(P, Q, X, Y)$ we can, in principle, solve the classical Hamiltonian equations of motion given initial data. To simplify the notation let $R = (P, Q),\ Z = (Y, X)$ with initial data (R_0, Z_0). Consider first an arbitrary function $R(\tau)$ and solve the Hamiltonian equations of motion $\dot{Z}^R_{Z_0}(\tau) = \{H, Z\}_{R=R(\tau), Z=Z^R_{Z_0}(\tau)},\ Z^R_{Z_0}(0) = Z_0$ where $H(\tau, Z) = H(Z(R(\tau), Z)$ is considered as an explicitly time-dependent Hamiltonian. The solution will be a function $Z^R_{Z_0}(\tau)$ which depends on the chosen $R(\tau)$. It can be obtained by Picard–Lindelöf iteration $Z^R_{Z_0}(\tau) = Z_0 + \int_0^\tau\ ds;\ \{H, Z\}_{R=R(\tau), Z=Z^R_{Z_0}(s)}$ and thus depends on nested integrals of $R(\tau)$. Now, we set $R(\tau) = R_{R_0,Z_0}(\tau)$ and solve the Hamiltonian equations of motion $\dot{R}_{R_0,Z_0}(\tau) = \{H, Z\}_{R=R_{R_0,Z_0}(\tau), Z=Z^{R_{R_0,Z_0}}_{Z_0}(\tau)},\ R_{R_0,Z_0}(0) = R_0$. This takes the form of an integro differential equation which contains memory and friction terms and whose parametric dependence on Z_0 is considered as "noise" or "environment". If one has only statistical knowledge about Z_0 one can consider it as a random variable leading to a Langevin type [107] of equation or one can average over the Z_0 dependence which leads to corresponding "master" equations. If one has specific knowledge about the initial state Z_0 and can motivate a certain specific Z_0 as given, one may try to obtain an effective Hamiltonian which governs the integro-differential equation.

In the quantum theory, we see that in the statistical approach we enter the regime of open quantum systems, decoherence, entanglement, partial tracing and non-equilibrium statistical mechanics [108] which leads to master equations of Lindbladt type for the "statistical operator", i.e., the density matrix that replaces Z_0. In the effective approach of the quantum theory one tries to solve the exact Schrödinger or Heisenberg equations following the above idea of the classical theory of solving first the equations for the X, Y

sector and after that for the Q, P sector. To conduct this one assumes that the physical Hilbert space is a tensor product $\mathcal{H} = \mathcal{H}_f \otimes \mathcal{H}_s$ where $\mathcal{H}_f,\ \mathcal{H}_s$, respectively, describe the "fast" X, Y and "slow" Q, P degrees of freedom. The terminology comes from the well-known Born–Oppenheimer-Approximation (BOA) scheme [109] that was invented for molecular physics and for which the huge differences in the masses of electrons and nuclei leads to a natural hierarchy of time scales of these two types of degrees of freedom so that the fast particles move essentially as if the slow particles were at rest with only a weak (adiabatic) correction governed by an adiabatic parameter ϵ (the quotient of electrons and nuclei masses). Thus, the BOA works very well for systems with 1. finitely many fast degrees of freedom, 2. finitely many slow degrees of freedom, such that 3. the interaction between the two subsystems depends only on a commuting set of slow degrees of freedom (typically Q), such that 4. a natural adiabatic parameter ϵ exists and such that 5. the Hilbert space representation is of the tensor product type as above.

In the application of black hole perturbation theory the first four assumptions all fail when incorporating matter "hair" in addition to Maxwell fields such as the Klein–Gordon or Fermion fields. First, assumption 3 is violated as the interaction involves both P, Q variables which do not commute in quantum theory. A natural extension of BOA which relaxes 3 is space adiabatic perturbation theory (SAPT) which However, still rests on the validity of assumptions 1, 2, 4 while 5 is trivially satisfied for finite dimensional systems. In [72] SAPT was applied to the simpler case of quantum cosmology for which the slow sector has only finitely many degrees of freedom, hence assumption 2 holds. The relaxation of assumption 1 is non-trivial because assumption 5 is now no longer granted as the Hilbert space representation of the fast sector depends on the slow sector variables and the corresponding are not necessarily unitarily equivalent. However, the obstacles can be overcome perturbatively. Already in quantum cosmology also assumption 4 is violated because there is no mass hierarchy between the homogeneous modes of a scalar inflaton field and its non-homogeneous perturbations. This obstacle can be overcome as follows: The adiabatic effective decoupling of the slow and fast sectors rests on the Weyl quantization of the slow system in terms of the variables $Q, P' := \epsilon P$ where ϵ is the adiabatic parameter. Now, even if the reduced Hamiltonian $H(X, Y, Q, P)$ does not have a natural such parameter, using that H depends polynomially on P we can multiply H by ϵ^N where N is the smallest positive integer such that $H_\epsilon(X, Y, Q, P') := \epsilon^N\ H(X, Y, Q, P = \frac{P'}{\epsilon})$ has no negative powers of ϵ. Then, SAPT can be formally applied to H_ϵ which allows to compute an effective Hamiltonian $H_{\epsilon,n,k}(Q, P')$ for each energy band n of the fast sector and k is the order of the adibatic expansion. In the end, we set $\epsilon := 1$ which can be considered as a kind of analytic extension. In this way the adiabatic parameter just serves to organize the adiabatic perturbation and is removed in the end. It is of course not granted that resulting effective Hamiltonians $H_{n,k} = H_{\epsilon=1,n,k}$ converge in any sense.

This still leaves condition 2, which in contrast to quantum cosmology is violated for quantum black holes: The symmetric degrees of freedom are just spherically symmetric and not homogeneous and thus defining an effectively 1+1 dimensional field theory on the radial z-axis rather than a 1+0 dimensional mechanical system. In order to apply SAPT this calls for the Weyl quantization of a field theory which is problematic [110]. As a first step one may apply the following regularization of the problem: Let $b_I,\ I = 0, 1, 2, \ldots$ be an on ONB of $\mathfrak{h} = L_2(\mathfrak{R}, dz)$ and consider the conjugate variables $Q_I =< b_I, Q >_{\mathfrak{h}},\ P_I =< b_I, Q >_{\mathfrak{h}}$. We now expand $H(X, Y, Q, P)$ into the Q_I, P_I using completeness $Q = \sum_I\ Q_I\ b_I$ and for given "mode cut-off" $0 < M < \infty$ set to zero for all instances of $Q_I, P_I,\ I > M$ which may be called a truncation. The resulting Hamiltonian $H_M(X, Y, \{Q_I, P_I\}_{I=0}^M)$ can then be treated by SAPT methods as above and one may study in which way one can remove the cut-off M.

10. Observation, Radiation Energy and Flux

Since we have a concrete expression for a physical Hamiltonian $H[P, Q, X, Y]$ at our disposal which depends only on the true degrees of freedom P, Q, X, Y we can write it in the form

$$H[P, Q, X, Y] = \int_\sigma d^3x\; h[P, Q, X, Y; x) \tag{275}$$

where h can be interpreted as the energy volume density observed by the free-falling observers. From the way it is constructed perturbatively in terms of nested radial integrals using the inverse core mass expansion, it is spatially non-local, explicit spatially but not explicitly τ dependent as the system is conservative and at any finite order in perturbation theory a polynomial in the canonical fields and their spatial derivatives up to a finite order N. Since h, therefore, depends generically spatially non-locally on the fields we used a square bracket notation with respect to the dependence of h on them and a round bracket notation with respect to the explicit x dependence.

To compactify the notation we write $R = (Q, X),\; Z = (P, Y)$. The variation of (275) is then given by

$$[\delta H][R, Z] = \sum_{k=0}^{N} \int_\sigma d^3y \int_\sigma d^3x\; \{r^{a_1 \ldots a_k}(y, x)\; [\delta R]_{,a_1 \ldots a_k}(x) + z^{a_1 \ldots a_k}(y, x)\; [\delta Z]_{,a_1 \ldots a_k}(x)\} \tag{276}$$

where the integral kernels displayed are themselves nested integrals over polynomials in R, Z and their spatial derivatives up to order N. They can be found by collecting in the expression for δH all instances of, e.g., $[\delta R]_{,a_1 \ldots a_k}(z)$ where z is one of the integration variables in the nested integrals and then relabeling integration variables $z \leftrightarrow x$. The Hamiltonian equations of motion are obtained by integrating parts, dropping boundary terms

$$\dot{R}(x) = \sum_{k=0}^{N} (-1)^k \int d^3y\; [r^{a_1 \ldots a_k}(y, x)]_{,a_1 \ldots a_k},\quad -\dot{Z}(x) = \sum_{k=0}^{N} (-1)^k \int d^3y\; [z^{a_1 \ldots a_k}(y, x)]_{,a_1 \ldots a_k}, \tag{277}$$

where the multiple partial derivatives are with respect to the argument x.

Let now $S(\tau) \subset \sigma$ be a compact region in σ then the object

$$E_{S(\tau)} = \int_{S(\tau)} d^3x\; h[R(\tau), Z(\tau); x) \tag{278}$$

is the energy content of the region $S(\tau)$ where the τ dependent fields satisfy the above Hamiltonian equations of motion, e.g., $\dot{X} = \{H, X\}$. Then, $P_{S(\tau)} = \frac{d}{d\tau} E_{S(\tau)}$ is the total power emitted/absorbed from $S(\tau)$. To obtain an energy flux area current one usually resorts to the Lagrangian framework and extracts the on-shell conserved Noether current from the symmetry of the Lagrangian under foliation time translations, formally corresponding to the conserved time component of the canonical energy momentum tensor. We could proceed like this here as well by formally computing the Legendre transform of the Hamiltonian but since we expect H to depend higher than quadratically on Z and since the relation between momenta and velocities will involve integro differential equations one will have trouble to compute the Legendre transform sufficiently explicitly.

Fortunately this is not necessary. All that is needed is the Hamiltonian. To see how this works in a familiar setting consider the Hamiltonian density $h = \frac{1}{2}[\vec{E}^2 + \vec{B}^2]$ of free Maxwell theory on Minkowski space where $\vec{B} = \vec{\nabla} \times \vec{A}$ is the magnetic field of the vector potential $\vec{A}$ which has canonical brackets with the electric field $\vec{E}$. The equations of motion resulting from $H = \int d^3x\; h$ are the familiar vacuum Maxwell equations $\dot{B} = \vec{\nabla} \times \vec{E},\; \dot{E} = -\vec{\nabla} \times \vec{B}$. Consider a compact region $S \subset \mathbb{R}^3$ and its energy content $E(S) = \int_S d^3x\; h$ evaluated on a solution of Maxwell's equations. Then,

$$\dot{E}(S) = -\int_S d^3x\; \vec{\nabla} \cdot [\vec{E} \times \vec{B}] = -\int_{\partial S} d\Sigma_a\; [\vec{E} \times \vec{B}]^a \tag{279}$$

which correctly yields the Poynting vector $\vec{J} = \vec{E} \times \vec{B}$ as energy current area density. In other words with $J^\tau = h$ the four-vector J^μ is conserved on shell.

We proceed analogously in the present more complicated situation. From (276) we have for a time independent set S

$$\dot{E}(S) = \sum_{k=0}^{N} \int_S d^3y \int_\sigma d^3x \; \{r^{a_1...a_k}(y,x) \; [\dot{R}]_{,a_1...a_k}(x) + z^{a_1...a_k}(y,x) \; [\dot{Z}]_{,a_1...a_k}(x)\} \tag{280}$$

We integrate the spatial derivatives successively by parts. In the course of this process we may pick up boundary terms or not depending on the distributional properties of the integral kernels r, z. Typically, if $r^{a_1...a_k}(y,x)$ depends on $l \leq k$ nested integrals, then the first l integrations by parts do not generate any boundary terms but each integration by parts removes one nested integral. Thus, rearranging terms by performing integrations by parts that do not generate boundary terms, one may rewrite (280) as

$$\dot{E}(S) = \int_S d^3y \int_\sigma d^3x \; \{\hat{r}(y,x) \; \dot{R}(x) + \hat{z}(y,x) \; \dot{Z}(x)\} + \sum_{k=1}^{N} \int_S d^3x \; \{\hat{r}^{a_1...a_k}(x) \; [\dot{R}]_{,a_1...a_k}(x) + \hat{z}^{a_1...a_k}(x) \; [\dot{Z}]_{,a_1...a_k}(x)\} \tag{281}$$

where the second term is now ultra-local. We now perform the remaining integrations by parts and obtain a bulk term and a surface term. The bulk term is given by (280) with all integrations by parts performed and all boundary terms dropped, that is

$$0 = \sum_{k=0}^{N} (-1)^k \int_S d^3y \int_\sigma d^3x \; \{r^{a_1...a_k}_{,a_1...a_k}(y,x) \; [\dot{R}](x) + z^{a_1...a_k}_{,a_1...a_k}(y,x) \; [\dot{Z}](x)\} \tag{282}$$

where the equations of motion (277) were used. The surface term is given by

$$-J^a := \sum_{k=1}^{N} \sum_{l=1}^{k} (-1)^{l+1} \int_{\partial S} d\Sigma_{a_1} \; \{\hat{r}^{a_1...a_k}_{,a_2...a_l}(x) \; [\dot{R}]_{,a_{l+1}...a_k}(x) + \hat{z}^{a_1...a_k}_{,a_2...a_l}(x) \; [\dot{Z}]_{,a_{l+1}...a_k}(x)\} \tag{283}$$

where it is understood that the spatial derivatives in (283) are simply absent when the indices are out of range.

The on-shell conserved energy Noether current can now be determined: it is given by J^μ with $J^\tau = h$ and J^a as in (283) where $\dot{R}, \dot{Z}$ are to be replaced by (277). In particular, given a surface element s, $\int_s d\Sigma_a \; J^a$ is the power flowing through s. Using appropriate solutions of the field equations one can now compute the classical radiation power through any surface similar as in usual second order perturbation theory [111].

Similarly, in the quantum theory, one can define at second order, the grey body factors $\sigma_{\omega,l,m}$ of the radiation in the usual way for each bosonic degree of freedom [62–64]

$$\lim_{r\to\infty} \omega_\beta[\int_{s(r)} d\Sigma_a J^a] =: -\sum_{l,m} \int d\omega \; \frac{\sigma_{\omega,l,m}}{\exp(\beta\,\omega) - 1} \tag{284}$$

where $s(r)$ is a round sphere at radius r and β is the inverse temperature, expected to scale as $1/M$, of a corresponding KMS state ω_β which we consider as restriction of the GP vacuum state to the SS portion in a similar way as the Unruh KMS state arises by restriction of the Minkowski vacuum state [13] to the Rindler wedge. The form of (284) in fact has been confirmed for second order perturbation theory using mode functions of the type discussed in Section 8 but restricted to an asymptotic SS region. More in detail, there one works with the turtoise coordinate $z = r_* = r + R\ln(r/R - 1),\; r > R = 2M$ rather than the GPG coordinate z and observes that the potential that enters the Schrödinger type equation rewritten in terms of z vanishes at both $z = \pm\infty$ being positive in between with a maximum around the photon sphere $r = 3M$. Hence, the mode function problem becomes a regular quantum mechanical scattering problem, see [111] for all the details. One can work with either SS null coordinates $u = t - z,\; v = t + z$ or corresponding Kruskal null coordinates V, U and the KMS state here arises by restricting the Kruskal vacuum state of one full Kruskal universe (SS, BH, WH, MSS; Hartle–Hawking state) to the SS portion (the quantum field is written in terms of u, v mode functions defining the Boulware state which are then expanded into U, V mode functions defining the Hartle–Hawking state which gives rise to non-vanishing Bogol'ubov coefficients in (284)).

Remark 9. It should be noted that there is some debate about which Noether current to use for the gravitational radiation in order to derive the radiation formulae, often the Landau–Lifshitz pseudo tensor is argued for [112], or one proceeds as sketched above, perturbs the Lagrangian to the second order and then computes the canonical (Noether) energy-momentum tensor. In the present situation we have a natural candidate as derived above and it would be interesting to compare the different formalisms at least at second-order.

Remark 10. Note, that the Schwarzschild stationary and Gullstrand–Painleveé free falling clocks at distances far away from the black hole tick at the same rate but they have a radius-dependent offset. Far away from the black hole, during a short amount of time, the GP observer is barely picking up speed if previously at rest and thus the radius is approximately constant during observation. An astronomer on Earth can be argued to be rather free falling toward a black hole rather than being stationary as one cannot prevent Earth from being attracted to the black hole. However, for both observers, the time passed during observation is the same to high accuracy.

Remark 11. When the set $S(\tau)$ itself is time-dependent then the radiation formula for $\frac{d}{d\tau}\, E(S(\tau))$ must be corrected by the term that takes the time change in $S(\tau)$ into account. The application would be a trapped region $S(\tau)$ with τ dependent profile function $\rho_\tau : S^2 \to \mathbb{R}_+$ and $S(\tau) = \{(r, \Omega),\ r \leq \rho_\tau(\Omega),\ \Omega \in S^2\}$. Then, the correction term for the time dependence of $E(S(\tau)) = \int\, d\Omega\, \int_0^{\rho_\tau(\Omega)}\, dr\, h$ is given by

$$\int_{S_2} d\Omega\, \dot{\rho}_\tau(\Omega)\, h(r = \rho_\tau(\Omega), \Omega) \tag{285}$$

which due to the dependence of ρ_τ on the gravitational radiation variables X, Y is by itself a rather complicated functional of the true degrees of freedom.

11. Conclusions and Outlook

To define interacting, gauge invariant black hole perturbations of geometry and matter is a complicated topic for which many conceptual and technical questions have to be answered. In this paper, we have attempted a concrete proposal. The basic idea is to divide the problems into several steps. The first step consists of disentangling gauge invariance from perturbation theory already in the classical theory. Thus, one first constructs the non-perturbative reduced phase space (true degrees of freedom) and physical Hamiltonian and then perturbs it directly in terms of the gauge invariant perturbations which are defined as those true degrees of freedom which are non (spherically or axi) symmetric. Having access to both the black hole interior and the exterior at the same time puts restrictions on the choice of the true degrees of freedom (equivalent to the choice of a congruence of observers), and therefore, we have opted for the Gullstrand–Painlevé gauge. The second step consists in quantizing the true degrees of freedom, both the symmetric and nonsymmetric ones, in suitable representations of the canonical commutation relations which are such that the physical Hamiltonian, perturbed to the desired order of accuracy is at least a well-defined quadratic form.

