Emergent modified gravity coupled to scalar matter

Martin Bojowald[*] and Erick I. Duque[†]

Institute for Gravitation and the Cosmos, The Pennsylvania State University, 104 Davey Lab, University Park, Pennsylvania 16802, USA

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Emergent modified gravity presents a new set of generally covariant gravitational theories in which the space-time metric is not directly given by one of the fundamental fields. A metric compatible with the modified dynamics of gravity is instead derived from covariance conditions for space-time in canonical form. By staying within the canonical setting throughout all the required steps, several assumptions about space-time made implicitly in modified action principles can be relaxed. This paper presents a significant extension of existing vacuum models to the case of a scalar field coupled to emergent modified gravity in a spherically symmetric setting. Unlike in previous attempts for instance in models of loop quantum gravity, it is possible to maintain general covariance in the presence of modified gravity-scalar couplings. In general, however, the emergent space-time metric depends not only on the phase-space degrees of freedom of the gravitational part of the coupled theory, but also on the scalar field. Matter therefore directly and profoundly affects the geometry of space-time, not only through the well-known dynamical coupling of stress-energy to curvature as in Einstein's equation, but even on a kinematical level before equations of motion are imposed. In addition to the covariance condition, this paper introduces further physical requirements that may be imposed in order to reduce modified gravity-scalar theories to more specific classes. In some cases, coupling emergent modified gravity to a scalar field eliminates some of the modifications that would be possible in a vacuum situation. Moreover, certain results about the removal of classical black hole singularities in vacuum emergent modified gravity are found to be unstable under the inclusion of matter fields. However, alternative modifications exist in which singularities are removed even in the presence of matter. Emergent modified gravity is seen to provide a large class of new scalar-tensor theories with second-order field equations.

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I. INTRODUCTION

The search for modified theories of gravity is motivated by both observational considerations as well as deep theoretical developments. Examples of the former are the desire to compare the increasing number of strong-field measurements with a sufficiently large class of consistent parametrized theoretical descriptions of black holes, or to explain puzzling cosmological features such as dark matter and dark energy. The latter are relevant in particular in the context of quantum gravity, or in the quest to find singularity-free models of black holes and the big bang. General covariance is a crucial property that makes it possible to introduce a space-time description for these phenomena and define the horizon of a black hole or the expanding geometry of the Universe. However, general covariance applied to an action principle for the gravitational field appears to be a strong and very restrictive consistency condition that does not seem to allow sufficiently many interesting and viable alternatives to general relativity [1–4].

Emergent modified gravity [5,6] presents a new version that can include modifications of general relativity even without going beyond second derivative order and without including extra fields, so far at least in a spherically symmetric setting. These theories can therefore be understood as new classical theories of gravity with gravitational and matter couplings that differ from general relativity. It is of interest to analyze them in their own right, but they may also be used as alternative starting points of quantization (quantum emergent modified gravity). If modifications of higher order in curvature are included, emergent modified gravity provides a broad effective framework for possible semiclassical regimes of various approaches to quantum gravity that is more general than standard higher-curvature effective actions. For instance, some of the higher-order modifications of emergent modified gravity can be interpreted as possible effects from loop quantum gravity, but with a full implementation of general covariance that restricts choices that have traditionally been made in this setting. In these examples, nonsingular models of static

[*]bojowald@psu.edu
[†]eqd5272@psu.edu

black holes can be found [7,8], demonstrating new features compared with general relativity.

The key observation of emergent modified gravity is that the metric used to describe space-time geometrically need not be one of the fundamental fields, which allows us to weaken some of the usual assumptions that lead for instance to higher-curvature effective actions as the main source of generally covariant modifications of vacuum general relativity. Moreover, emergent modified gravity works on a canonical level and therefore does not require assumptions about space-time integrations and 4-volume measures. In particular, while it is possible to define a corresponding Lagrangian via a Legendre transformation of the modified Hamiltonian, the former does not provide a mechanism to derive the emergent metric, which is obtained from the Poisson brackets of the canonical constraints. There is therefore no self-contained Lagrangian approach or action principle for emergent modified gravity, making it possible to find previously unrecognized gravitational theories. In this way, emergent modified gravity provides a new source of modified gravity for phenomenological studies, and it helps to analyze questions such as whether proposed quantum effects, for instance in models of loop quantum gravity [9], have a chance of being consistent with space-time covariance. Emergent modified gravity is well suited to the latter applications because it is inherently canonical, and it is able to test the covariance for instance of holonomy modifications suggested by the eponymous loop integrations in loop quantum gravity [10].