Since the dependence of the perturbed Hamiltonian on the symmetric true degrees of freedom typically is non-polynomial while it depends non polynomially on the symmetric true degrees of freedom, one has to use different quantization techniques for these two sets of degrees of freedom. This observation has already been made in quantum cosmology where one uses a so-called "hybrid" approach [59,60] and uses a Narnhofer–Thirring type representation [77,78] for the symmetric (homogeneous) degrees of freedom while the non-symmetric ones are treated in a Fock representation. In [113,114] we have recently shown that one can in fact also use Fock representations for the non-polynomial dependence of the Hamiltonian if one carefully chooses the dense domain of the quadratic form, for instance, as the span of the excitations of a coherent state concentrated on a 3-metric Euclidean signature. This stresses once more the importance of states that describe non-degenerate quantum metrics as emphasized in [115,116] in a different context.

In this paper we only have proposed a possible framework but of course the real task to describe black hole evaporation is still to be conducted. In our companion papers [67–69] we perform the first steps. These consist of showing that our approach reproduces the known classical second-order results due to Regge–Wheeler, Zerilli and Moncrief [52–55] outside the Horizon in the Einstein–Maxwell sector after one translates our reduced Hamiltonian into the Schwarzschild coordinates used in [52–55]. More in detail, in [67] we consider pure gravity perturbations while in [68] we add electromagnetic perturbations. While in [67,68] we perform the reduced phase space analysis in the GP gauge, in [69] one considers more general gauges which are merely asymptotically GP, directly for both gravity and electromagnetic perturbations. In all cases, non-trivial canonical transformations on the reduced phase space have to be performed to show that the equations of motion generated by the reduced Hamiltonian agree with those of [52–55]. However, this is just a consistency check. The real virtue of our method is that it enables to construct the reduced Hamiltonian also to higher than second orders without the necessity to change the gauge invariant (true) degrees of freedom when increasing the order and thus to describe self-interactions among the symmetric and non-symmetric true degrees of freedom, respectively, as well as interaction (backreaction) between them. This requires a better understanding of the Fock representation that is suggested by the second order part of the reduced Hamiltonian. We have started this investigation in the present paper but the construction of the mode functions in a black hole–white hole transition spacetime that we considered is an interesting mathematical challenge in itself and we certainly must know more about their properties before we can proceed. This is not even under full control in an asymptotic end of a black hole. However, once this is conducted, one can study the quantum dynamics of interesting measures of evaporation such as the quantum area of the apparent horizon for which we have given a perturbative formula in the present paper and which can be quantized by the tools provided in [113,114]. This will be the subject of future publications within this series which will allow us to study the (perturbative) mass spectrum defined by the apparent horizon.

The methodology of the present manuscript can be readily applied also to cosmology or rotating black holes. But even for spherically symmetric black holes there is a huge amount of work to be conducted whose steps we described rather concretely in the present work. The list of these steps is not at all exhaustive, many interesting questions were not touched upon. For instance, in the asymptotically flat context of black hole spacetimes one has access to the ten Poincaré generators as Dirac observables. It would be interesting to derive the (perturbative) reduced phase space formulae for those and to quantize them. In the present paper we have sketched the corresponding tasks only for one of these generators, the reduced Hamiltonian, but the same methods can be used to construct the remaining Poincaré generators.

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Appendix A. Reduced Phase Space and Gauge Fixing of Constraints with Spatial Derivatives

The reduced phase space of the constrained system is conveniently obtained by solving the constraints for suitable momenta, imposing gauge fixing conditions on the conjugate configuration degrees of freedom and determining the values of the smearing functions of the constraints from the corresponding stability conditions of the gauge imposed. The physical Hamiltonian is then determined by those three solutions of the constraints, gauge fixing conditions and stability conditions.

In this section, we review that there is an important difference between A. constraints depending purely algebraically on the canonical fields and B. constraints involving spatial derivatives of these. Namely in case A, the reduced phase space is smaller by at least one canonical pair than in case B. This section serves as a preparation to understand in later sections why even in spherically symmetric vacuum GR there are two rather than one Dirac observable and why this is not in conflict with Birkhoff's theorem.

To understand this in non-technical terms, consider a 1 + 1 dimensional field theory on $\mathbb{R}^2$ with canonically conjugate fields $(q(x), p(x)),\ x \in \mathbb{R}$ and the following constraints

$$A.\quad C(x) = p(x),\ B.\quad C(x) = p'(x) \tag{A1}$$

where $(.)' = \frac{d}{dx}$.

For a field theory, it is not sufficient just to state that $\{p(x), q(y)\} = \delta(x, y)$, a complete characterization of the phase space must also specify the space of functions to which q, p belong which among other things involves their decay behavior at spatial infinity. One of the conditions is that the symplectic structure

$$\Omega = \int_{-\infty}^{\infty} [\delta p](x) \wedge [\delta q](x) \tag{A2}$$

converges where δ is the functional exterior derivative. For instance, we could impose that both $\delta q, \delta p$ decay as $1/x$ which allows both q, p to asymptote to fixed values $q_\pm, p_\pm$ at $x = \pm\infty$ which are not variable on the phase space. If on the other hand $p_\pm$ is considered a variable on the phase space and $p = p_\pm + O(1/x)$ then $q_\pm$ must not be a variable on the phase space and we need the integral of δq to converge which either requires a stronger fall off condition on δq, say as $1/x^2$ or an asymptotic parity condition, e.g., that $\delta q = \delta c/x$ in leading order where c is another variable on the phase space. The leading order then vanishes when defined as a principal value integral. This specification of the decay behavior has also consequences for the treatment of the constraints.

We smear the constraints with test functions f which are treated as constants on the phase space ($\delta f(x) \equiv 0$), that is, we consider $C(f) := \int_{\mathbb{R}} dx\ f(x)\ C(x)$. The exterior derivative of $C(f)$ enters the computation of the Poisson brackets

$$A.\quad [\delta C(f)] = \int dx\ f(x)\ [\delta p](x),\quad B.\quad [\delta C(f)] = -\int dx\ f'(x)\ [\delta p](x) - [\delta B(f)],\quad B[f] := -[f(x) p(x)]_{x=-\infty}^{\infty} \tag{A3}$$

For model A the functional $C(f)$ is functionally differentiable without any condition on f while for model B it is functionally differentiable if and only if $f_+ \delta p_+ - f_- \delta p_- = 0$ where $f_\pm = f(\pm\infty)$. This is automatically the case if $p_\pm$ do not vary on the phase space (in which case we can drop $B(f)$ altogether) or if, e.g., f decays at both infinities. We can, however, define for both models

$$A.\quad H(f) := C(f),\quad B.\quad H(f) := C(f) + B(f) \tag{A4}$$

which are functionally differentiable with no condition on f in both cases no matter what the decay behavior of p is. In contrast to model A, in model B the functional $H(f)$ is different from the functional $C(f)$ unless $B(f) = 0$. We call canonical transformations generated by $H(f)$, with f such that $B(f) = 0$, *gauge transformations* because C is the constraint and not H. We call canonical transformations generated by $H(f)$ with f such that $B(f) \neq 0$ *symmetry transformations*. For model A there is no difference between the two because $B(f) \equiv 0$.

For both models, the unconstrained phase space is infinite dimensional. The constraint surface is the kernel of the constraint $C(x) = 0$ for all x. The reduced phase space is the constraint surface with points identified that lie on the same gauge orbit. In the present case, the reduced phase space is very simple to compute. In both models p is gauge invariant because $C(f)$ depends only on p.

In model A any f corresponds to a gauge transformation and the gauge transformation of q is

$$[\Delta_f q](x) = \{C(f), q(x)\} = f(x) \tag{A5}$$

We are allowed to pick f from the same function space that q belongs to and see that $q(x)$ can be gauged to any value, say $q_*(x) = 0$ for all x. As the constraint requires $p(x) = 0$ for all x we see that the reduced phase space is the single point $p \equiv q \equiv 0$. The gauge $q_* = 0$ is also complete, i.e., there are no non-trivial stability transformations that preserve $q = 0$ as $\{H(f), q(x)\} = f(x) = 0$ imposes $f(x) = f_*(x) = 0$ for all x.

In model B, we have to be more careful. The constraint $C(x) = 0$ now only imposes that $p(x) = M$ is a spatial integration constant but it is allowed to be considered a variable on the phase space. Thus, we have, in particular, $p_\pm = M$. Thus, $B(f) = -M(f_+ - f_-)$ on the constraint surface. Thus, the weakest condition we can impose for f to define a gauge transformation is that $f_+ = f_-$. For $f_+ \neq f_-$ we obtain a symmetry transformation. Then, a possible condition on the decay behavior of q is that δq decays as $[\delta c]/x$ in leading order so that we have odd parity conditions at infinity. The gauge transformation of q is

$$[\Delta_f q](x) = \{H(f), q(x)\} = -f'(x) \tag{A6}$$

To gauge a given $q(x)$ to zero we must solve $\Delta_f q = -q$, i.e., $f' = q$ which is solved by

$$f_q(x) = f_- + \int_{-\infty}^{x} dy\; q(y) \tag{A7}$$

However, unless

$$Q := \int_{-\infty}^{\infty} dy\; q(x) \tag{A8}$$

equals zero, the function (A7) does not correspond to a gauge transformation because $f_+ \neq f_-$. It follows that $q(x)$ cannot be gauged to zero for all x. Indeed for a gauge transformation we have

$$[\Delta_f Q] = \{H(f), Q\} = -\int_{-\infty}^{\infty} dy f'(y) = -[f_+ - f_-] = 0 \tag{A9}$$

whence Q is gauge invariant, i.e., a Dirac observable. We require the function space space of q to be such that Q is well defined. Pick $\infty > L$. We can then set for $x \in (-\infty, L]$

$$f_q(x) = f_- + Q - \int_{x}^{\infty} dy\; q(y) \tag{A10}$$

and interpolate smoothly between $f_q(L)$ and f_- in $x \in (L, \infty)$. As this can be conducted for any $L < \infty$ we see that $q(x)$ for $x < \infty$ is pure gauge. Note, that $q(x) = 0$ for $x < \infty$ does not fix the gauge completely because we have $f_+ = f_-$ possibly non-vanishing. Equivalently, let $w(x)$ be a fixed weight function belonging to the function space of q with $\int_{\mathbb{R}} dx\; w(x) = 1$. Then, we can gauge $q(x)$ to $q_*(x) = Q\, w(x)$ for all x because the required gauge transformation is now given by

$$f_q(x) = f_- + \int_{-\infty}^{x} dy\; [q(y) - Q\, w(y)] \tag{A11}$$

which satisfies $f_q(\infty) = f_- = f_q(-\infty)$. Again the constant f_- is unspecified corresponding to a residual gauge freedom which is also clear from the stability condition $\delta_f(q - Qw) = -f' = 0$, i.e., the solution (A11) is only unique up to adding a constant $f_q \to f_q + c$ which corresponds to shifting f_-.

On the other hand, for a symmetry transformation we have

$$[\Delta_f Q] = \{H(f), Q\} = -\int_{-\infty}^{\infty} dy f'(y) = -[f_+ - f_-] \neq 0 \tag{A12}$$

Since $\{p(x), Q\} = 1$ for any x and as we have $p(x) = M$ on the constraint surface, it follows that (A12) has the canonical generator

$$H = -(f_+ - f_-)M =: \kappa\, M = B(f) \tag{A13}$$

called the physical Hamiltonian. The more systematic way to obtain H is the condition that for any function $F = F(M, Q)$ we require

$$\{H, F\} = \{H(f), F\}_{f=f_*, C=0, q=q_*} = -(f_+^* - f_-^*)\,\frac{\partial F}{\partial Q} \tag{A14}$$

where $f = f^*$ is the general solution of the stability condition

$$\{H(f), [q - q_*](x)\} = \{H(f), q(x)\} - \{H(f), Q\}\, w(x) = -f'(x) + [f_+ - f_-]\, w(x) = 0 \tag{A15}$$

which has the solution

$$f^*(x) = f_- + (f_+ - f_-)\int_{-\infty}^{x} dy\; w(y) \tag{A16}$$

depending on two free parameters f_+, f_-. Thus, the general solution of the stability condition is a symmetry transformation when $f_+ \neq f_-$ and it is only sensitive to the single parameter $\kappa = -(f_+ - f_-)$. Thus, the systematic analysis reproduces (A13).

To summarize, the innocent looking spatial derivative of canonical variables in constraints have drastic consequences on the reduction of the system: the reduced phase space is augmented by canonical pairs and there is a residual transformation freedom even after all possible gauge freedom has been exploited and the gauge has been maximally fixed. This residual transformation freedom parameter finds its way into the physical Hamiltonian on which it depends linearly. That parameter, therefore, can be interpreted as the clicking rate of the clock that measures time.

Appendix B. Consequences for Black Hole Physics

For spherically symmetric spacetimes, the existence of a *pair* of Dirac observables rather than just the black hole mass has been discovered, to the best knowledge of the author, for the first time in [23,73] which provides a complete quantum theory of spherically symmetric black holes in terms of complex connection variables. In [74] a similar analysis is performed in terms of ADM variables. In view of the previous section and as we will review below, the origin of the second Dirac observable is due to the fact that the constraints of spherically symmetric gravity involve momentum derivatives. This means that the constraints cannot be used to completely gauge away all configuration degrees of freedom and that there is an integration constant when solving the constraints for the momenta. These degrees of freedom are the analogs of M, Q above.

How can this be reconciled with Birkhoff's theorem which states that every spherically symmetric vacuum solution is static and completely characterized by a *single* degree of freedom, namely the mass of the black hole [6]? As we will show, the freedom corresponding to Q can be considered as associated with a one-parameter family of temporal diffeomorphism corresponding to the choice of the time coordinate which is supposed to coincide with the Cartesian time coordinate at spatial infinity. If one considers this freedom as a gauge degree of freedom as it is customary in the Lagrangian framework, then indeed one can discard Q. On the other hand, in the Hamiltonian framework one is instructed not to consider that freedom as a gauge.

We repeat here from the main text why this is significant: Suppose there would be no variable conjugate to the mass at all. Then, because the mass has vanishing Poisson brackets with the matter and the gravitational multiple degrees of freedom, it would have vanishing Poisson brackets with the reduced Hamiltonian, which is a constant of motion, and thus would be a constant of motion itself. It would be present also after all Hawking processes have ceased and thus could also be called *remnant* mass. If on the other hand we respect the existence of that Dirac observable conjugate to the mass, then the gauge fixing condition must be consistent with its existence. This can be granted, for instance, when the gauge fixing condition keeps a one parameter freedom which is able to capture the existence of the conjugate variable, let us call it Q. It can also find its way into the reduced Hamiltonian and now both Q, M can change in time and, in particular, we can have the *backreaction* from the multipole and matter degrees of freedom to Q, M.

We will now give a self-contained exposition of how the time variable comes into existence. The mechanism at work is a one-parameter family of purely temporal diffeomorphisms that we use to pull back the Schwarzschild metric away from the GPG. This leaves the radial coordinate intact but changes lapse, shift and the radial-radial component of the spatial metric. For instance, we can choose that one-parameter family such that the pulled-back metric deviates from the exact GPG only in an arbitrarily small neighborhood of the core $r = 0$, say in a Planck-length neighborhood which is the region of spacetime in which we do not trust classical GR anyway, in fact, from a strictly classical point of view the point of view, $r = 0$ or a neighborhood of it should be cut out from the physical spacetime. The parameter Q is directly determined by that temporal diffeomorphism. If one considers that diffeomorphism as a *gauge* transformation then Q would be considered as a gauge degree of freedom. If one considers that diffeomorphism as a *symmetry* transformation then Q would be considered as a Dirac observable. It is the first point of view that is taken in Birkhoff's theorem coming from a Lagrangean point of view, thereby explaining why one only has the mass parameter as an observable. It is the second point of view which is taken coming from the Hamiltonian point of view.

We thus follow the Hamiltonian path in order to keep the possibility open that also the remnant mass can change dynamically. In the main text and Appendix D we show that one can also have Q existent without that it leaves a trace in the physical Hamiltonian by exploiting that the expression that defines Q requires regularization which introduces the required one-parameter freedom without implementing it into the gauge fixing condition. Still, evaporation is not excluded because $2M$ is not the event horizon or apparent horizon when there is radiation present.

Appendix B.1. The Reduced Phase Space of Spherically Symmetric Vacuum GR

Proceeding to the details, following the notation of Section 4 in the purely spherically symmetric sector we have the following two constraints prior to any gauge fixing of $2\, q_0 = \Omega^{AB} q_{AB}, q_3 = q_{33}$ with conjugate momenta $p^0 = P^{AB}\Omega_{AB}/\omega,\ p^3 = P^{33}/\omega$

$$v_3 := V_3/\omega = p^0\, q_0' + p^3\, q_3' - 2(q_3 p^3)',\ v_0 := V_0\sqrt{\det(q)}/\omega^2 = \frac{1}{2}(q_3 p^3)^2 - (q_0 p^0)(q_3 p^3) - \det(q) R/\omega^2 \tag{A17}$$

By introducing $p^0 = (p^3 q_3' + 2[p^3]' q_3)/q_0'$ into V_0 relying on $q_0' > 0$ as $\sqrt{q_0}$ should be the radial coordinate up to a radial diffeomorphism, we have

$$v_0 = -\frac{q_3\, q_0^{3/2}}{q_0'}\, [\frac{q_3 [p^3]^2}{q_0^{1/2}}]' - \det(q) R/\omega^2 \tag{A18}$$

By working out the Ricci scalar explicitly for the non-vanishing components $q_{33}, q_{AB} = q_0/2\, \Omega_{AB}$ one finds after a longer calculation

$$v_0 = -4\, \frac{q_3\, q_0^{3/2}}{q_0'}\, \{\frac{q_3 [p^3]^2}{4\, q_0^{1/2}} + q_0^{1/2}[1 - (\frac{\sqrt{q_0}'}{\sqrt{q_3}})^2]\}' \tag{A19}$$

In the exact GPG $q_0 = r^2, q_3 = 1, p^3 = 2\sqrt{2Mr}$ we see that the curly bracket is just twice the black hole mass M. Without imposing any gauge, let us call this quantity m. Then, a non-trivial calculation confirms that we can pass to new canonical coordinates

$$\gamma = \sqrt{q_{33}},\ p_\gamma = -2\gamma p^3,\ \delta = \sqrt{q_0},\ p_\delta = 2\delta\ p^0 \tag{A20}$$

and after that

$$m = \frac{p_\gamma^2}{16\delta} + \delta(1 - [\frac{\delta'}{\gamma}]^2),\ p_m = \frac{\gamma\ p_\gamma}{2\delta\Phi},\ \Phi = 1 - \frac{m}{\delta},\ X = \delta,\ p_X = p_\delta - (\gamma\ p'_\gamma + m' p_m)/\delta' \tag{A21}$$

which enables us to express the constraints in the equivalent form

$$\tilde{v}_3 = p_m\ m' + p_X\ X',\ \tilde{v}_0 = m' \tag{A22}$$

which simply enforce $p_X = 0,\ m' = 0$.