While consistency conditions for a space-time formulation within canonical quantum gravity, such as having first-class constraints that may generate hypersurface deformations, have been imposed to varying degrees in vacuum spherically symmetric models, attempts to include scalar matter [11] (or, more generally, local physical degrees of freedom [12]) had for some time led only to no-go results. This outcome presents a major challenge to models of canonical or loop-quantum gravity, not only conceptually because including matter with local degrees of freedom is important to test whether proposed modifications have a chance of being sufficiently general for physical applications, but also for important practical questions of how to study matter collapse or Hawking radiation in the presence of such modifications. For instance, if quantum effects may avoid the classical black hole singularity only in vacuum models, they would be of little use when it comes to the physical question of stellar collapse. Recently, the constructions in [13,14] showed that the first-class nature of spherically symmetric constraints can be maintained in the presence of matter if a specific coupling term to spatial derivatives of the gravitational momenta is included. Such terms are not directly suggested by loop-quantum gravity and therefore had been omitted in earlier attempts.

The canonical analysis underlying emergent modified gravity includes the conditions that the gravitational constraints remain first class, but [5], building on [15], has also shown that this property is not sufficient for the theory to be consistent with a geometrical space-time interpretation of its solutions. First-class modifications of the constraints in general imply modifications not only of the constraint functionals themselves but also of the structure function in their Poisson brackets. Classically, and in all standard higher-curvature effective actions, this structure function equals the inverse spatial part of a space-time metric compatible with its solutions, reflecting a general geometrical property of deformations of embedded hypersurfaces. If the structure function is modified, the compatible space-time geometry in which hypersurfaces can be embedded must therefore be adapted to the new theory; it must be derived from the modified constraints through the structure function. Classically, the structure function is closely related to the configuration variables among the gravitational phase-space degrees of freedom, given by metric or triad components, but this need not be the case in a modified theory in which the structure function could also depend on the gravitational momenta. Even if the modified constraints are first class, it is not guaranteed that the modified structure function can be part of a consistent space-time metric. There are therefore first-class modifications of the classical gravitational constraints that are not compatible with a covariant space-time interpretation.

Imposing the condition that modified canonical solutions can be used to describe space-time geometrically therefore goes beyond the algebraic condition that the constraints remain first class. In spherically symmetric models, including scalar matter, the first-class property has been analyzed in [13,14], but the condition that the structure function be compatible with a space-time interpretation remains to be analyzed. The recent [6] proposed a minimal coupling for scalar matter to modified gravity in canonical form, but it is not sufficiently general to encompass all possibilities of modified structure functions of interest in emergent modified gravity. Moreover, the possibility of minimal coupling for momentum-dependent structure functions is nontrivial and requires a proof of existence, which we provide in this paper as a corollary of our general theory.

We present the required analysis for covariant scalar-field couplings in spherically symmetric emergent modified gravity in the main part of this paper, with several surprising outcomes. In particular, even in the presence of matter with local degrees of freedom it is still possible to find new versions of emergent modified gravity that are not of higher-curvature form. The emergent space-time geometry is determined by a line element whose components, expressed as functions of the original phase-space degrees of freedom, depend on the gravitational as well as matter fields. It is therefore impossible to separate the geometrical roles of gravitational and matter degrees of freedom on phase space, as initially defined by their appearance in different contributions to the constraints. Instead, for a given theory of modified gravity, the covariance condition predicts a unique combination of these fields that can serve as the spatial part of a space-time line element.

In Sec. II, we review the vacuum covariance conditions for a consistent space-time geometry in emergent modified gravity, following [5], and formulate a new covariance condition for the scalar field. The same section contains our proof that minimal coupling of a scalar field is consistent in emergent modified gravity. We formulate and discuss several additional requirements of physical interest in Sec. III. These covariance and other conditions, specialized to spherical symmetry, are evaluated in various combinations in Sec. IV. In order to manage the large space of possible theories, we will take a viewpoint of effective field theory in which generic constraints are formulated by including terms up to a certain order in spatial derivatives, and then subjected to several consistency conditions. Section V contains the derivation of three classes of modified theories with different physically desirable properties, and Sec. VI discusses some of their equations of motion and some solutions with the additional assumption of spatial homogeneity, drawing conclusions about the potential to resolve classical singularities. After giving an outlook on new possibilities for the phenomenology of scalar-tensor theories in Sec. VII, our main results, several characteristic properties, and possible future applications are discussed in Sec. VIII.

II. COVARIANCE IN CANONICAL GRAVITY

New theories of canonical gravity can be formulated by modifying the classical Hamiltonian constraint H, derived from general relativity, to a new Hamiltonian constraint $\tilde{H}$ such that the classical expression is obtained in a specific limit of suitable parameters. One could also try to modify the diffoemorphism constraint $\vec{H}$, but this is not necessary if one is interested in new space-time structures that retain the well-understood classical structure of space on spacelike hypersurfaces. A canonical formulation also requires a phase space, providing the variables on which the constraints depend. In a minimal modification, one may assume that the phase space remains unchanged, with configuration variables q_{ab} with momenta p^{ab} for gravity that, in the classical limit, equal the spatial metric and a q_{qb}-dependent linear combination of extrinsic-curvature components. We will maintain this assumption and use it to identify q_{ab} and p^{ab} as the gravitational variables distinct from matter degrees of freedom. Therefore, we will not allow for higher-derivative theories that would require an extended phase space in canonical form. However, unlike other approaches to modified gravity (where such a condition may appear only implicitly if they are not formulated canonically), in emergent modified gravity we impose the relationship between the gravitational phase-space variables and the spatial metric and extrinsic curvature of spacelike hypersurfaces only in the classical limit. In a modified theory of this form, there is therefore no *a priori* relationship between q_{ab} and a spatial metric and between momenta p^{ab} and extrinsic curvature. Such relationships and geometrical interpretations rather have to be derived (and therefore emerge) from covariance conditions imposed on the modified constraints.

A. General theory

A modified Hamiltonian constraint in general has a nonclassical Poisson bracket with the diffeomorphism constraint, such that covariance will be completely removed if the modification is not chosen with sufficient care. It is therefore necessary to restrict modified constraints to a form that preserves the classical brackets as much as possible, implementing the classical gauge symmetry of hypersurface deformations. The constraints must remain first class in order to ensure that the number of independent gauge transformations is not reduced and still equals the required number of independent infinitesimal space-time diffeomorphisms. Moreover, the brackets should resemble the classical brackets of hypersurface deformations in order for a space-time interpretation to remain possible. These condition lead to the requirement that the modified Hamiltonian constraint $\tilde{H}$ together with the classical diffeomoprhism constraint $\vec{H}$ obey

$$\{\vec{H}[\vec{N}],\vec{H}[\vec{M}]\} = \vec{H}[\mathcal{L}_{\vec{N}}\vec{M}], \tag{1a}$$

$$\{\tilde{H}[N],\vec{H}[\vec{N}]\} = -\tilde{H}[N^b\partial_b N], \tag{1b}$$

$$\{\tilde{H}[N],\tilde{H}[M]\} = -\vec{H}[\tilde{q}^{ab}(N\partial_b M - M\partial_b N)], \tag{1c}$$

with a structure function $\tilde{q}^{ab}$ that approaches the inverse q^{ab} of the configuration variables q_{ab} in the classical limit, but not necessarily for all parameter choices in the modified Hamiltonian constraint. If the first-class condition is satisfied and the general structure of the hypersurface deformation brackets is maintained, the new structure function $\tilde{q}^{ab}$ is uniquely determined by the modified $\tilde{H}$.

The constraints generate gauge transformations of the phase-space variables in the usual way, given by Poisson brackets $\delta_\epsilon f(q_{ab},p^{ab}) = \{f, H[\epsilon^0]+\vec{H}[\vec{\epsilon}]\}$. Since evolution is a gauge transformation in a generally covariant theory, evolution is generated by the same constraints, but with specific gauge functions N and $\vec{N}$ for a given choice of a time-evolution vector field; $\dot{f} = \{f, H[N]+\vec{H}[\vec{N}]\}$ for a phase-space function f. Standard results in canonical gravity [16,17] show that the evolutionary gauge functions N and $\vec{N}$ in $\tilde{H}[N]$ and $\vec{H}[\vec{N}]$, respectively, are subject to gauge transformations that follow from the requirement that Hamiltonian evolution generated by $\tilde{H}[N]+\vec{H}[\vec{N}]$

must be compatible with gauge transformations generated by the same functionals $\tilde{H}$ and $\vec{H}$ but with different gauge functions, $\tilde{H}[\epsilon^0] + \vec{H}[\vec{\epsilon}]$. The evolution and gauge generators are the same because the theory is completely constrained, but in a space-time interpretation (if it exists), the multipliers N and $\vec{N}$ for evolution play a different role than the gauge functions ϵ^0 and $\vec{\epsilon}$: The former appear as time components of the space-time line element compatible with the constraints, identified as the lapse function and the shift vector, while the latter parametrize generic gauge changes or transformation between different slicings in the resulting space-time. The compatibility condition that the evolution of a gauge-transformed configuration be the gauge-transformation of the evolved original configuration then implies that the lapse function and shift vector transform as

$$\delta_\epsilon N = \dot{\epsilon}^0 + \epsilon^a \partial_a N - N^a \partial_a \epsilon^0, \tag{2a}$$

$$\delta_\epsilon N^a = \dot{\epsilon}^a + \epsilon^b \partial_b N^a - N^b \partial_b \epsilon^a + \tilde{q}^{ab}(\epsilon^0 \partial_b N - N \partial_b \epsilon^0). \tag{2b}$$

Since the condition involves the commutator of gauge and evolution equations, it is sensitive to the structure function $\tilde{q}^{ab}$ in the constraint brackets, which implies the only modification in these equations.