The transformation (A20) is easy but (A21) is non-trivial to check, see [23,73,74]. A short-cut is as follows:

The spatial diffeomorphism constraint $v_3 = \delta'\ p_\delta - \gamma\ p'_\gamma$ identifies δ, p_γ radial scalars and p_δ, γ as radial scalars of density weight one. Thus, $p_\delta/\delta', \gamma/\delta'$ as radial scalars. For any radial scalar F the function $\hat{F}(s) = F(r = \delta^{-1}(s))$ is spatially diffeomorphism invariant for any value of s relying on $\delta : \mathbb{R} \to \mathbb{R}; r \mapsto \delta(r) = s$ to be a diffeomorphism (if one wants to consider one asymptotic end only, one just has to restrict r to positive or negative values, respectively). Explicitly, one has

$$\hat{F}(s) = \int_{-\infty}^{\infty} dr\ \delta'(r)\ \Delta(\delta(r), s)\ F(r) \tag{A23}$$

where Δ is the δ distribution. This makes it possible to compute the Poisson brackets among $\hat{\gamma}(s), \hat{P}_\gamma(s)$ and with v_3. That computation shows that $\{\hat{P}_\gamma(s), \hat{\gamma}(\tilde{s})\} = \delta(s, \tilde{s})$ and that they have vanishing Poisson brackets with v_3. The function $\hat{m}(s)$ can now be expressed just in terms of these

$$\hat{m}(s) = \frac{\hat{P}_\gamma^2(s)}{16s} + s\ [1 - \hat{\gamma}^{-2}(s)] \tag{A24}$$

and the Hamiltonian constraint becomes $\hat{m}'(s) = 0$. As (A24) has no derivatives with respect to s we have $\{\hat{m}(s), \hat{m}(\tilde{s})\} = 0$. To construct a momentum $\hat{P}_m$ conjugate to $\hat{m}$ we solve (A24) for $\hat{P}_\gamma(s) = 4\ s\ \sigma\sqrt{\frac{\hat{m}(s)}{s} + \hat{\gamma}^{-2}(s) - 1}$ with $\sigma = \pm 1$ and plug it into the symplectic potential $\hat{\Theta} = -\int\ ds\ \hat{\gamma}\ \delta\hat{P}_\gamma$. Then, we take the functional exterior derivative

$$\hat{\Omega} = \delta\hat{\Theta} = -\int\ ds\ \delta\hat{\gamma}\ \wedge\ \delta\hat{P}_\gamma = -\int\ ds\ [\frac{\partial\hat{P}_\gamma}{\partial\hat{m}}\ \delta\hat{\gamma}]\ \wedge\ \delta m \tag{A25}$$

so that $\delta\hat{p}_m$ at fixed $\hat{m}$ must be $-\frac{\partial\hat{P}_\gamma}{\partial\hat{m}}\ \delta\hat{\gamma}$. This is indeed solved by

$$\hat{P}_m = 2\sigma\frac{\sqrt{1 - \hat{\gamma}^2\hat{\Phi}}}{\hat{\Phi}},\ \ \hat{\Phi} = 1 - \frac{\hat{m}}{s} \tag{A26}$$

modulo addition of a function that just depends on $\hat{m}$. It is instructive to check by hand that $\hat{P}_m, \hat{m}$ are conjugate. For this one needs to plug (A24) into (A26) which yields

$$\hat{P}_m = \frac{\hat{\gamma}}{2}\frac{[\hat{P}_\gamma/s]}{\hat{\gamma}^{-2} - \frac{1}{16}[\hat{P}_\gamma/s]^2} \tag{A27}$$

The two constraints $p_X(r) = 0$ and $m'(r) = 0$, respectively, bring us exactly into the situation of models A and B of the previous section. In terms of these canonical coordinates and setting $p = m, q = -p_m$ we have the symplectic structure

$$\Theta = \int dx\ [p_X(x)\delta X(x) + p(x)\delta q(x)] \tag{A28}$$

Note, that our aim is to solve the original constraints for p^0, p^3 which are encoded in p_X, m and not p_X, p_m which is why we switched the roles of momentum and configuration coordinates with respect to m.

By the results of the previous section, the coordinatization of the reduced phase of the equivalent set of constraints $p_X(x) = 0,\ p'(x) = 0$ is now very transparent: X is pure gauge while q must carry one degree of freedom Q. Also, $p_X(x) = 0$ fixes p_X completely while $p'(x) = 0$ retains one parameter P (integration constant) as unconstrained. The reduced phase space of the system is thus two-dimensional encoded by Q, P and the reduced Hamiltonian is $H = \kappa P$ up to a constant κ. Thus, up to a constant κ, the physical Hamiltonian is the ADM mass or energy as one would have expected. The conjugate variable Q thus plays the role of an intrinsic time variable whose ticking rate is given by κ which can be chosen to be any value (reparametrisation of the coordinate time).

Appendix B.2. Gauge Fixings Consistent with the Existence of Q

The task left over is to pick a suitable set of gauge fixings which gives rise to Q, i.e., yields

$$Q = \int_{-\infty}^{\infty} dr\ q(r) = -\int_{-\infty}^{\infty} dr\ p_m(r) \tag{A29}$$

We have the freedom to subtract from Q an arbitrary function of P because that will change the reduced symplectic potential $\Theta = P\delta Q$ only by a total differential, hence we require

$$Q = -\int_0^{\infty} dr\ [p_m(r) - f_P(r)] \tag{A30}$$

Without specifying $q_{33} = \gamma^2, q_0 = \delta^2$ for the moment, we can solve $m'(r) = 0$ as $m(r) = P$ and solve for p_m in terms of γ, δ, P which yields

$$p_m = \frac{\gamma p_\gamma}{2\delta\Phi} = \frac{2\gamma}{\Phi}\ \frac{p_\gamma}{4\delta} = \frac{2\gamma\sigma}{\Phi}\ \sqrt{[\frac{\delta'}{\gamma}]^2 - \Phi},\ \ \Phi = 1 - \frac{P}{|\delta|} \tag{A31}$$

where σ is the sign freedom left over from solving the quadratic equation $m = P$ for P_γ and we note that when solving that equation one finds that the argument of the square root in (A31) is constrained to be non-negative.

We note that in the exact GPG, we would choose $\delta = r,\ \gamma = 1$ which would give $[\frac{\delta'}{\gamma}]^2 - \Phi = \frac{P}{|r|} \geq 0$ constraining P to be positive. In order to give Q an independent value that gauge must be relaxed by a one-parameter family of gauges. Among the many possible choices, we will discuss here two simple possibilities.

Range restriction

This is motivated by Appendix C.3 where we construct a non-singular spacetime by gluing a black hole and a white hole spacetime along a cylinder $|r| = l < R = 2M$. We then have for $q = -p_m,\ f_P = 0$

$$Q = \int_{|r|\geq l} dr\ q(r) = \int_{-l}^{l} dr\ q(r) + \int_{\mathbb{R}} dr\ q(r) \tag{A32}$$

The second integral in (A32) is ill-defined as it stands and must be defined by a limiting procedure (principal value). Alternatively, we can simply drop it because it just depends on M thus drops out of the symplectic structure. The calculation is carried out in Appendix C.6. It can be given any value and thus can be used to define Q for $l \equiv 0$, see that section for details. Here, we use that regularization freedom to make the second integral vanish. The first integral then gives

$$Q = -4\sigma \int_0^l dr \, \frac{\sqrt{R/r}}{1 - R/r} = -4\sigma \, R \, [2\sqrt{\frac{l}{R}} - \ln(\frac{1 + \sqrt{\frac{l}{R}}}{1 - \sqrt{\frac{l}{R}}})] \tag{A33}$$

Since the reduced Hamiltonian is $H = \kappa \, M, \kappa > 0$ and M, Q are conjugate this gives the equations of motion $\dot{Q} = \kappa > 0, \; \dot{M} = 0$, hence the variable Q is eventually positive which means that $\sigma.0$ so that for large times τ and with $c = \kappa/4$

$$\frac{c\tau}{R} = -2\sqrt{\frac{l}{R}} + \ln(\frac{1 + \sqrt{\frac{l}{R}}}{1 - \sqrt{\frac{l}{R}}}) \tag{A34}$$

Since this diverges with τ, $l(\tau) \to R-$. Thus, for large τ

$$l = R \, \text{th}^2(\frac{c\tau}{R}) \tag{A35}$$

i.e., the solution approaches exponentially fast the *Einstein – Rosen bridge solution* $|r| \geq R$ with two asymptotic ends. Thus for late times, the second parameter l gets frozen to R and the metric depends only on a single parameter R. However, in this implementation, the interior of the black hole is cut out from spacetime. We will, therefore, not consider this possibility further in what follows.

Local deviation from exact GPG

We generalize the gauge to $\delta = r, \gamma = \sqrt{1 + \Delta}$ where Δ will be further specified below and which will be non-vanishing only in compact subsets of $\mathbb{R}^+$ and carries the information about Q. In particular, $\Delta > -1$ in order that the metric stays non-degenerate. As P is constrained to be a constant, this still imposes $P > 0$. The motivation for that particular generalization within the Hamiltonian analysis is that the spatial diffeomorphism constraint generates radial reparametrizations, and therefore, we can always choose $\delta = r$. On the other hand the relation between temporal spacetime diffeomorphisms and the gauge transformations generated by the Hamiltonian constraint is more tricky: These two notions only coincide *on shell*, i.e., when the equations of motion (e.g., vacuum Einstein equations) hold. We will not violate those equations at all, we simply pull back the exact GPG form of the Schwarzschild metric by a temporal diffeomorphism which encodes Δ and that pulled back metric then still solves the Einstein equations. In particular, we will not at all contradict Birkhoff's theorem because in contrast to the Hamiltonian picture, in the Lagrangian picture one considers *all* diffeomorphisms as a gauge transformation.

In that parametrized GPG (PGPG – by Q) the spatial line element reads

$$q_{33} \, dr^2 + q_0 \, \Omega_{AB} \, dy^A \, dy^B = \gamma^2 \, dr^2 + r^2 \, \Omega_{AB} \, dy^A \, dy^B \tag{A36}$$

Then, (A31) becomes

$$p_m = \frac{2\sigma}{\Phi} \, \sqrt{1 - \gamma^2 \Phi}, \tag{A37}$$

In order for the square root to be well-defined it is sufficient to require that $\gamma^2 \Phi \leq 1$ for $|r| > P$. This will be, in particular, the case for $\gamma^2 \leq 1$ for all r. We will choose $\Delta \neq 0$ for some subset of $[-P, P]$ which thus satisfies this requirement. Accordingly the integral of p_m approaches for large $|r|$ the function $|r|^{-1/2}$ and thus would diverge. We thus use the freedom to add to Q a function that depends just on P which does not change the reduced symplectic structure and makes the integral defining Q converge. The natural choice is to subtract from (A37) its value in the exact GPG (i.e., for $\gamma = 1$), i.e., we define

$$Q = -2\sigma \int_{-\infty}^{\infty} \frac{\sqrt{1-\gamma^2\Phi} - \sqrt{1-\Phi}}{\Phi} = 4\sigma \int_0^{\infty} \frac{\Delta}{\sqrt{1-[1+\Delta]\Phi} + \sqrt{1-\Phi}} \tag{A38}$$

where we focus on even functions $\Delta(r) = \Delta(-r)$ so that we can restrict to the positive axis. The integral is now confined to the support of Δ which will lie in the region where $\Phi < 0$. We will choose $\Delta \geq 0$ there so that we obtain the interpretation

$$\sigma = \text{sgn}(Q) \tag{A39}$$

Let now $w \geq 0$ be a function of compact support in $[0, P]$ such that $\int_0^\infty dr\ w = 1$ then we pick Δ such that

$$\frac{w\ |Q|}{2} = \frac{\Delta}{\sqrt{1-[1+\Delta]\Phi} + \sqrt{1-\Phi}} \tag{A40}$$

This can be solved for Δ and yields either $\Delta = w = 0$ or

$$\Delta = |Q|\ w\ [\sqrt{1-\Phi} - |Q|\ w\ \Phi/4] \tag{A41}$$

which is manifestly nonnegative as $\Phi < 0$ in the support of w. If we want the support of w to be independent of the value of P we can restrict it to the interval $[0, \ell],\ l = \epsilon \ell_P]$ with $\epsilon \leq 1$ because a Planck size black hole mass is believed to be outside of the regime of classical GR and within classical GR it is well-motivated to cut out the region $r \leq \ell_P$ from the physical manifold. Alternatively, we may pick $\ell = \min(\epsilon \ell_P, P/2)$. Then, with $\chi_{[0,\ell]}$ the characteristic function of that interval we make the Ansatz

$$w(r) = \chi_{[0,\ell]} f(r),\ f \geq 0 \tag{A42}$$

so that

$$\Delta = |Q|\ \chi_{[0,\ell]}\ [\frac{f}{r^{1/2}}\ \sqrt{P} + |Q|\ \frac{f^2}{r}\ (P-r)/4] \tag{A43}$$

This is regular at $r = 0$ e.g., for the choice $f(r) = h\sqrt{r}$ for some height amplitude h and yields

$$\Delta = |Q|\ \chi_{[0,\ell]}\ [h\ \sqrt{P} + |Q|\ h^2\ (P-r)/4] \tag{A44}$$

The height h is fixed by the requirement

$$\int_0^\infty dr\ w = h\ \int_0^\ell dr\ \sqrt{r} = \frac{2h}{3}[\ell]^{3/2} = 1 \tag{A45}$$

so that we finally obtain

$$\Delta = \frac{|Q|}{\ell}\ \chi_{[0,\ell]}\ [\frac{3}{2}\ \sqrt{\frac{P}{\ell}} + \frac{9}{16}\ \frac{|Q|}{\ell}\ \ \frac{P-r}{\ell}] \tag{A46}$$

in particular

$$\Delta(0) = \frac{3}{2}\ z^{1/2} + \frac{9}{16}\ z,\ \ z = \frac{P\ Q^2}{[\ell]^3} \tag{A47}$$

which is also the maximal value that Δ can be taken for this particular gauge. Note, that the range of Q is all of $\mathbb{R}$ which is compatible with the equation of motion $\dot{Q} = \kappa$ that follows from the reduced Hamiltonian $H = \kappa P$. The non-differentiable step function can be mollified to obtain a smooth function which would yield qualitatively similar formulae.

This proves that a suitable gauge for γ exists that produces a given value of Q independent of the value of P and that deviates from the exact GPG only very *locally*, i.e., $\gamma^2 = 1$ except for a neighborhood of zero of at most of Planck size behind the event horizon.

Appendix B.3. Relation between Existence of Q and Temporal Diffeomorphisms

To relate a deviation from the strict GPG to a spacetime diffeomorphism we write the Schwarzschild metric in exact GPG

$$ds^2 = -[1 - \frac{2M}{|r|}]\, d\tau^2 + 2\sqrt{\frac{2M}{|r|}}\, dr\, dt\; + dr^2 + r^2\, \Omega_{AB}\, dy^A\, dy^B \tag{A48}$$

and pull it back by a temporal diffeomorphism

$$r = \rho(\tilde{\tau}, \tilde{r}) := \tilde{r},\; \tau = T(\tilde{\tau}, \tilde{r}) \tag{A49}$$

and rewriting (A48) in terms of the coordinate $\tilde{\tau}$. That reparametrized metric still solves the Einstein equations, no matter what the function T is, as long as $\partial_{\tilde{t}} T > 0$, since then we have just carried out a diffeomorphism (A49) as $\det(\partial(\tau, r)/\partial(\tilde{\tau}, \tilde{r})) = \partial_{\tilde{t}} T(\tilde{\tau}, \tilde{r})$. That the pulled back metric still solves the Einstein equations is obvious from its tensorial character but can of course also be verified by hand.

The spatial part of the metric pulled back by this diffeomorphism starting from GPG $q_3 =:= \gamma^2 = 1, q_0 = r^2$ becomes

$$\tilde{q}_3(\tilde{\tau}, \tilde{r}) = \tilde{\gamma}^2(\tilde{\tau}, \tilde{r}) = 1 - \Phi(\tilde{r})\; [\partial_{\tilde{r}}\; T(\tilde{\tau}, \tilde{r})]^2 + 2\sqrt{1 - \Phi(\tilde{r})}\; [\partial_{\tilde{r}}\; T(\tilde{\tau}, \tilde{r})], \tilde{q}_A = 0,\; \tilde{q}_0(\tilde{t}, \tilde{r}) = \; \tilde{r}^2 \tag{A50}$$

where $\Phi(r) = 1 - 2M/|r|$. It is, therefore, still flat in regions where $\partial_{\tilde{r}}\; T(\tilde{t}, \tilde{r}) = 0$. If we compare (A50) with $q_3 =: \gamma^2 =: 1 + \Delta, m := 2M$ from the previous subsection we obtain the relation

$$\frac{|Q| w}{2} = \partial_{\tilde{r}}\; T(\tilde{t}, \tilde{r}) \tag{A51}$$

where w has compact support in an at-most Planck size neighborhood of the origin and Q is the aforementioned second Dirac observable which can, in principle, be an arbitrary function of coordinate time $\tilde{t}$ and which is canonically conjugate to the mass m. As the physical Hamiltonian is just m up to a constant, Q is actually linear in $\tilde{\tau}$ on shell.

The GPG lapse $\alpha = 1$ and shift $\beta = \sqrt{1 - \Phi}$ become upon pull-back

$$\tilde{\alpha}^2 - \tilde{\beta}^2 = \Phi[\partial_{\tilde{\tau}}\; T(\tilde{\tau}, \tilde{r})]^2,\;\; \tilde{\beta}\tilde{\gamma} = [\sqrt{1 - \Phi}\; - \Phi\partial_{\tilde{r}}\; T(\tilde{t}, \tilde{r})]\; \partial_{\tilde{\tau}}\; T(\tilde{\tau}, \tilde{r}) \tag{A52}$$

This can be combined with (A50) to

$$(\tilde{\alpha}\tilde{\gamma})^2 = (\partial_{\tilde{\tau}}\; T(\tilde{\tau}, \tilde{r}))^2 \tag{A53}$$

Here, we have employed a general parameterization of spherically symmetric spacetimes in coordinates τ, r given by $g_{\tau\tau} = -\alpha^2 + \beta^2,\; g_{\tau r} = \beta\gamma,\; g_{rr} = \gamma^2,\; g_{AB} = \delta^2\, \Omega_{AB}$ and in the *radial gauge* $\delta = r$ chosen here the Einstein equations are equivalent to (we drop the tilde again)

$$1 - \gamma^{-2} + \frac{\beta^2}{\gamma^2\alpha^2} = 1 - \frac{2M}{r},\;\; \partial_t M = \partial_r M = 0,\;\; \partial_t \gamma = \frac{\beta}{\gamma\alpha}\, \partial_r[\gamma\alpha] \tag{A54}$$

which can be combined and integrated to parameterize the metric as a function of γ

$$\beta = \sigma\alpha\sqrt{1 - \gamma^2\Phi},\; (\gamma\alpha)(\tau, r) = [\partial_\tau\; \hat{T}](\tau) - \sigma\; \partial_\tau[\int_0^r\;\; ds\; [\frac{\sqrt{1 - \gamma^2\Phi} - \sqrt{1 - \Phi}}{\Phi}](\tau, s)] \tag{A55}$$

where $\hat{T}(\tau)$ is an arbitrary function of time and σ a sign which determines whether we consider the out/ingoing patch ($\sigma = \pm 1$). If we compare this with the definition of Q in the previous section and with (A53) we find

$$(\gamma\alpha)(\tau, r) = [\partial_\tau\; \hat{T}](\tau) + [\partial_\tau Q]\; \frac{1}{2}[\int_{-\infty}^r\;\; ds\; w(s)],\;\; \lim_{r\to\infty} \alpha\gamma = \partial_\tau[\hat{T}(\tau) + Q/2] = \partial_\tau T,\;\; \beta\gamma \to \sigma\alpha\gamma\sqrt{1 - \gamma^2\Phi} \tag{A56}$$

As $\gamma \to 1$ at infinity, we see that α, β approach their exact lapse and shift value value in GPG up to a pure time reparametrisation. The result of the previous section $\kappa := \alpha(\infty) - \alpha(-\infty) = \dot{Q}$ agrees with the Hamiltonian equations of motion.

Thus, the physical meaning of the time function Q has been worked out: It is canonically conjugated to m and its clicking rate at infinity coincides both with the asymptotic lapse value and the asymptotic clicking rate of the temporal diffeomorphism. The temporal diffeomorphism obeys $T' = |Q|w$ and $\dot{T} = \dot{\hat{T}} + \partial_\tau[\int\ dsT']$ and this PDE system is solved by

$$T(\tau, r) = \hat{T}(\tau) + \frac{Q(\tau)}{2} \int_{-\infty}^{r} dsw(s) \tag{A57}$$

This diffeomorphism is generically not an asymptotic identity even if $\hat{T}(\tau) = \tau$ unless $Q = 0$ and thus should not be considered as a gauge transformation but rather a symmetry transformation in agreement with the Hamiltonian distinction between symmetry and gauge reviewed in the previous section.

The choice of a one-parameter set of gauge fixings consistent with Q given in the previous subsection that deviates from the exact GPG only *locally* in a neighborhood of the origin $r = 0$ of at most Planck size has the advantage that it is not observable from the outside of the black hole. On the other hand, it makes the analysis of mode functions in such a spacetime very hard. In the next section we, therefore, consider another one-parameter set of gauge fixings consistent with Q which has a *non-local* effect on the spacetime metric and which has an intuitively quite appealing interpretation in terms of the energy of timelike observers called generalized Painlevé Gullstrand coordinates.

Appendix C. Generalized Gullstrand–Painlevé Coordinates

We review here the theory of radial timelike geodesics in Schwarzschild spacetime with mass M [56–58]. These define a one-parameter set $e \mapsto C_e^\pm$ of congruences $C_e^\pm$ of free-falling observers that fill the spacetime starting (ending) at timelike infinity and ending (starting) at the singularity for the ingoing (outgoing) congruence C_e^- (C_e^+), respectively. The parameter $e \geq 1$ has the physical interpretation of the special relativistic energy per unit mass at spatial infinity (i.e., $e = [1 - (v/c)^2]^{-1/2}$ if v is the velocity at spatial infinity). For each congruence $C_e^\pm$ the geodesics fill an asymptotic end and the white (black) hole region of the Kruskal extension, respectively. The radial geodesics $c^\pm_{e,\rho,\Omega} \in C_e^\pm$ are labeled, besides the angular direction Ω, by a parameter $\rho \in \mathbb{R}$ that labels the range of the affine parameter τ along the geodesic where $\tau \in (-\infty, \rho)$ for $c^-_{e;\rho,\Omega}$ and $\tau \in (\rho, \infty)$ for $c^+_{e;\rho,\Omega}$ and at $\tau = \rho$ the geodesic intersects the singularity $r = 0$.

The set of synchronous points $\Sigma^\pm_{e,\tau} = \{c^\pm_{e;\rho,\Omega}(\tau);\ \pm(\tau - \rho) \geq 0,\ \Omega \in S^2\}$ defines the leaf of a foliation of the white (black) hole and asymptotic region by spacelike hypersurfaces. However, since they start (end) at the singularity, none of them is a Cauchy surface, i.e., there exist inextendible causal curves not intersecting them. Thus, one cannot use them for the initial value formulation. One could use a segment of the singularity to turn them into Cauchy surfaces but then different leaves of the foliation would not be disjointed. One could use two asymptotic ends in the *same* Kruskal spacetime and join say the two ingoing geodesics from the two ends that hit the same point of the singularity in the black hole region to form Cauchy surfaces but these intersect and do not form a foliation. However, one can join an ingoing geodesic in the part of a *past* Kruskal spacetime covering the Schwarzschild (SS) and black hole (BH) region with an outgoing geodesic in a *different*, i.e., *future* Kruskal spacetime covering the mirror Schwarzschild (MSS) and white hole (WH) region that hit the same point of the singularity. We may then consider the geodesics $c_{e;\rho,\Omega}$ with $c_{e;\rho,\Omega}(\tau) := c^\pm_{e;\rho,\Omega}(\tau)$ for $\pm(\tau - \rho) \geq 0$ and their synchronous hypersurfaces $\Sigma_{e,\tau} = \{c^\pm_{e;\rho,\Omega}(\tau);\ \rho \in \mathbb{R},\ \Omega \in S^2\}$. The resulting *black hole white hole transition* spacetime M consisting of the four pieces SS, BH, WH, MSS is then foliated by the $\Sigma_{e,\tau}$ which are Cauchy surfaces for (M, g), where g is the extension of the Schwarzschild metric just outlined, is then globally hyperbolic (but singular) in the usual sense in the future and past Kruskal patches. We also consider a non singular wormhole regularization of that spacetime.

Therefore, (M,g) is an interesting spacetime to study when analyzing questions such as black hole–white hole transition (BHWHT) and singularity resolution in quantum gravity as we explore both interior and exterior regions of spactime. Moreover, the free falling observer congruences labeled by e define a natural 1-parameter family of gauge fixing conditions for black hole spacetimes and corresponding preferred generalized Gullstrand–Painlevé (GGP) coordinates. A parameter like e is motivated by the result of the previous Appendix because the constraints depend on spatial derivatives giving rise to two Dirac observables even in vacuum. These will be related to the mass M and e as we will see in the course of this appendix which are natural observables to consider in spherically symmetric spacetimes. Finally, each foliation $\tau \mapsto \Sigma_{e,\tau}$ makes it possible to use the machinery of QFT in CST and to define 1-particle inner products, etc., to study Hawking radiation, etc.

Appendix C.1. Radial Timelike Geodesics in Spherically Symmetric Vacuum Spacetimes

We consider the exterior static region of a spherically symmetric black hole with mass $M > 0$, usual Schwarzschild coordinates $t \in \mathbb{R}, r > 2M, \Omega = (\theta,\phi) \in S^2$ and line element

$$ds^2 = -\Phi\, dt^2 + \Phi^{-1}\, dr^2 + r^2\, d\Omega^2,\ \ \Phi = 1 - \frac{2M}{r} \tag{A58}$$

which has a timelike Killing vector field $\xi = \partial_t = \delta^\mu_t \partial_\mu$.

A radial $\Omega =$ const., timelike $g(u,u) < 0;\ u = \dot{c}$ geodesic $\tau \to c(\tau)$ with affine parameter τ i.e., $\nabla_u u = 0$ obeys $\nabla_u g(u,u) = 0$ and provides two constants of motion $K := g(u,u)$ and $e := -g(u,\xi)$. As usual, we may fix $K = -1$ by rescaling the affine parameter so that

$$-1 = -\Phi(r(\tau))\, \dot{t}(\tau)^2 + \Phi^{-1}(r(\tau))\, \dot{r}(\tau)^2,\ e = \Phi(r(\tau))\, t(\dot{\tau}) \tag{A59}$$

It follows with $R := 2M$

$$\dot{r}^2 = e^2 - \Phi = e^2 - 1 + \frac{R}{r} \tag{A60}$$

We are interested in geodesics that extend all the way to spatial infinity $r = +\infty$ which requires that

$$e^2 \geq 1 \tag{A61}$$

The geodesic label by e has an outgoing and ingoing branch corresponding to the choice of the square root of (A60)

$$\dot{r} = \pm\sqrt{e^2 - 1 + \frac{R}{r}} \tag{A62}$$

Although the coordinate system is a priori only defined for $r > R$, Equation (A62) is meaningful for $r \in \mathbb{R}_+$. We note that

$$u_t = g_{t\mu} u^\mu = -\Phi u^t = -\Phi \dot{t} = -e,\ u_r = g_{r\mu} u^\mu = \Phi^{-1} u^r = \Phi^{-1} \dot{r} = \pm \Phi^{-1}\sqrt{e^2 - \Phi} =: \pm f'(r),\ u_\theta = u_\phi = 0 \tag{A63}$$

which means that $u_\mu = -\nabla_\mu \tau_e^\pm$ where

$$\tau_e^\pm := e\, t \mp f(r), f'(r) = \Phi^{-1}(r)\sqrt{e^2 - \Phi(r)} \tag{A64}$$

Thus, $\nabla_{[\mu} u_{\nu]} = 0$ so that the geodesics are hypersurface orthogonal, forming a foliation by $\tau_e^\pm =$ const. hypersurfaces.

The coordinates $(\tau = \tau_e^\pm, r)$ are called out(in) going generalized Gullstrand–Painlevé (GGP) coordinates. The line element in terms of them is obtained from

$$t(\tau,r) = e^{-1}[\tau \pm f(r)],\ f'(r) = \sqrt{e^2 - \Phi}\, \Phi^{-1} \ \ \Rightarrow\ \ ds^2 = -e^{-2}\Phi\, d\tau^2 \mp 2\, e^{-2}\sqrt{e^2 - \Phi}\, d\tau\, dr + e^{-2}\, dr^2 + r^2\, d\Omega^2 \tag{A65}$$

which does not require to solve for $f(r)$ explicitly. The line element (A65) is no longer static but still stationary. It is easy to check that the outgoing (ingoing) future oriented (with respect to τ) unit timelike geodesics with congruence parameter $e' \geq 1$ in the outgoing (ingoing) version of the line element (A65) have full range $r \in \mathbb{R}^+$ but intersect $r = 0$ at finite τ. The future oriented ingoing (outgoing) geodesics in the outgoing (ingoing) version of (A65) on the other hand are confined to $r > 2M$.

The ADM data of (A65) are

$$q_{rr} = e^{-2},\ q_{AB} = r^2\Omega_{AB},\ q_{rA} = 0,\ N^a = \mp\delta^a_r\sqrt{e^2 - \Phi},\ N = 1 \tag{A66}$$

which gives the future-oriented timelike unit normal to the $\tau =$ const. leaves $n = N^{-1}(\partial_\tau - N^a\partial_a) = \partial_\tau \pm \sqrt{e^2 - \Phi}\partial_r$. Note, that the vector field ∂_τ in these (τ, r) coordinates is a Killing vector field but it is not everywhere timelike and nowhere orthogonal to the $\tau =$ const. foliation.

On the other hand, Gaussian or synchronous coordinates are characterized by unit lapse squared and vanishing shift. One obtains them most easily from (A65) by computing the function $r = a(\tau, \rho)$

$$ds^2 = e^{-2}\ (-\Phi \mp 2\ \dot{a}\ \sqrt{e^2 - \Phi} + \dot{a}^2)\ d\tau^2 + 2\ a'\ e^{-2}\ (\dot{a} \mp \sqrt{e^2 - 1 - \Phi})\ d\tau\ d\rho + [a']^2\ d\rho^2 + a^2\ d\Omega^2 \tag{A67}$$

with $\dot{a} = \partial_\tau a,\ a' = \partial_\rho a$. The shift vanishes if

$$\dot{a} = \pm\sqrt{e^2 - \Phi} \tag{A68}$$

It follows

$$ds^2 = -d\tau^2 + e^{-2}\ (a')^2\ d\rho^2 + a^2\ d\Omega^2 \tag{A69}$$

We call the integration constant $\rho = \rho_e^\pm$ in (A68) and find

$$\pm(\tau - \rho) = \int\ da\ [e^2 - \Phi(a)]^{-1/2} \tag{A70}$$

which shows that $\dot{a} = -a'$ hence without further calculation

$$ds^2 = -d\tau^2 + e^{-2}[e^2 - \Phi(a)]\ d\rho^2 + a^2\ d\Omega^2 \tag{A71}$$

with a implicitly determined by (A70).

To actually determine a we have to treat the case $e^2 = 1$ separately. The integral is elementary

$$\pm(\tau - \rho) = \frac{2}{3}\ a^{3/2}\ R^{-1/2}\ \ \Leftrightarrow\ \ r = a(\tau, \rho) = [\pm\frac{3}{2}\sqrt{R}(\tau - \rho)]^{2/3} \tag{A72}$$

valid for $\pm(\tau - \rho) > 0$. Then, (A71) simplifies

$$ds^2 = -d\tau^2 + \frac{R}{a}\ d\rho^2 + a^2\ d\Omega^2 \tag{A73}$$

For $e^2 > 1$ we introduce the quantity

$$z := \sqrt{(e^2 - 1)\frac{a}{R}} \tag{A74}$$

then

$$\pm(\tau - \rho) = R\ (e^2 - 1)^{3/2}\ h(z),\ h(z) = [z\sqrt{z^2 + 1} - \ln(z + \sqrt{z^2 + 1})],\ h'(z) = 2\frac{z^2}{\sqrt{z^2 + 1}} \tag{A75}$$

which determines $r = a(\tau, \rho)$ implicitly. Since h is monotonously increasing and $h(0) = 0$, again the range of τ, ρ is constrained by $\pm(\tau - \rho) > 0$.

Note, that the metric coefficients $g_{\tau\tau}, g_{\rho\rho}, g_{AB},\ A, B = 1, 2$ in (A71) only depend on a and thus $\tau - \rho$. Therefore, $\xi_e := \partial_\tau + \partial_\rho$ is a Killing vector field $[\mathcal{L}_{\xi_e} g]_{\mu\nu} = \xi_e^\sigma\ g_{\mu\nu,\sigma} = 0$ with norm $g(\xi_e, \xi_e) = -1 + 1 - \frac{\Phi}{e^2} = -\frac{\Phi}{e^2}$ that is timelike for $r = a > M$. Thus, ξ_e must coincide for $a > R$ with $\xi = \partial_t$ up to a constant, which can be confirmed. Evaluating the norm at spatial infinity $a = \infty$ we find $\xi_e = e^{-1}\xi$.

Note, also that the change between GGP coordinates (τ, r) and synchronous coordinates $\tilde{\tau}, \rho$ with $\tau = \tilde{\tau}, r = a(\tilde{\tau}, \rho)$ gives $\partial_\tau = \partial_{\tilde{\tau}} + ([\partial_\tau b(\tau, r)]_{r=a(\tau,\rho)})_{\tau=\tilde{\tau}}\ \partial_\rho$ where $b(\tau, a(\tau, \rho)) = \rho$ inverts $r = a(\tau, \rho)$ for $\rho = b(\tau, r)$ at fixed τ. Thus, $0 = b_{,\tau}(\tau, r = a) + b_{,r}(\tau, r = a)\ a_{,\tau},\ 1 = b_{,r}(\tau, r = a)\ a_{,\rho}$ and since $a_{,\rho} + a_{,\tau} = 0$ it follows $\partial_\tau = \partial_{\tilde{\tau}} + \partial_\rho$. Thus, while $\tilde{\tau} = \tau$ there is a non-trivial transformation between $\partial_\tau, \partial_{\tilde{\tau}}$ as vector fields when changing from GGP to synchronous coordinates. This also explains why ∂_τ is a KVF but not hypersurface orthogonal while $\partial_{\tilde{\tau}}$ is no KVF but hypersurface orthogonal. With this clarification out of the way, we keep the notation ∂_τ for both coordinate systems but have to remember the difference between the roles that ∂_τ plays in them.

We consider the geodesic congruence with congruence parameter e' and geodesic tangent $u = \partial_s = u^\tau \partial_\tau + u^\rho \partial_\rho,\ u^\tau = d\tau/ds,\ u^\rho = d\rho/ds$ in the coordinates $\tau = \tau_e^\pm$, $\rho = \rho_e^\pm$. Then,

$$-e' = g(u, \xi) = e[-d\tau/ds + (1 - \Phi/e^2)\ d\rho/ds],\ \ -1 = g(u, u) = \frac{d\tau}{ds}^2 + [1 - \frac{\Phi}{e^2}]\ [\frac{d\rho}{ds}]^2 \tag{A76}$$

These have two solutions. The outgoing solution for $\tau - \rho > 0$ and the ingoing solution for $\tau - \rho < 0$, respectively, correspond to $\rho =$ const. and $d\tau/ds = \frac{e'}{e}$ which can be seen from the fact that $a(\tau, \rho)$ is monotonously increasing and, respectively, decreasing with increasing τ thanks to the monotonocity of h in (A72). For the geodesic congruence $e' = e$ we see that $\tau = s$ coincides with the proper time along the geodesics.

Thus, the out(in) going geodesic congruence with $e' = e$ becomes especially simple in out(in)going synchronous coordinates $\tau = \tau_e^\pm, \rho = \rho_e^\pm$, they are just the lines $\rho =$ const. and $s \mapsto \tau = s$ and are valid for $\tau > \rho$ and $\tau < \rho$, respectively. All geodesic observers are synchronized on the $\tau =$ const. hypersurface $\Sigma_{e,\tau}^\pm = \{\pm(\tau - \rho) > 0,\ \Omega \in S^2\}$. The hypersurfaces are mutually disjointed and cover one exterior region and the white (black) hole region of the Kruskal extension. Since $1 - \Phi(a)/e^2 > 0$ for all $a \in \mathbb{R}_+$ and $e^2 \geq 1$ the hypersurfaces $\tau =$ const have the intrinsic metric of manifestly positive signature and are thus spacelike. The vector field ∂_τ is everywhere timelike and in fact the future oriented timelike unit normal to the hypersurfaces; however, it is not a Killing vector field, and therefore, for the geodesic observer the metric is eigentime τ dependent both in the exterior and interior region. Yet, the observer (in the ideal limit of vanishing spatial extension) feels no tidal forces and thus considers themselves in an inertial frame.