The geometrical structure of hypersurface deformations, algebraically expressed by constraint brackets of a specific form, suggests that the modified theory is compatible with a space-time interpretation of its solutions given in terms of the emergent line element,

$$\mathrm{d}s^2 = -N^2 \mathrm{d}t^2 + \tilde{q}_{ab}(\mathrm{d}x^a + N^a \mathrm{d}t)(\mathrm{d}x^b + N^b \mathrm{d}t), \tag{3}$$

where the inverse $\tilde{q}_{ab}$ of the modified structure function appears as the spatial metric. [If the modified structure function is not invertible, the emergent line element may have to be split into separate expressions with varying signatures depending on the sign of $\det(\tilde{q}^{ab})$, see [5].] However, gauge transformations generated by the modified constraints, applied to $\tilde{q}_{ab}$, N, and N^z, are not guaranteed to be compatible with coordinate transformations applied to $\mathrm{d}t$ and $\mathrm{d}x^a$. If this is not the case, expression (3) is not invariant and therefore meaningless as a line element or distance measure. The condition that the emergent line element be invariant imposes additional conditions on the modified Hamiltonian constraint through conditions on the modified structure function implied by it.

We say that the modified canonical theory is generally covariant if the emergent space-time line element is coordinate invariant. Coordinate changes applied to $\mathrm{d}x^\mu$ must therefore be dual to canonical gauge transformations applied to the components of (3). The case of the time components with coefficients given by N and N^a has been considered in [15], but not the spatial part. As a complete equation, this condition implies that gauge transformations in the modified canonical theory have a strict correspondence with infinitesimal space-time diffeomorphisms or space-time Lie derivatives, at least on shell when the constraints and equations of motion are satisfied (indicated by a subscript O.S.),

$$\delta_\epsilon \tilde{g}_{\mu\nu}|_{\mathrm{O.S.}} = \mathcal{L}_\xi \tilde{g}_{\mu\nu}. \tag{4}$$

(There is an analogous relationship between gauge transformations and infinitesimal diffeomorphisms acting on extrinsic curvature of spacelike hypersurfaces in the emergent space-time, but, as shown in [5], it does not imply a new covariance condition in addition to the equation for $\tilde{q}_{ab}$.)

The canonical gauge transformations with gauge functions (ϵ^0, ϵ^a), taken on shell, then reproduce space-time diffeomorphisms with a space-time vector ξ related to the gauge functions by

$$\xi^\mu = \epsilon^0 n^\mu + \epsilon^a s^\mu_a = \xi^t t^\mu + \xi^a s^\mu_a, \tag{5a}$$

$$\xi^t = \frac{\epsilon^0}{N}, \qquad \xi^a = \epsilon^a - \frac{\epsilon^0}{N} N^a, \tag{5b}$$

because the former has components referring to the time direction in space-time, while the latter refer to the normal direction of embedded spacelike hypersurfaces. Following [15], the timelike components of the covariance condition are satisfied by virtue of the hypersurface-deformation brackets, (1), if we use (2) and assume that the spatial metric is covariant, $\delta_\epsilon q_{ab}|_{\mathrm{O.S.}} = \mathcal{L}_\xi q_{ab}$. This latter equation is not true for any first-class modification of the constraints, but only if [5]

$$\frac{\partial(\delta_{\epsilon^0} \tilde{q}^{ab})}{\partial(\partial_c \epsilon^0)}\bigg|_{\mathrm{O.S.}} = \frac{\partial(\delta_{\epsilon^0} \tilde{q}^{ab})}{\partial(\partial_c \partial_d \epsilon^0)}\bigg|_{\mathrm{O.S.}} = \cdots = 0, \tag{6}$$

where $\delta_{\epsilon^0} \tilde{q}^{ab} = \{\tilde{q}^{ab}, H[\epsilon^0]\}$ without a spatial shift.