Appendix C.2. Black Hole White Hole Transition

The geodesic congruence C_e^+, C_e^- determines a spacelike foliation of the WH and MSS region or BH and SS region, respectively. However, none of the leaves $\Sigma_{e,\tau}^\pm$ of the foliation is a Cauchy surface for those parts of the Kruskal spacetime because ρ is not allowed to take full range $\mathbb{R}$, rather it is restricted by $\pm(\tau - \rho) > 0$. The obvious idea to turn them into Cauchy surfaces is to consider a gluing of a past SS and BH part of one Kruskal spacetime with a future WH and MSS part of another Kruskal spacetime along the singularity $a = 0$. Accordingly, we consider fixed e coordinates $\tau, \rho \in \mathbb{R}$ and the metric

$$ds^2 = -d\tau^2 + [1 - \frac{\Phi(a)}{e^2}]\ d\rho^2 + a^2\ d\Omega^2 \tag{A77}$$

where $a(\tau, \rho)$ is the function implicitly defined by

$$|\tau - \rho| = \begin{cases} R\ (e^2 - 1)^{3/2})\ h(z),\ h(z) = [z\sqrt{z^2 + 1} - \ln(z + \sqrt{z^2 + 1})],\ z = [(e^2 - 1)a/R]^{1/2} & e^2 > 1 \\ \frac{2}{3}\frac{a^{3/2}}{R^{1/2}} & e^2 = 1 \end{cases} \tag{A78}$$

The metric (A77) is singular at the singularity "hypersurface" $\tau = \rho$ where $a = 0$. In the (τ, ρ) diagram the geodesics $\rho = \text{const.}$ cross the singularity at the proper time $\tau = \rho$ smoothly. The radial coordinate $a(\tau, \rho) \to 0$ is also continuous at $\tau = \rho$ but the radial velocity $da/d\tau \to \mp\infty$ as $\tau \to \rho\mp$. The $\tau = \text{const.}$ surfaces also intersect the singularity transversally in the (τ, ρ) diagram. Nevertheless, they are geometrically tangential: The reason for this is that the co-normals n, n' to the $\tau = \text{const.}$ and the $\tau - \rho = 0$ surface, respectively, are given by $n_\mu = \nabla_\mu \tau = \delta^\tau_\mu$, $n'_\mu = \nabla_\mu(\tau - \rho) = \delta^\tau_\mu - \delta^\rho_\mu$, hence the normal is given by $n^\mu = g^{\mu\nu} n_\nu = -\delta^\mu_\tau$ and $n'^\mu = g^{\mu\nu} n'_\nu = -\delta^\mu_\tau + \frac{a}{R}\delta^\mu_\rho$, respectively, thus $n = n'$ at $a = 0$.

We can return to GGP coordinates but need two radial coordinates, i.e., a past radial coordinate r and a future radial coordinate $\bar{r}$ which are related to τ, ρ by

$$r = a(\tau, \rho);\ t < \rho;\ \bar{r} = a(\tau, \rho);\ t > \rho \tag{A79}$$

These can be combined into a single coordinate

$$z = -\text{sgn}(\tau - \rho) a(\tau, \rho) = \begin{cases} -\bar{r} & \tau > \rho \\ r & \tau < \rho \end{cases} \tag{A80}$$

which like ρ takes full range in $\mathbb{R}$. Then, $dz/d\tau < 0$ (thus, z is monotonous along the geodesic) taking its minimal value $-\infty$ at $\tau = \rho$ and its maximal value $-\sqrt{e^2 - 1}$ at $\tau = \pm\infty$. Note, that if we use the same τ, θ, ϕ coordinates for the whole spacetime; therefore, the radial geodesics $\rho, \theta, \phi = \text{const.}$ change to the opposite direction when passing through the singularity.

Appendix C.3. Non-Singular Spacetime

In terms of the synchronous coordinates, the surface $a(\tau, \rho) = 0$ is three-dimensional but in terms of the Cartesian coordinates $x^a = r\Omega^a$, $\bar{x}^a = \bar{r}\Omega^a$, $a = 1, 2, 3$ which vanish at the singularity, it is just a one-dimensional line. This can be seen also by considering the surface $\tau = \rho + \epsilon$, $\epsilon \neq 0$ which has induced line element

$$ds^2 = -\frac{\Phi(a)}{e^2}\, d\rho^2 + a^2\, d\Omega^2 \tag{A81}$$

which for $\epsilon \to 0$ results in $R > a \to 0$ so that $0 < -\Phi(a) \to +\infty$ while $a \to 0$ so that (A80) formally has the signature $(1, 0, 0)$.

Following ideas about non-singular and wormhole spacetimes such as [117,118] we may exclude the singularity in an ad-hoc manner by simply restricting the range of $r, \bar{r}$ to (l, ∞), $l > 0$ and perform the gluing for each τ at $r = \bar{r} = l$, $\theta = \bar{\theta}, \phi = \bar{\phi}$ or at $r = \bar{r} = l$, $\theta = \pi - \bar{\theta}, \phi = \pi + \bar{\phi}$. which now has the the topology of $\mathbb{R} \times S^2$. In contrast to [117] and similar to [118] this still defines a *vacuum solution* for any $r, \bar{r} > l$, i.e., the energy-momentum tensor vanishes. This has the following mild disadvantage: The geodesic $\rho = \text{const.}$ in the region $\pm(\tau - \rho) > 0$ hits the value $r = a(\tau, \rho) = l$ at a value $\tau^\pm_l(\rho) = \rho \pm \epsilon_l$ where $a(\tau^\pm_l(\rho), \rho) = l$. Thus, the geodesic that starts at $\rho = \text{const.}$ in the $\tau < \rho$ region cannot continue as the geodesic with the same value of ρ in the $\tau > \rho$ region if the affine parameter is to be continuous. Rather, the geodesic parameter must change to ρ' where $\tau^+_l(\rho') = \tau^-_l(\rho)$. In the first gluing option the geodesic then continues in the opposite direction, in the second gluing option it continues into the same direction (remember that the geodesics are in/outgoing, respectively). If one wishes to interpret this in a τ, z diagram in which the angular dimension is suppressed, then it appears as if the geodesic jumps between $z = \pm l$. However, if we consider a three-dimensional diagram in which we depict the angular dependence by circles, then we should consider two copies of $\mathbb{R}^3$ covered by coordinates τ, r, φ and $\bar{\tau}, \bar{r}, \bar{\varphi}$ from which we cut out the solid cylinders $0 \leq r \leq l$ and $0 \leq \bar{r} \leq l$, respectively. We then glue the surfaces $r = l$ and $\bar{r} = l$ of the cylinders at either $\tau = \bar{\tau}, \varphi = \bar{\varphi}$ or $\tau = \bar{\tau}, \varphi = \pi + \bar{\varphi}$. A radial inward geodesic $\varphi = \text{const.}$

starting in the first copy then hits $r = l$ at some τ and continues either as the geodesic $\bar{\varphi} = \varphi =$ const. into the opposite or as the geodesic $\bar{\varphi} = \pi + \varphi =$ const. into the same direction. In both cases the geodesic is continuous because of the prescription in which we identified the points. In the second gluing option also the first derivative of the geodesic is continuous. W.l.g. consider the ingoing radial geodesic in 1-direction $\tau \mapsto (r_\rho(\tau), 0, 0)$ with $\tau \in (-\infty, \tau_l),\ r_\rho(\tau_l) = l$. Then, it continues as the outgoing geodesic $(\bar{r}_{\bar{\rho}}(\tau), 0, 0)$ with $\tau \in (\tau_l, \infty),\ r_{\bar{\rho}}(\tau_l) = l$ in the first option and as $(-\bar{r}_{\bar{\rho}}(\tau), 0, 0)$ in the second. We have by construction $-\dot{r}_\rho(\tau_l) = \dot{\bar{r}}_{\bar{\rho}}(\tau_l) > 0$. This spacetime is, therefore, geodesically complete with respect to the observers in these congruences and in that sense singularity-free. In the first option, an observer considers themselves as "bounced" off $r = l$ when entering the second universe while in the second option, they consider themselves as "gone through" the cylinder.

Note, that no causal geodesic can stay on the cylinder surface $r = l$ as it is spacelike. The $r =$ const. surfaces are timelike/null/spacelike for $r > / = / < R$ as may be seen easiest from (A82) while the hypersurfaces $\tau = const.$ are always spacelike. Therefore, the cylinder surfaces $r = l$ are for $l < R$ certainly spacelike and thus causal geodesics must cross them transversally. The cylinder surface replaces the singularity by a spacelike surface with coordinates τ, θ, ϕ and thus has the topology $\mathbb{R} \times S^2$. It maybe disturbing that the time τ here serves as a coordinate on a spacelike hypersurface but we can interpret it as the point of eigentime at which geodesic observers cross the gluing cylinder between the universes.

One may consider the introduction of l also as a regularization of the singular spacetime which maybe used to construct QFT in CST. This is relevant in the construction of mode systems (solutions of Klein–Gordon like equations) and 1-particle inner products which rely on the presence of Cauchy surfaces such as the leaves of this BHWHT foliation. From that perspective, the corresponding wave equations for a function $f(\tau, z, \Omega) = e^{i\omega\tau} f_\omega(z, \Omega)$ become stationary Schrödinger type of eigenvalue equations for f_ω in a singular potential as $l \to 0$ as we have shown in Section 8.

Appendix C.4. Causal Structure and Penrose Diagramme

In order to understand the causal structure of this singular BHWHT spacetime we consider the simpler case $e^2 = 1$ for which we can write the line element in terms of τ, z, θ, ϕ using (A65) and (A81)

$$ds^2 = -\Phi(|z|)\, d\tau^2 + 2\sqrt{\frac{R}{|z|}}\, d\tau\, dz + dz^2 + z^2 d\Omega^2 \tag{A82}$$

Its radial null geodesics are determined by

$$ds^2 = -|z|^{-1}\ (d\tau\ [1 + |z|^{-1/2}] + dz)\ (d\tau\ [1 - |z|^{-1/2}] - dz)\ = 0 \tag{A83}$$

where we switched to $\hat{\tau} = \tau/R,\ \hat{z} = z/R$ and removed the hat again. We use $z \in \mathbb{R}$ as a parameter so that we obtain two types of null geodesics

$$\frac{d\tau}{dz} = \mp \frac{|z|^{1/2}}{|z|^{1/2} \pm 1} \tag{A84}$$

For the upper sign, $d\tau/dz$ is everywhere regularly, at $z = \pm\infty$ taking the value -1, at the two horizons $z = \pm 1$ taking the value $-1/2$ and at the singularity of the value 0. For the lower sign we have four kinds of null geodesics, namely those that are stuck in either of the intervals $(1, \infty),\ (-1, 1),\ (-\infty, -1)$ and those that are stuck at the horizions $|z| = 1$. For the first interval the null geodesic starts at $z = 1$ with $d\tau/dz = +\infty$ moving to $z = \infty$ with $d\tau/dz = 1$. For the third interval the null geodesic ends at $z = -1$ with $d\tau/dz = +\infty$ having moved from $z = -\infty$ with $d\tau/dz = 1$. For the second interval the geodesic starts at $z = 1$ in the infinite past with $d\tau/dz = -\infty$, passes through $z = 0$ with $d\tau/dz = 0$ and ends at $z=-1$ in the infinite future with $d\tau/dz=-\infty$. Accordingly, in the τ, z diagram the lightcone structure is as follows: For $|z|>1$ there are ingoing and outgoing light rays (i.e., moving to smaller and larger $|z|$), for $z=1$ there is one ingoing one and one that is tangential to the horizon, for $z=-1$ there is one outgoing one and one that is tangential to the horizon, for $0<z<1$ there are only ingoing lightrays (trapped region), for $-1<z<0$ there are only outgoing lightrays (anti-trapped region) and for $-\infty<z<-1$ there are both ingoing and outgoing lightrays. This is of course exactly the BHWHT spacetime structure. The discussion also shows that the restriction to $z>0$ ($z<0$), respectively, covers precisely an ingoing (outgoing) GP spacetime or equivalently an advanced (retarded) Finkelstein spacetime (covered by v, r or u, r coordinates, respectively, with $v=t+r_*,\ u=t-r_*$ on the SS portion where t is SS time and r_* is the turtoise coordinate, i.e., there is always the ingoing (outgoing) null geodesic $v=$ const. ($u=$ const.)).

It is helpful to construct the corresponding Penrose diagram which can be conducted analytically in the case $e^2=1$ in terms of Kruskal coordinates. From (A64) we have

$$\tau=\bar{t}-f(\bar{r})=t+f(r),\ f(r)=R(2y+\ln(\frac{y-1}{y+1})),\ y=\sqrt{\frac{r}{R}} \tag{A85}$$

for Schwarzschild coordinates $r, \bar{r}>1$ and Schwarzschild asymptotic times $t, \bar{t}$ in the SS and MSS regions, respectively. In terms of the null coordinates $v=t+r_*,\ u=t-r_*$, $r_*=r+R\ln(\frac{r}{R}-1)$ and analogously for the barred quantities we set

$$V:=e^{\frac{v}{2R}},\ U:=-e^{-\frac{u}{2R}},\ \bar{V}:=-e^{\frac{\bar{v}}{2R}},\ \bar{U}:=e^{-\frac{\bar{u}}{2R}}, \tag{A86}$$

By substituting $r_*/R=y+\ln(y^2-1)$ and for $t, \bar{t}$ according to (A85) one finds with $\kappa=\tau/(2R)$

$$V=e^{\kappa+\frac{y^2}{2}-y}\ (y+1),\ U=-e^{-\kappa+\frac{y^2}{2}+y}\ (y-1),\ \bar{V}=-e^{\kappa+\frac{\bar{y}^2}{2}+\bar{y}}\ (\bar{y}-1),\ \bar{U}=e^{-\kappa+\frac{\bar{y}^2}{2}-\bar{y}}\ (\bar{y}+1) \tag{A87}$$

The choice of signs is here uniquely determined by the continuity requirement that at the singularity $y=\bar{y}=0$ we have $\bar{V}=V, \bar{U}=U$. Thus, for $y, \bar{y}\in\mathbb{R}^+,\ \tau\in\mathbb{R}$ we have $U, \bar{V}\in\mathbb{R},\ V, \bar{U}\in\mathbb{R}^+$ and the Kruskal relations

$$U\ V=-e^{y^2}(y^2-1),\ \ \bar{U}\ \bar{V}=-e^{\bar{y}^2}(\bar{y}^2-1) \tag{A88}$$

which are bounded from above by $+1$. The SS, BH, WH, MSS regions are, respectively, covered by $V>0>U$, $U, V>0$, $\bar{U}, \bar{V}>0$, $\bar{U}>0>\bar{V}$ separated, respectively, by the BH horizon $y=1$, the singularity $y=\bar{y}=0$ and the WH horizon $\bar{y}=1$ in chronological order. We introduce compactified null coordinates

$$\hat{v}=\mathrm{arctan}(V),\ \hat{u}=\mathrm{arctan}(U),\ \hat{\bar{v}}=\mathrm{arctan}(\bar{V}),\ \hat{\bar{u}}=\mathrm{arctan}(\bar{U}), \tag{A89}$$

with $\hat{v}, \hat{\bar{u}}\in(0, \frac{\pi}{2}),\ \hat{u}, \hat{\bar{v}}\in(-\frac{\pi}{2}, \frac{\pi}{2})$ and finally

$$\hat{t}:=\begin{cases}\hat{v}+\hat{u} & \mathsf{SS, BH}\\ \pi-(\hat{\bar{v}}+\hat{\bar{u}}) & \mathsf{WH, MSS}\end{cases},\quad \hat{x}:=\begin{cases}\hat{v}-\hat{u} & \mathsf{SS, BH}\\ \hat{\bar{v}}-\hat{\bar{u}} & \mathsf{WH, MSS}\end{cases} \tag{A90}$$

It follows that in SS $-\pi/2\le\hat{u}\le0\le\hat{v}$ we have

$$0\le2\hat{v}=\hat{t}+\hat{x}\le\pi,\ -\pi\le2\hat{u}=\hat{t}-\hat{x}\le0,\ 0\le\hat{x}\le\pi\ \ \Rightarrow\ \mathsf{max}(-\hat{x}, \hat{x}-\pi)\le\hat{t}\le\mathsf{min}(\hat{x}, \pi-\hat{x}) \tag{A91}$$

in BH $0\le\hat{u}, \hat{v}\le\pi/2$ and $U\ V=\frac{\cos(\hat{v}-\hat{u})-\cos(\hat{v}-\hat{u})}{\cos(\hat{v}-\hat{u})+\cos(\hat{v}-\hat{u})}\le1$, i.e., $\cos(\hat{v}+\hat{u})\ge0$ i.e., $\hat{t}\le\pi/2$ and

$$0\le2\hat{v}=\hat{t}+\hat{x}\le\pi,\ 0\le2\hat{u}=\hat{t}-\hat{x}\le\pi,\ 0\le\hat{t}\le\pi/2\ \ \Rightarrow\ -\hat{t}\le\hat{x}\le\hat{t} \tag{A92}$$

in WH $0 \leq \hat{u}, \hat{v} \leq \pi/2$ and $\bar{U}\ \bar{V} = \frac{\cos(\hat{v}-\hat{u})-\cos(\hat{v}-\hat{u})}{\cos(\hat{v}-\hat{u})+\cos(\hat{v}-\hat{u})} \leq 1$, i.e., $\cos(\hat{v}+\hat{u}) \geq 0$, i.e., $\hat{u}+\hat{v} \leq \pi/2$, i.e., $\hat{t} \geq \pi/2$ and

$$0 \leq 2\hat{v} = \pi - \hat{t} + \hat{x} \leq \pi,\ 0 \leq 2\hat{u} = \pi - \hat{t} - \hat{x} \leq \pi,\ \pi/2 \leq \hat{t}\ \Rightarrow\ \hat{t} - \pi \leq \hat{x} \leq \pi - \hat{t} \tag{A93}$$

and in MSS $-\pi/2 \leq \hat{v} \leq 0 \leq \hat{u} \leq \pi/2$ and $-\pi \leq \hat{x} \leq 0$ and

$$-\pi \leq 2\hat{v} = \pi - \hat{t} + \hat{x} \leq 0,\ 0 \leq 2\hat{u} = \pi - \hat{t} - \hat{x} \leq \pi,\ \Rightarrow\ \max(-\hat{x}, \hat{x}+\pi) \leq \hat{t} \leq \min(2\pi+\hat{x}, \pi-\hat{x}) \tag{A94}$$

It is not difficult to see that in the $\hat{x}, \hat{t}$ diagram SS is a diamond with corners $b_P = (0,0)$, $i^-_P = (\pi/2, -\pi/2)$, $i^0_P = (\pi, 0), i^+_P = (\pi/2, \pi/2)$, BH is a triangle with corners $b_P, i^+_P, i^-_F = (-\pi/2, \pi/2)$, WH is a triangle with corners $b_F = (0, \pi), i^-_F, i^+_P$ and MSS is a diamond with corners $i^0_F = (-\pi, \pi)$, i^-_F, b_F, $i^+_F = (-\pi/2, 3\pi/2)$. Here, the subscripts refer to past and future Kruskal portions. The singularity is the line between i^-_F, i^+_P, the BH horizon is the line between b_P, i^+_P, the WH horizon is the line between i^-_F, b_F. Past and future null infinity in SS are the lines between i^-_P, i^0_P and i^0_P, i^+_P, respectively, while past and future null infinity in MSS are the lines between $i-_F, i^0_F$ and i^0_F, i^+_F, respectively. All other diagonal lines are at $r = R$ or $\bar{r} = R$, respectively. The points b_P, b_F are the bifurcation points in the full past and future Kruskal spacetimes.

This BHWHT spacetime can be extended indefinitely to the future and the past by gluing identical pieces along the $r = R, \bar{r} = R$ lines. Or we can complete it by a Minkowski part of spacetime both in the past and the future by adding the points $I^-_P = (-\pi/2, -3\pi/2)$ and $I^+_F = (\pi/2, 5\pi/2)$, respectively, and adding the triangles with corners I^-_P, i^-_P, i^-_F and I^+_F, i^+_F, i^+_P, respectively. The vertical lines between I^-_P, I^+_F and the singularity then represent $r = 0$ during the formation of the black hole and evaporation of the white hole, respectively. In this completed spacetime the free-falling hypersurfaces are still Cauchy surfaces and we can complete the foliation in the Minkowski regions by segments along past and future null infinity between i^0_P, I^-_P and i^0_F, I^+_F and Cauchy surfaces in the Minkowksi parts. In the completed spacetime past null infinity in the past part and and future null infinity in the future part got extended by the Minkowski parts and we have two spacelike infinities i^0_P, i^0_F and one past and future timelike infinity I^-_P, I^+_F, respectively.

We now explore the radial timelike geodesics and the free-falling orthogonal foliation they generate. For a geodesic $\rho =$ const. we are interested in the limits $\tau \to \pm\infty$. For $\tau \to +\infty$ we eventually enter the region $\tau > \rho$ covered by $\bar{y} = (\bar{r}/R)^{1/2} = [\frac{3}{2}(\tau-\rho)/R]^{1/3}$ which grows as $[\tau/R]^{1/3}$. Hence, even $\bar{y}^2$ grows slower than τ/R and the behavior of $\bar{V}, \bar{U}$ is governed by $e^{\pm\tau/(2R)}$. Thus, $\bar{V} \to -\infty, \bar{U} \to 0$ hence $\hat{v} \to -\pi/2$, $\hat{u} \to 0$ i.e., $\hat{t} = \pi - \hat{v} - \hat{u} \to 3\pi/2$, $\hat{x} = \hat{v} - \hat{u} \to -\pi/2$ i.e., the geodesic ends up in i^+_F. For $\tau \to -\infty$ we eventually enter the region $\tau < \rho$ covered by $y = (r/R)^{1/2} = [-\frac{3}{2}(\tau-\rho)/R]^{1/3}$ which grows as $[-\tau/R]^{1/3}$. Hence, even y^2 grows slower than $-\tau/R$ and the behavior of V, U is governed by $e^{\pm\tau/(2R)}$. Thus, $V \to 0, \bar{U} \to -\infty$ hence $\hat{v} \to 0$, $\hat{u} \to -\pi/2$, i.e., $\hat{t} = \hat{v} + \hat{u} \to -\pi/2$, $\hat{x} = \hat{v} - \hat{u} \to \pi/2$, i.e., the geodesic ends up in i^-_P.

For the $\tau =$ const. slices we are interested in $\rho \to \pm\infty$. For $\rho \to \infty$ we eventually enter the region $\tau - \rho < 0$ covered by $y = [-\frac{3}{2}(\tau-\rho)/R]^{1/3}$ which grows as $[\rho/R]^{1/3}$ and the behavior of V, U is governed by $e^{y^2/2}$. Thus, $V \to +\infty, U \to -\infty$ i.e., $\hat{v} \to \pi/2$, $\hat{u} \to -\pi/2$ hence $\hat{t} \to 0$, $\hat{x} \to \pi$, i.e., we end up in i^0_P. For $\rho \to -\infty$ we eventually enter the region $\tau - \rho > 0$ covered by $\bar{y} = [\frac{3}{2}(\tau-\rho)/R]^{1/3}$ which grows as $[-\rho/R]^{1/3}$ and the behavior of V, U is governed by $e^{\bar{y}^2/2}$. Thus, $\bar{V} \to -\infty, \bar{U} \to \infty$, i.e., $\hat{v} \to -\pi/2$, $\hat{u} \to \pi/2$ hence $\hat{t} \to \pi$, $\hat{x} \to -\pi$, i.e., we end up in i^0_F.

Thus, the following geometric picture emerges: All geodesics start at i^-_P and end in i^+_F as τ grows, all leaves start in i^0_F and end in i^0_P as ρ grows. The geodesic labeled by ρ intersects at $\tau = \rho$ the singularity in a point while the hypersurface labeled by τ intersects the singularity at the coordinate label $\rho = \tau$ in a sphere. One can work out $d\hat{t}, d\hat{x}$ explicitly in terms of the differentials $d\tau, d\rho$ using the coordinate transformation between these coordinates by the same technique as below for T, X coordinates. One then shows by computing $\frac{d\hat{t}}{d\hat{x}}$ that in the Penrose diagram all $\tau =$ const. surfaces coordinated by ρ are tangent to the horizontal line representing the singularity ($\rho = \tau$) and have inclination of +45 degrees at the spatial infinities ($\rho = \pm\infty$) while the geodesics $\rho =$ const. coordinated by τ intersect the singularity line at 90 degrees ($\tau = \rho$) and have an inclination of +45 degrees at the timelike infinities ($\tau = \pm\infty$).

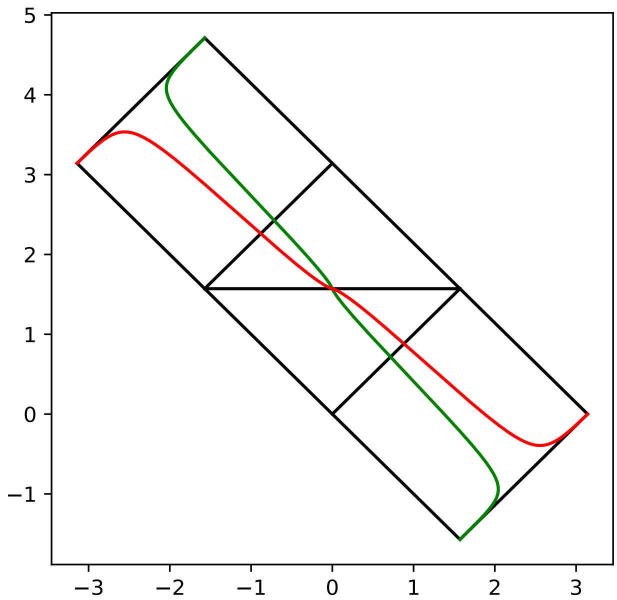

Figure A1. Penrose diagram of a globally hyperbolic region of a black hole–white hole transition with timelike geodesic labeled by $\rho = c$ (green) and Cauchy hypersurface labeled by $\tau = c$ for a constant c. The geodesic starts in i_P^- and ends in i_F^+ (bottom to top) intersecting the singularity $r = 0$ at proper time $\tau = c$ vertically. The Cauchy surface starts at i_F^0 and ends in i_P^0 (left to right) intersecting the singularity at spatial coordinate $\rho = c$ horizontally. The spacetime can be extended indefinitely to the future and past by gluing identical regions along the 45 degree lines $r = 2M$ of the boundaries of the black hole and white hole regions, respectively. Or it can be completed by adding a triangular Minkowski region in the past and the future along the 45 lines $r = 2M$ between i_P^-, i_F^+ and the line $r = 0$, respectively.

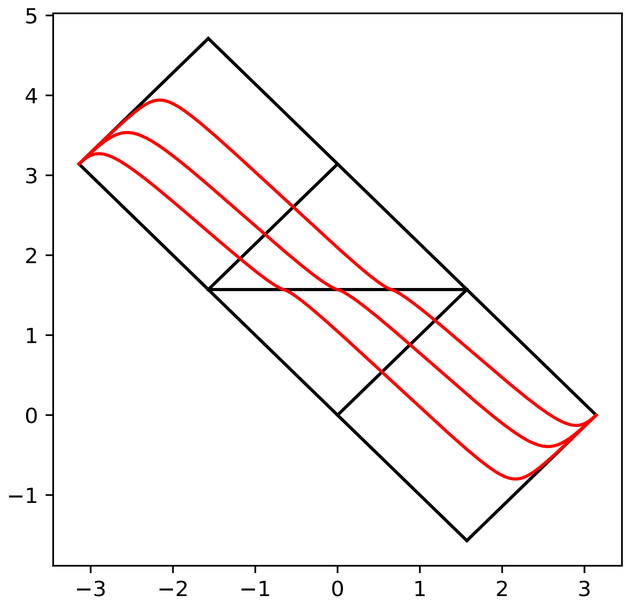

Figure A2. Foliation of a globally hyperbolic portion of a BHWHT spacetime by synchronous proper time free falling Cauchy surfaces. The portion is the common domain of dependence of all leaves of the foliation.

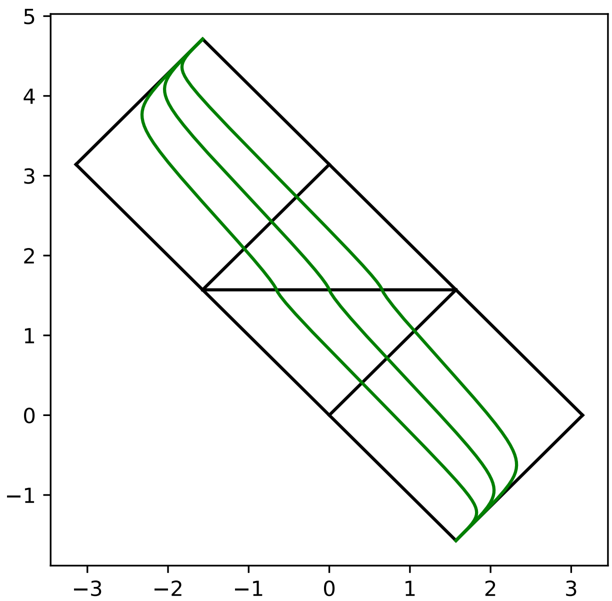

Figure A3. Congruence of free-falling timelike observers in a globally hyperbolic portion of a BHWHT spacetime.

In order to determine the finer details of this intersection we introduce the coordinates $T, X, \bar{T}, \bar{X}$ defined by

$$2T = V + U,\ 2X = V - U,\ 2\bar{T} = -(\bar{V} + \bar{U}),\ 2\bar{X} = \bar{V} - \bar{U} \tag{A95}$$

Thus, $\bar{X} = X,\ \bar{T} = -T$ at the singularity. Since $U\ V = T^2 - X^2 = 1 = \bar{V}\ \bar{U} = \bar{T}^2 - \bar{X}^2$ at the singularity and $U = \bar{U}, V = \bar{V} > 0$ it follows $T = \sqrt{1+X^2},\ \bar{T} = -\sqrt{1+\bar{X}^2}$ describes the singularity curves in terms of these coordinates. These have inclinations $dT/dX = \frac{X}{\sqrt{1+X^2}},\ d\bar{T}/d\bar{X} = -\frac{\bar{X}}{\sqrt{1+\bar{X}^2}}$, respectively.

We now compute for $y = y(\tau, \rho),\ \bar{y} = \bar{y}(\tau, \rho)$, respectively, and $\tau < \rho,\ \tau > \rho$, respectively, using

$$dy^2/2 = \frac{1}{2Ry}(d\rho - d\tau),\ d\bar{y}^2/2 = \frac{1}{2R\bar{y}}(d\tau - d\rho),\ d[(y \pm 1)\ e^{y^2/2 - \mp y}] = y^2\ e^{y^2/2 \mp y}\ dy \tag{A96}$$

the differentials

$$\begin{aligned}
dV &= \frac{V}{2R}\ (d\tau + \frac{1}{y+1}(d\rho - d\tau)) = \frac{V}{2R(y+1)}(y\ d\tau + d\rho) \\
dU &= \frac{U}{2R}\ (-d\tau + \frac{1}{y-1}(d\rho - d\tau) = \frac{U}{2R(y-1)}\ (-y\ d\tau + d\rho) \\
d\bar{V} &= \frac{\bar{V}}{2R}\ (d\tau + \frac{1}{\bar{y}-1}(d\tau - d\rho)) = \frac{\bar{V}}{2R(\bar{y}-1)}(\bar{y}\ d\tau - d\rho) \\
d\bar{U} &= \frac{\bar{U}}{2R}\ (-d\tau + \frac{1}{\bar{y}+1}(d\tau - d\rho) = \frac{\bar{U}}{2R(\bar{y}+1)}\ (-\bar{y}\ d\tau - d\rho)
\end{aligned} \tag{A97}$$

It follows

$$\begin{aligned} 2dT &= \frac{e^{y^2/2}}{2R}\,[e^{\kappa-y}\,(d\rho+yd\tau)-e^{-\kappa+y}\,(d\rho-yd\tau)] \\ 2dX &= \frac{e^{y^2/2}}{2R}\,[e^{\kappa-y}\,(d\rho+yd\tau)+e^{-\kappa+y}\,(d\rho-yd\tau)] \\ 2d\bar{T} &= \frac{e^{\bar{y}^2/2}}{2R}\,[-e^{\kappa+\bar{y}}\,(d\rho-\bar{y}d\tau)+e^{-\kappa-\bar{y}}\,(d\rho+\bar{y}d\tau)] \\ 2d\bar{X} &= \frac{e^{\bar{y}^2/2}}{2R}\,[e^{\kappa+\bar{y}}\,(d\rho-\bar{y}d\tau)+e^{-\kappa-\bar{y}}\,(d\rho+\bar{y}d\tau)] \end{aligned} \tag{A98}$$

This gives

$$\begin{aligned} \frac{dT}{dX} &= \frac{\mathrm{sh}(\kappa-y)\,d\rho+y\,\mathrm{ch}(\kappa-y)\,d\tau}{\mathrm{ch}(\kappa-y)\,d\rho+y\,\mathrm{sh}(\kappa-y)\,d\tau} \\ \frac{d\bar{T}}{d\bar{X}} &= \frac{-\mathrm{sh}(\kappa+\bar{y})\,d\rho+\bar{y}\,\mathrm{ch}(\kappa+\bar{y})\,d\tau}{\mathrm{ch}(\kappa+\bar{y})\,d\rho-\bar{y}\,\mathrm{sh}(\kappa+\bar{y})\,d\tau} \end{aligned} \tag{A99}$$

This enables us to conveniently compute the inclinations. For geodesics $d\rho = 0$

$$\frac{dT}{dX} = \mathrm{coth}(\kappa-y),\;\; \frac{d\bar{T}}{d\bar{X}} = -\mathrm{coth}(\kappa+\bar{y}) \tag{A100}$$

and for hypersurfaces $d\tau = 0$

$$\frac{dT}{dX} = \mathrm{th}(\kappa-y),\;\; \frac{d\bar{T}}{d\bar{X}} = -\mathrm{th}(\kappa+\bar{y}) \tag{A101}$$

Thus, in the T, X and $\bar{T}, \bar{X}$ diagram, respectively, the geodesics and hypersurfaces have anti-reciprocal inclinations.

Since at $y = 0$ we have $2X = 2\mathrm{sh}(\kappa)$ and at $\bar{y} = 0$ we have $2\bar{X} = 2\mathrm{sh}(\kappa)$ it follows that the singularity inclination is $\mathrm{th}(\kappa)$ in terms of T, X and $-\mathrm{th}(\kappa)$ in terms of $\bar{T}, \bar{X}$, respectively. It follows that the hypersurfaces are tangent to the singularity while the geodesics are transversal. Thus, in these coordinates, a $\tau =$ const. hypersurface can be described in terms of the T, X coordinates until it intersects the singularity tangentially ($T = \mathrm{ch}(\kappa), X = \mathrm{sh}(\kappa)$). Then, it continues from the tangential point ($\bar{T} = -\mathrm{ch}(\kappa), \bar{X} = \mathrm{sh}(\kappa)$) in terms of $\bar{T}, \bar{X}$ coordinates.

If one wants to avoid the jump by $-2\sqrt{1+X^2}$ between T and $\bar{T}$ at the singularity, we may substitute $T, \bar{T}$ by $T - \sqrt{1+X^2},\; \bar{T} + \sqrt{1+\bar{X}^2}$ which maps the singularity to the common line $T = \bar{T} = 0$.

Appendix C.5. Relation between Different GGP Coordinates

A GGP coordinate system is determined by two parameters M, e. It determines a geodesic congruence C_e in the BHWHT spacetime which by construction is isometric to two copies of two complementary halves (namely SS, BH and WH, MSS parts) of Kruskal spacetime where the latter carries a single parameter M. From this point of view the additional parameter e is redundant and can be fixed to any desired value by a spacetime diffeomorphism. To change between two different values, say e, e' we relate them through the Schwarzschild time

$$\tau_e^{\pm} = e\;t \mp \int\;dr\;\frac{\sqrt{e^2-\Phi(r)}}{\Phi(r)} \tag{A102}$$

which means

$$\frac{1}{e}[\tau_e^{\pm} \pm \int\;dr\;\frac{\sqrt{e^2-\Phi(r)}}{\Phi(r)}] = t = \frac{1}{e'}[\tau_{e'}^{\pm} \pm \int\;dr\;\frac{\sqrt{(e')^2-\Phi(r)}}{\Phi(r)}] \tag{A103}$$

This corresponds to a temporal diffeomorphism (consider $e, e' > 0$)

$$\tau^{\pm}_{e'} = \frac{e'}{e}\tau^{\pm}_{e} \pm [e'] \int dr\ \Phi(r)^{-1}[\sqrt{1-e^{-2}\ \Phi(r)} - \sqrt{1-(e')^{-2}\ \Phi(r)}] \tag{A104}$$

while the radial coordinate is unchanged. Noticing that $g^e_{rr} = q^e_{rr} = e^{-2}$ we see that the right hand side of (A104) is exactly the second Dirac observable conjugate to the mass as derived from the Hamiltonian formulation. This shows that in the Lagrangian formulation the second Dirac observable is considered as a gauge degree of freedom.

Appendix C.6. Dirac Observable Conjugate to Mass in GGP

We evaluate the Dirac observable conjugate to the mass M (dropping inessential constants)

$$Q = \int_{\mathbb{R}} dz\ \delta'\ \frac{\sqrt{1-\gamma^2\Phi}}{\Phi},\ q_{ab}\ dx^a\ dx^b = \gamma^2(z)dz^2 + \delta(z)^2 d\Omega^2,\ \ \Phi = 1 - \frac{R}{|\delta(z)|},\ R = 2M \tag{A105}$$

in the GGP gauge $\delta(z) = z,\ \gamma(z) = e^{-2},\ e^2 \geq 1,\ e = \text{const}$. This gives

$$Q = 2\int_{\mathbb{R}^+} dr\ \frac{\sqrt{1-\gamma^2\Phi(r)}}{\Phi(r)},\ \Phi(r) = 1 - \frac{R}{r} \tag{A106}$$

The integral (A106) is ill-defined as it stands due to a singularity at $r = R$ and $r = \infty$ while it is regular at $r = 0$. It, therefore, needs a more detailed definition. We regularize it with three parameters $c < R, d < R, L > 2\,R$

$$\frac{Q_{c,d,L}}{2} = \int_0^{R-c} dr\ \frac{\sqrt{1-\gamma^2\Phi}}{\Phi},\ + \int_{R+d}^{L} dr\ \frac{\sqrt{1-\gamma^2\Phi}}{\Phi}, \tag{A107}$$

and eventually, take $c, d, L^{-1} \to 0+$. Note, that $\gamma^2 \leq 1$. We treat the case $\gamma^2 = 1$ separately from the case $\gamma^2 < 1$.

Case 1. $\gamma^2 = 1$: *We have*

$$\begin{aligned}
\frac{Q_{c,d,L}}{2} &= \sqrt{R}\,[\int_0^{R-c} dr\ \frac{\sqrt{r}}{r-R} + \int_{R+d}^{L} dr\ \frac{\sqrt{r}}{r-R}] \\
&= R\,[\int_0^{1-c/R} dx\ \frac{\sqrt{x}}{x-1} + \int_{1+d/R}^{L/R} dx\ \frac{\sqrt{x}}{x-1}] \\
&= 2\,R\,[\int_0^{\sqrt{1-c/R}} dy\ \frac{y^2}{y^2-1} + \int_{\sqrt{1+d/R}}^{\sqrt{L/R}} dy\ \frac{y^2}{y^2-1}] \\
&= 2\,R\,[\sqrt{L/R} - \sqrt{1+d/R} + \sqrt{1-c/R} - \int_0^{\sqrt{1-c/R}} dy\ \frac{1}{1-y^2} + \int_{\sqrt{1+d/R}}^{\sqrt{L/R}} dy\ \frac{1}{y^2-1}] \\
&= 2\,R\,[\sqrt{L/R} - \sqrt{1+d/R} + \sqrt{1-c/R} - \frac{1}{2}\,[\ln(\frac{1+y}{1-y})]_0^{\sqrt{1-c/R}} + \frac{1}{2}\,[\ln(\frac{y-1}{y+1})]_{\sqrt{1+d/R}}^{\sqrt{L/R}}] \\
&= 2\,R\,[\sqrt{L/R} - \sqrt{1+d/R} + \sqrt{1-c/R} \\
&\quad -\frac{1}{2}\,[\ln(\frac{[1+y]^2}{1-y^2})]_{y=\sqrt{1-c/R}} - \frac{1}{2}\,[\ln(\frac{y^2-1}{[y+1]^2})]_{y=\sqrt{1+d/R}} + \frac{1}{2}\,[\ln(\frac{y-1}{y+1})]_{y=\sqrt{L/R}}]
\end{aligned} \tag{A108}$$

with $x = r/R = y^2$. The terms $\sqrt{1-c/R} - \sqrt{1+d/R},\ [\ln(y+1)]^{\sqrt{1+d/R}}_{\sqrt{1-c/R}},\ \ln((y+1)/(y-1))_{y=\sqrt{L/R}}$ vanish independently of how we take the limit $c, d, L^{-1} \to 0$. Thus, up to those terms, (A108) becomes

$$\frac{Q_{c,d,L}}{2} = 2\,R\,[\sqrt{L/R} - \frac{1}{2}\ln(\frac{d}{c})] \tag{A109}$$

Case 2. $\gamma^2 < 1$ *We have with* $a^2 := \frac{\gamma^2}{1-\gamma^2}$

$$\frac{Q_{c,d,L}}{2} = 2\,R\,\sqrt{1-\gamma^2}\,[\int_0^{\sqrt{1-c/R}} dy\,\frac{y^2\sqrt{y^2+a^2}}{y^2-1} + \int_{\sqrt{1+d/R}}^{\sqrt{L/R}} dy\,\frac{y^2\sqrt{y^2+a^2}}{y^2-1}] \tag{A110}$$
$$= 2\,R\,\sqrt{1-\gamma^2}\,[\int_0^{\sqrt{1-c/R}} dy\,\{\sqrt{y^2+a^2} + \frac{\sqrt{y^2+a^2}}{y^2-1}\} + \int_{\sqrt{1+d/R}}^{\sqrt{L/R}} dy\,\{\sqrt{y^2+a^2} + \frac{\sqrt{y^2+a^2}}{y^2-1}\}]$$

We have the elementary integrals

$$\int dy\,\sqrt{y^2+a^2} = \frac{1}{2}[y\sqrt{y^2+a^2} + \ln(y+\sqrt{y^2+a^2})]$$
$$\int dy\,\frac{1}{\sqrt{y^2+a^2}} = \ln(y+\sqrt{y^2+a^2})$$
$$\int dy\,\frac{\sqrt{y^2+a^2}}{y^2-b^2} = \ln(y+\sqrt{y^2+a^2}) + \int dy\,\frac{1}{\sqrt{y^2+a^2}}\,[\frac{y^2+a^2}{y^2-b^2} - 1]$$
$$= \ln(y+\sqrt{y^2+a^2}) + (a^2+b^2)\int dy\,\frac{1}{\sqrt{y^2+a^2}}\,\frac{1}{y^2-b^2} \tag{A111}$$

We have

$$\frac{d}{dy}\mathrm{arth}(h\frac{y}{\sqrt{y^2+a^2}}) = \frac{d}{dy}\mathrm{arcoth}(h\frac{y}{\sqrt{y^2+a^2}}) = -\frac{1}{\sqrt{y^2+a^2}}\,\frac{ha^2}{h^2-1}\,\frac{1}{y^2-\frac{a^2}{h^2-1}} \tag{A112}$$

To match this to last integral in (A111) we pick $a^2/(h^2-1) = b^2,\ h^2 = 1 + a^2/b^2$ so that $ha^2/(h^2-1) = b\sqrt{a^2+b^2}$. Then, the argument of the hyperbolic function becomes $\sqrt{1+a^2/b^2}y/\sqrt{y^2+a^2})$ which must take values in $(-1,1)$ and $\mathbb{R}-[-1,1]$, respectively, for hyperbolic tangens and cotangens, respectively. For the tangens function this implies due to $b=1$ in our case that $|y|<1$ while $|y|>1$ for the cotangens function. Assembling these findings we have with $b^2=1$ in our case

$$\frac{Q_{c,d,L}}{2} = 2\,R\,\sqrt{1-\gamma^2}\,\{\frac{1}{2}[y\sqrt{y^2+a^2} + 3\,\ln(y+\sqrt{y^2+a^2})]_0^{\sqrt{1-c/R}}$$
$$+\frac{1}{2}[y\sqrt{y^2+a^2} + 3\,\ln(y+\sqrt{y^2+a^2})]_{\sqrt{1+d/R}}^{\sqrt{L/R}}$$
$$-\sqrt{a^2+1}\,[\mathrm{arth}(\sqrt{a^2+1}\frac{y}{\sqrt{y^2+a^2}})]_0^{\sqrt{1-c/R}} - \sqrt{a^2+1}\,[\mathrm{arcoth}(\sqrt{a^2+1}\frac{y}{\sqrt{y^2+a^2}})]_{\sqrt{1+d/R}}^{\sqrt{L/R}}\} \tag{A113}$$

where we may use

$$\mathrm{arth}(z) = \frac{1}{2}\ln(\frac{1+z}{1-z}),\ \mathrm{arcoth}(z) = \frac{1}{2}\ln(\frac{z+1}{z-1}), \tag{A114}$$

for $|z|<1, |z|>1$, respectively. Up to terms that vanish no matter how we take $c,d,L^{-1}\to 0$ the first two terms in (A113) may be combined into

$$2\,R\,\sqrt{1-\gamma^2}\,\frac{1}{2}[y\sqrt{y^2+a^2} + 3\ln(y+\sqrt{y^2+1})]_0^{\sqrt{L/R}} \tag{A115}$$

where the contribution from $y=0$ vanishes. The last two terms in (A113) are with $z(y) = \sqrt{a^2+1}\frac{y}{\sqrt{y^2+a^2}}$

$$2\,R\,\sqrt{1-\gamma^2}\,(-\frac{1}{2}\sqrt{1+a^2})\ln([\frac{1+z}{1-z}]_{y=\sqrt{1-c/R}}\,[\frac{1-z}{1+z}]_{y=0}\,[\frac{z+1}{z-1}]_{y=\sqrt{L/R}}\,[\frac{z-1}{z+1}]_{y=\sqrt{1+d/R}}) \tag{A116}$$

We have

$$\frac{z+1}{z-1} = \frac{\sqrt{1+a^2}\, y + \sqrt{y^2+a^2}}{\sqrt{1+a^2}\, y - \sqrt{y^2+a^2}} \tag{A117}$$

which for $y = 0$ equals -1 and for $y = \sqrt{L/R}$ equals

$$\frac{\sqrt{1+a^2} + \sqrt{1+a^2 R/L}}{\sqrt{1+a^2} - \sqrt{1+a^2 R/L}} \to \frac{\sqrt{1+a^2}+1}{\sqrt{1+a^2}-1} \tag{A118}$$

which is finite no matter how $c, d, L^{-1} \to 0$. For $y = \sqrt{1+d/R}$ (A117) becomes

$$\begin{aligned} \frac{\sqrt{1+a^2}\,\sqrt{1+d/R} + \sqrt{1+a^2+d/R}}{\sqrt{1+a^2}\,\sqrt{1+d/R} - \sqrt{1+a^2+d/R}} &= \frac{[\sqrt{1+a^2}\,\sqrt{1+d/R} + \sqrt{1+a^2+d/R}]^2}{(1+a^2)\,(1+d/R) - (1+a^2+d/R)} \\ = \frac{[\sqrt{1+a^2}\,\sqrt{1+d/R} + \sqrt{1+a^2+d/R}]^2}{a^2\, d/R} &\to \frac{4(1+a^2)^2}{a^2\, d/R} \end{aligned} \tag{A119}$$

while for $y = \sqrt{1-c/R}$ (A117) becomes

$$\begin{aligned} \frac{\sqrt{1+a^2}\,\sqrt{1-c/R} + \sqrt{1+a^2-c/R}}{\sqrt{1+a^2}\,\sqrt{1-d/R} - \sqrt{1+a^2-d/R}} &= \frac{[\sqrt{1+a^2}\,\sqrt{1-d/R} + \sqrt{1+a^2-d/R}]^2}{(1+a^2)\,(1-c/R) - (1+a^2-d/R)} \\ = \frac{[\sqrt{1+a^2}\,\sqrt{1-c/R} + \sqrt{1+a^2-c/R}]^2}{-a^2\, c/R} &\to -\frac{4(1+a^2)^2}{a^2\, c/R} \end{aligned} \tag{A120}$$

Hence, the last two terms in (A113) approach

$$\begin{aligned} & 2\, R\, \sqrt{1-\gamma^2}\, (-\frac{1}{2}\sqrt{1+a^2})\ln(\frac{4(1+a^2)^2}{a^2\, c/R}\, \frac{\sqrt{1+a^2}+1}{\sqrt{1+a^2}-1}\, \frac{a^2\, d/R}{4(1+a^2)^2}) \\ = \;& 2\, R\, \sqrt{1-\gamma^2}\, (-\frac{1}{2}\sqrt{1+a^2})\ln(\frac{d}{c}\, \frac{\sqrt{1+a^2}+1}{\sqrt{1+a^2}-1}) \end{aligned} \tag{A121}$$

Altogether with $a^2 = \gamma^2/(1-\gamma^2), 1+a^2 = 1/(1-\gamma^2))$

$$\frac{Q_{c,d,L}}{2} = \frac{2\, R}{\sqrt{1+a^2}}\, \{\frac{1}{2}[y\sqrt{y^2+a^2} + 3\ln(y+\sqrt{y^2+a^2})]_{y=\sqrt{L/R}} - \frac{1}{2}\sqrt{1+a^2}\, \ln(\frac{d}{c}\, \frac{\sqrt{1+a^2}+1}{\sqrt{1+a^2}-1})\} \tag{A122}$$

In the limit $\gamma \to 1-$ this becomes

$$\frac{Q_{c,d,L}}{2} = 2\, R\, \{\frac{1}{2}\sqrt{L/R} - \frac{1}{2}\ln(\frac{d}{c})\} \tag{A123}$$

which differs by a factor $1/2$ from the result (A109), i.e., the integral and the limit $\gamma \to 1-$ do not commute.

Yet, we find for all values of γ that

$$\frac{Q_{c,d,L}}{4R} = g(\gamma, L/R) - \frac{1}{2}\ln(d/c) \tag{A124}$$

where $g(\gamma, L/R) = Q_{c,d,}/(4R) + \frac{1}{2}\ln(d/c)$ is given explicitly in (A109) and (A122) for $\gamma^2 = 1, \gamma^2 < 1$, respectively, and diverges as $\sqrt{L/R}$ as $L \to \infty$. The fact that (A109) is not the limit of (A122) as $\gamma \to 1-$ suggests to consider two different strategies:

Strategy 1:

We consider the exact GPG $\gamma^2 \equiv 1$, i.e., γ is not a dynamical variable. Then, we pick the following limit $c, d, L^{-1} \to 0$ in (A109)

$$\ln(\frac{d}{c}) = 2\sqrt{L/R} + \frac{Q}{2R}, \quad c = e^{-L/R} \tag{A125}$$

Then, the large L behavior of d is $d \propto e^{2\sqrt{L/R}-L/R}$, thus both c, d decay exponentially in L/R. Thus, the value of Q comes about simply because of the ambiguity in the *principal value regularization* of the integral defining it. However, Q is not a parameter on which the spatial metric depends, it is the variable conjugate to M but its existence has no further consequences for the theory. The advantage of this strategy is that it yields a consistent picture, i.e., the integral defining Q is actually able to produce that value while the exact GPG is imposed, without introducing additional observable consequences. Furthermore, it agrees with the Kantowski–Sachs picture that we review in the next subsection which also yields two Dirac observables one of which is M and the other one is related to a time rescaling freedom κ which in the GPG also arises, however, not as a Dirac observable but rather as a residual gauge freedom in choosing the physical Hamiltonian, see Appendices A and B.
Strategy 2:

We consider $0 < \gamma^2 < 1$ as a dynamic variable. Then, we pick the following limit $c, d, L^{-1} \to 0$ in (A122)

$$\frac{1}{2}\ln(\frac{d}{c}) = g(\gamma, L/R) - \frac{\zeta}{2}\,\mathsf{arth}(\gamma), \; c = e^{-L/R} \tag{A126}$$

for $\zeta > 0$ some numerical constant. Then, the large L behavior of d is $d \propto e^{\sqrt{L/R}-L/R}$ and thus both c, d decay exponentially in L/R. The limit $L \to \infty$ then yields

$$\frac{Q}{R} = \zeta\mathsf{arth}(\mathsf{fl}) \tag{A127}$$

Now the physical Hamiltonian of spherically symmetric vacuum gravity is just $R = 2M$ up to a constant which yields the equations of motion $M =$ const. and $\dot{Q} =$ const. Thus, Q diverges linearly in τ. Thus, $\gamma = \mathsf{th}(Q/(\zeta R))$ approaches exponentially fast (the faster the smaller ζ) the value ± 1 from below/above. Thus, $e^2 = 1/\gamma^2$ approaches the value $e^2 = 1$ exponentially fast from above, i.e., the *generalized* GP coordinates become *dynamically* exponentially fast the *exact* GP coordinates.

This conclusion is of course dependent on the choice of the finite part in the regularization (A125) which is a regularization ambiguity. It is motivated by the desire to reconcile the fact that in the Lagrangian picture, the parameter e is a choice of gauge that can be removed by a temporal diffeomorphism while in the Hamiltonian picture it is a function of the Dirac observables M, Q and thus cannot be gauged away. Thus, the only way to bring both pictures into agreement with Birkhoff's theorem that there is only one physical degree of freedom in the Lagrangian picture is to ensure that in the Hamiltonian picture the additional degree of freedom *dynamically* settles to the value it can be assigned to in the Lagrangian picture. This can be viewed as a temporal diffeomorphism as well but that diffeomorphism in the Hamiltonian picture is a symmetry transformation. This requirement still does not fix the finite part of $f(\gamma)$ (A125) uniquely, any bijection $f : (-1, 1) \to \mathbb{R};\ \gamma \mapsto f(\gamma)$ with the property that $\lim_{\gamma \to \pm 1\mp} = \pm\infty$ will do such as $f(\gamma) = \frac{1+\gamma}{1-\gamma}$. However, the faster $\gamma^2 \to 1$ dynamically, the faster the black hole becomes truly static observationally no matter which picture is used.

Note, that these conclusions hold only in the strictly spherical symmetric vacuum case. With the presence of gravitational perturbations and matter, the physical Hamiltonian will be of the form $H = M + H_1(M, Q)$ where H_1 contains the information about perturbations and matter and which will depend on both M, Q when expanding the background metric parametrized by M, e and thus M, Q. This means that M is no longer a constant of motion and that Q is not necessarily diverging which means that γ^2 does not necessarily become unity as time progresses. In this case, we must use the SAPT framework [71,72] to capture the corresponding quantum backreaction.

We will not follow the second strategy in the present paper because it also requires revisiting the decay behavior of the fields and the whole boundary structure analysis that leads to the reduced Hamiltonian as developed in Section 4 and which may lead to some restriction on the freedom to choose $f(\gamma)$. However, the advantage of the second strategy is that it offers the possibility to change the integration constant M dynamically, a possibility that one may want to keep in mind for future investigations.

Appendix D. Kantowski–Sachs Spacetimes

The purpose of this section is to provide the link with the substantial amount of work [23–32] that has been devoted to the interior of quantum black holes. In particular, we show that there is no contradiction between the presence of two independent and canonically conjugate Dirac observables on which the metric depends non-trivially and Birkhoff's theorem: While the reduced or physical phase space is manifestly two-dimensional, one of the degrees of freedom corresponds to a time rescaling of the spacetime coordinates which is considered a gauge transformation in the Lagrangian formulation but certainly not in the Hamiltonian formulation (by definition a Dirac observable is gauge-invariant). This is a general phenomenon for cosmological models as has been pointed out in [76].

Kantowski–Sachs (KS) spacetimes are homogeneous and spherically symmetric rather than isotropic spacetimes described by the line element

$$ds^2 = -D(T)^2\, dT^2 \; + A(T)^2\, dX^2 \; + B(T)^2\, d\Omega^2 \tag{A128}$$

where $d\Omega^2$ is the standard line element of the round sphere metric Ω_{EF} while $X \in [-K/2, K/2]$ is a KS "radial" coordinate with spatial cut-off $K \in \mathbb{R}_+$ and A, B, D are functions of KS time $T \in \mathbb{R}$ only. We consider all coordinates T, X, θ, φ dimension-free while D, A, B have dimension of length. Alternatively, we may want to introduce dimensionful coordinates $\hat{T} = L\, T,\ \hat{X} = LX$ where L is some unit of length and $\hat{A} = \frac{A}{L},\ \hat{B} = \frac{B}{L},\ \hat{D} = \frac{D}{L}$ become dimensionless.

To obtain the Hamiltonian description of these models, we identify the ADM variables

$$N = D,\ N^a = 0,\ q_{ab} = A^2\, \delta^X_a\, \delta^X_b + B^2\, \delta^E_a\, \delta^F_b \Omega_{EF},\ =: q_X\, \delta^X_a\, \delta^X_b + q_S\, \delta^E_a\, \delta^F_b \Omega_{EF}, \tag{A129}$$

and

$$k_{ab} = \frac{1}{2N}[\dot{q}_{ab} - (\mathcal{L}_{\vec{N}} q)_{ab}] = \frac{1}{D}[A\dot{A}\delta^X_a\, \delta^X_b + B\, \dot{B}\delta^E_a\, \delta^F_b \Omega_{EF}] =: k_X\, \delta^X_a\, \delta^X_b + k_S\, \delta^E_a\, \delta^F_b \Omega_{EF}, \tag{A130}$$

whence

$$\begin{aligned} p^{ab} &= \sqrt{\det(q)}[q^{ac}\, q^{bd} - q^{ab}\, q^{cd}]\, k_{cd} \\ &= A\, B^2 \sqrt{\det(\Omega)}\, [\delta^a_X \delta^b_X\, (A^{-4} k_X - A^{-2}(A^{-2} k_X + 2\, B^{-2} k_S)) \\ &\quad + \delta^a_E \delta^b_F \Omega^{EF}\, (B^{-4} k_S - B^{-2}(A^{-2} k_X + 2\, B^{-2} k_S))] \\ &=: \sqrt{\det(\Omega)}\, (p^X\, \delta^a_X\, \delta^b_X + p^S\, \delta^a_E\, \delta^b_F \Omega^{EF}) \end{aligned} \tag{A131}$$

Here, $q_X, q_S, k_X, k_S, p^X, p^S$ do not depend on the spatial coordinates and k_X, k_S have the dimension of length so that p^X, p^S are dimension-free.

We rescale the Einstein-Hilbert action by $\frac{1}{K}$ and pull back the symplectic potential

$$\begin{aligned} G_N\, \Theta &= \frac{1}{K} \int d^3x\;\; p^{ab}\, [\delta q]_{ab} = \frac{1}{K} \int dX \int d\theta\, d\varphi\, \sqrt{\det(\Omega)}\, (2A\, p^X\, [\delta A] + 4B\;\; p^S\, [\delta B]) \\ &= 4\pi\, (2A\, p^X\, [\delta A] + 4B\, p^S\, [\delta B]) \end{aligned} \tag{A132}$$

where G_N is Newton's constant which has a dimension of length squared in units in which $\hbar = 1$. We define

$$p_A = 2\, A\, p^X,\ p_B = 4\, B\, p^S \tag{A133}$$

which have a dimension of length. Accordingly, we have the non-vanishing Poisson brackets

$$\{p_A, A\} = \{p_B, B\} = g_N, \quad g_N = \frac{G_N}{4\pi} \tag{A134}$$

Next, we compute the constraints

$$\begin{aligned} G_N\, C_a(N^a) &= -\frac{2}{K} \int d^3x\, N^a D_b p_a^b \equiv 0, \\ G_N\, C(N) &= \frac{1}{K} \int d^3x\, N\, [\det(q)]^{-1/2}(p^{ab}\, p_{ab} - [p_a^a]^2) - \det(q)]^{1/2} R(q)] \\ &= \frac{4\pi\, D}{A\, B^2}\, (\frac{1}{8}\, [A\, p_A]^2 - \frac{1}{4}\, [A\, p_A]\, [B\, p_B] - 2[A\, B]^2) \end{aligned} \tag{A135}$$

where the results of Section 2 were used, in particular, that $R[\Omega] = 2$. The appearance of (A134) suggests to transform from $A, B > 0$ to $x := \ln(A/L),\ y := \ln(B/L) \in \mathbb{R}$ and to introduce $p_x := L^{-2}\, Ap_A,\ p_y = L^{-2}\, B\, p_B$. Then with $\tilde{D} = \frac{D\, L^2}{A\, B^2}$

$$\{p_x, x\} = \{p_y, y\} = g = \frac{g_N}{L^2}, \quad C(N) = \frac{\tilde{D}}{g}\, (\frac{1}{8}\, p_x^2 - \frac{1}{4}\, p_x\, p_y - 2e^{2(x+y)}) =: \frac{\tilde{D}}{g}\, \tilde{C} \tag{A136}$$

We can now develop three equivalent descriptions of the system:

1. The reduced phase space description in terms of a physical Hamiltonian and true degrees of freedom.
2. The description in terms of non-relational Dirac observables.
3. The description in terms of relational Dirac observables.

Appendix D.1. Reduced Phase Space Description

Since $\tilde{C}$ is linear in momentum p_y we choose y as a clock and rewrite the constraint as

$$\tilde{D}\, \tilde{C} = \hat{D}\, \hat{C}, \quad \hat{D} = -\frac{\tilde{D} p_x}{4}, \quad \hat{C} = p_y + h, \quad h = 8\, \frac{e^{2(x+y)}}{p_x} - \frac{p_x}{2} \tag{A137}$$

We impose the explicitly time-dependent gauge fixing condition

$$\hat{G}_T := y - T \tag{A138}$$

It is preserved in time on the constraint surface $\hat{C} = 0$ if (note the distinction between the total and explicit time derivative)

$$\frac{d}{dT}\hat{G}_T = \{\hat{D}\hat{C}/g, \hat{G}_T\} + \frac{\partial}{\partial T}\hat{G}_T = \hat{D} - 1 = 0 \tag{A139}$$

which fixes $\hat{D}_* = 1$. Thus, the gauge degrees of freedom are y, p_y while the true degrees of freedom are x, p_x. The reduced Hamiltonian is defined for functions F depending only on x, p_x by

$$\{H, F\} := \{\hat{D}\hat{C}/g, F\}_{\hat{D}=\hat{D}_*, y=T, p_y=-h} = \hat{D}_*/g\{h, F\}_{y=T} = \{h_{y=T}, F\} \tag{A140}$$

hence

$$H = H_T = \frac{1}{g}\, (8\, \frac{e^{2(x+T)}}{p_x} - \frac{p_x}{2}) \tag{A141}$$

which is explicitly time-dependent.

We now solve the resulting equations of motion

$$\dot{x}(T) = \{H_T(x, p_x), x\}_{x=x(T), p_x=p_x(T)}, \quad \dot{p}_x(T) = \{H_T(x, p_x), p_x\}_{x=x(T), p_x=p_x(T)} \tag{A142}$$

We note that
$$\frac{d}{dT}H_T = \frac{\partial}{\partial T}H_T = g^{-1}\ 16\ e^{2(x+T)}\ p_x^{-1} \tag{A143}$$
while
$$\frac{d}{dT}p_x = -16\ e^{2(x+T)}\ p_x^{-1} \tag{A144}$$
Hence,
$$E_T(x,p_x) := H_T(x,p_x) + g^{-1}p_x = \frac{1}{g}\ (8\ \frac{e^{2(x+T)}}{p_x} + \frac{p_x}{2}) \tag{A145}$$
is a constant of motion $E_T = \epsilon$ on the trajectories. As a function of the reduced phase space it is explicitly time dependent. Next, by combining (A144) and (A145) we have
$$\dot{p}_x = -2\ g\ E_T + p_x \tag{A146}$$
which is solved by
$$p_x(T) = \kappa\ e^T + 2\ g\ E_T \tag{A147}$$
where κ is an integration constant. It follows
$$16\ e^{2(x+T)} = p_x(2\ \ E_T - p_x) = -c\ e^T\ (2\ E_T + c\ e^T)\ \ \Rightarrow\ \ e^{2\ x(T)} = -\frac{\kappa}{16}\ (\kappa + 2\ g\ E_T\ e^{-T}) \tag{A148}$$
which provides the general and explicit solution. Since (A148) is positive, for a solution parametrized by ϵ, κ, we must necessarily have $\epsilon\kappa < 0$ and the range of T becomes confined to the set
$$2\ g\ \frac{|\epsilon|}{|\kappa|}\ e^{-T} > 1 \tag{A149}$$
We may also combine (A147) and (A148) into the statement that
$$c_T(x,p_x) := -16\ \frac{e^{2x+T}}{p_x} \tag{A150}$$
is an explicitly time-dependent function on the phase space which is a constant $c_T = \kappa$ on a trajectory.

In terms of E_T, c_T the description of this dynamical system is, therefore, especially convenient. The reduced Hamiltonian and true degrees of freedom are given by
$$H_T = -\frac{1}{g}\ (g\ E_T + c_T\ e^T),\ \ p_x = c_T\ e^T + 2\ g\ E_T,\ e^{2x} = -\frac{c_T}{16}\ (c_T + 2\ g\ E_T\ e^{-T}) \tag{A151}$$
where we denoted objects with explicit time dependence with subscript T. The inversion (A151) is given by (A145) and (A150) which yields
$$\{E_T, c_T\}(x,p_x) = \frac{1}{g}\ \{8\ \frac{e^{2(x+T)}}{p_x} + \frac{p_x}{2}, (-16)\ \frac{e^{2x+T}}{p_x}\} = \{\frac{p_x}{2\ g}, (-16)\ \frac{e^{2x+T}}{p_x}\} = (-16)\ \frac{e^{2x+T}}{p_x} = c_T \tag{A152}$$
To interpret E_T, c_T geometrically, we express D, A, B in terms of them. We have
$$\begin{aligned}
[\frac{B}{L}]^2 &= e^{2y} = e^{2T} \\
[\frac{A}{L}]^2 &= e^{2x} = -\frac{c_T^2}{16}\ (1 + 2\ g\ \frac{E_T}{c_T}\ e^{-T}) \\
D &= \frac{A\ B^2\ \tilde{D}}{L^2} = -4\ \frac{A\ B^2\ \hat{D}_*}{L^2\ p_x} = -4\ \frac{A\ B^2}{L^2\ (c_T\ e^T + 2\ g\ E_T)} \\
D^2 &= 16\ L^2\ e^{4T}\ (-\frac{c_T^2}{16}\ (1 + 2\ g\ \frac{E_T}{c_T}\ e^{-T})\frac{1}{(c_T\ e^T + 2\ g\ E_T)^2} \\
&= -L^2\ e^{2T}\ \frac{1}{1 + 2\ g\frac{E_T}{c_T}e^{-T}}
\end{aligned} \tag{A153}$$

This suggests to introduce the new coordinates and functions

$$r := L\, e^T,\ t := L\, X,\ M_T := -L^{-1}\, \frac{E_T}{c_T} \tag{A154}$$

In terms of these, the line element takes the form ($g_N = L^2 g$)

$$ds^2 = -\frac{1}{\frac{2\, g_N\, M_T}{r} - 1}\, dr^2 + [\frac{c_T}{4}]^2\, (\frac{2\, g_N\, M_T}{r} - 1)\, dt^2 + r^2\, d\Omega^2 \tag{A155}$$

This is precisely the interior Schwarzschild solution with the roles of r, t of being spatial and temporal coordinates switched since in the range (A149), i.e., $r < 2g_N M_T$ the coefficients of dr^2 and dt^2 are negative and positive, respectively. The metric depends on the explicitly time T dependent functions of the reduced phase space given by M_T, c_T which are conjugated up to a factor of L^{-1}

$$\{M_T, c_T\} = L^{-1} \tag{A156}$$

as follows from (A151). Clearly, M_T which is a positive constant on solutions is nothing but the mass of the black hole while c_T which is a dimensionless constant on solutions is nothing but a rescaling freedom of t.

The interesting point is that although 1. the reduced Hamiltonian H_T, 2. the mass M_T and 3. the rescaling freedom c_T are explicitly time T dependent and although M_T, c_T are canonically conjugate coordinates of the *2-dimensional* reduced phase space, nevertheless, solutions M_T, c_T are in fact time T independent.

Appendix D.2. Non-Relational Dirac Observables

We consider the full phase space with conjugate pairs $(x, p_x), (y, p_y)$ and the constraint in the form $\hat{C} = p_y + h(x, p_x, p_y)$. We note that x, y appear only in the combination $x + y$ in h. Thus, $x - y$ is cyclic, and therefore, $p_x - p_y$ is gauge invariant, i.e., a Dirac observable. Since $\hat{C}$ is trivially a Dirac observable also

$$E(x, p_x, y) := g^{-1}(p_x - p_y) + \hat{C} = g^{-1}[8\frac{e^{2(x+y)}}{p_x} + \frac{p_x}{2}] \tag{A157}$$

is a Dirac observable. In the gauge $y = T$ it coincides with $E_T(x, p_x)$. Correspondingly, we conjecture that

$$c(x, p_x, y) := -16\, \frac{e^{2x+y}}{p_x} \tag{A158}$$

is a second independent Dirac observable because in the gauge $y = T$ it coincides with $c_T(x, p_x)$. This is readily confirmed

$$\{\hat{C}, c\} = -16\, g^{-1}\{8\, \frac{e^{2(x+y)}}{p_x} + p_y - \frac{p_x}{2}, \frac{e^{2x+y}}{p_x}\} = -\frac{16}{p_x\, g}\, \{p_y - \frac{p_x}{2}, e^{2x+y}\} = 0 \tag{A159}$$

This provides an independent interpretation of the true degrees of freedom M_T, c_T of the previous subsection: They correspond to the Dirac observables $M := L^{-1}E/c, c$ evaluated on the gauge cut $y = T$. In particular, they are canonically conjugate

$$\{M, c\} = L^{-1} \tag{A160}$$

Being Dirac observables, they have trivial "evolution" with respect to $\hat{C}$ by construction. This is equivalent to the statement that E_T, c_T are constants of motion with respect to the reduced Hamiltonian because

$$\frac{d}{dT}E_T = \frac{\partial}{\partial T}E_T + \{H_T, E_T\} = \{\hat{C}, E\}_{y=T} \tag{A161}$$

and similar for c.

Appendix D.3. Relational Dirac Observables

The relational Dirac observables corresponding to a function F of the true degrees of freedom x, p_x are given by the explicit formula

$$O_F(T) := \sum_{n=0}^{\infty} \frac{(T-y)^n}{n!} \{\hat{C}, F\}_{(n)} \tag{A162}$$

where $\{\hat{C}, F\}_{(0)} = F,\ \{\hat{C}, F\}_{(n+1)} = \{\hat{C}, \{\hat{C}, F\}\}$ is the iterated Poisson bracket. The direct evaluation of the infinite series is quite non-trivial.

However, we may avoid the direct evaluation whenever we have a complete set of Dirac observables at our disposal as follows: Suppose that (x, p_x) are the true degrees of freedom, (y, p_y) the gauge degrees of freedom, the constraints are given in the form $\hat{C} = p_y + h(x, p_x, y)$, the gauge fixing condition is given in the form $G = y - k(T)$ with T dependent constants $k(T)$ and D a complete set of Dirac observables, i.e., their Hamiltonian vector fields are linearly independent on the constraint surface $\hat{C} = 0$. Now, for any function $F = F(x, p_x, y, p_y)$ in the full phase space we have the identity (see [50] and references therein)

$$O_F(T) := [e^{\{s \cdot \hat{C}, .\}} \cdot F]_{s=k(T)-y} = F(O_x(T), O_{p_x}(T), T, -h(O_x(T), O_{p_x}(T), T)) \tag{A163}$$

Applied to the system of Dirac observables $O_D(T) = D$ we thus find the relations

$$D(x, p_x, y, -h(x, p_x, y)) = D(O_x(T), O_{p_x}(T), T, -h(O_x(T), O_{p_x}(T), T)) \tag{A164}$$

which can be solved algebraically for $(O_x(T), O_{p_x}(T))$.

Applied to our system and using the Dirac observables of the previous section we find with $Q := O_x(T),\ P := O_{p_x}(T)$

$$\begin{aligned} E(x, p_x, y) &= \frac{1}{g}(8\frac{e^{2(x+y)}}{p_x} + \frac{p_x}{2} = \frac{1}{g}(8\frac{e^{2(Q+T)}}{P} + \frac{P}{2}) \\ c(x, p_x, y) &= -16\frac{e^{2x+y}}{p_x} = -16\frac{e^{2Q+T}}{P} \end{aligned} \tag{A165}$$

which can be solved for

$$\begin{aligned} P &= p_x + 16\,\frac{e^{2(x+y)}}{p_x}(1 - e^{T-y}) \\ e^{2Q} &= e^{2x}\, e^{-(T-y)}(1 + 16\frac{e^{2(x+y)}}{p_x^2}(1 - e^{T-y})) \end{aligned} \tag{A166}$$

This maybe Taylor expanded in powers of $y - T$ thus providing explicit formulae for the iterated Poisson brackets. In particular, the zeroth order gives $Q = x, P = p_x$ as it should be.

The physical Hamiltonian, i.e., the Dirac observable, that drives the evolution of the relational observables is given by [50]

$$H(x, p_x, y) = O_h(T) = h(x = O_x(T), p_x = O_{p_x}(T), y = T) \tag{A167}$$

and coincides with $H_T(x, p_x)$ at the gauge cut $y = T$.

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