B. Scalar fields

As a new result, we now extend the covariance condition to scalar fields. We begin with the case of a single-component scalar ϕ with momentum P_ϕ, introduced as an additional phase-space degree of freedom that couples to the gravitational degrees of freedom through a matter Hamiltonian added to $\tilde{H}$, and then consider additional structures available in the case of scalar multiplets.

1. Single scalar field

For a canonical theory with hypersurface-deformation brackets (1) for the combined constraints of gravitational and matter variables, $\tilde{H}_{\mathrm{grav}}[N] + \tilde{H}_{\mathrm{matter}}[N]$ and $\vec{H}_{\mathrm{grav}}[\vec{N}] + \vec{H}_{\mathrm{matter}}[\vec{N}]$, we say that a scalar field ϕ is covariant if

$$\delta_\epsilon\phi|_{\text{O.S.}} = \mathcal{L}_\xi\phi. \tag{7}$$

Just as the gravitational configuration variable q_{ab}, the canonical scalar field ϕ is initially defined only on a spatial slice. However, on shell we can use equations of motion to relate the momentum of ϕ to its time derivative, defined by $\dot\phi = \{\phi, \tilde H[N] + \vec H[\vec N]\}$. This time derivative, available on shell, can then be used in a comparison with the time component of the space-time Lie derivative.

Written in the basis adjusted to the foliation into spacelike hypersurfaces, the scalar covariance condition takes the form,

$$\delta_\epsilon\phi|_{\text{O.S.}} = \frac{\epsilon^0}{N}\dot\phi + \left(\epsilon^a - \frac{\epsilon^0}{N}\epsilon^a\right)\partial_a\phi. \tag{8}$$

Using of the canonical gauge transformation $\delta_\epsilon\phi = \{\phi, \tilde H[\epsilon^0] + H_a[\epsilon^a]\}$ on the left-hand side and Hamilton's equation of motion $\dot\phi = \{\phi, \tilde H[N] + H_a[N^a]\}$ on the right-hand side, the equation can be simplified to

$$\frac{1}{\epsilon^0}\{\phi, \tilde H[\epsilon^0]\}|_{\text{O.S.}} = \frac{1}{N}\{\phi, \tilde H[N]\} \tag{9}$$

using the assumption that the diffeomorphism constraint is unmodified, and the fact that a scalar field ϕ has spatial density weight zero.

The normal gauge transformation of the scalar field has the generic form $\{\phi, \tilde H[\epsilon^0]\} = \Phi\epsilon^0 + \Phi^c\partial_c\epsilon^0 + \Phi^{cd}\partial_c\partial_d\epsilon^0 + \cdots$, where the Φ tensors are phase-space functions. Substituting this expansion into the covariance condition, we obtain

$$\begin{aligned}\Phi^c\frac{\partial_c\epsilon^0}{\epsilon^0} + \Phi^{cd}\frac{\partial_c\partial_d\epsilon^0}{\epsilon^0} + \cdots|_{\text{O.S.}} \\ = \Phi^c\frac{\partial_c N}{N} + \Phi^{cd}\frac{\partial_c\partial_d N}{N} + \cdots|_{\text{O.S.}}\end{aligned} \tag{10}$$

for independent ϵ^0 and N. We can now use $\{\phi, H[\epsilon^0]\} = \delta\tilde H[\epsilon^0]/\delta P_\phi$ to write the Φ tensors in (10) as

$$\Phi^c = -\frac{\partial\tilde H}{\partial(\partial_c P_\phi)} + \partial_d\left(\frac{\partial\tilde H}{\partial(\partial_c\partial_d P_\phi)}\right) - \cdots, \tag{11a}$$

$$\Phi^{cd} = \frac{\partial\tilde H}{\partial(\partial_c\partial_d P_\phi)} - \partial_d\partial_e\left(\frac{\partial\tilde H}{\partial(\partial_c\partial_d\partial_e P_\phi)}\right) + \cdots, \tag{11b}$$

and so on. The space-time Lie derivative of a scalar field of density weight zero does not contain terms with spatial derivatives of the lapse function. Therefore, Φ^c, Φ^{cd} and so on must vanish on shell, such that

$$\frac{\partial\tilde H}{\partial(\partial_c P_\phi)} = \frac{\partial\tilde H}{\partial(\partial_c\partial_d P_\phi)} = \cdots = 0. \tag{12}$$

These equations, as derived, are required to hold on shell, but since partial derivatives of the Hamiltonian constraint by spatial derivatives of the momentum are neither constraints nor equations of motion, they must vanish identically. Therefore, no derivatives of the scalar momentum P_ϕ are allowed in a modified Hamiltonian constraint.

2. General scalar multiplets

It is straightforward to generalize the covariance condition from a single scalar field ϕ with momentum P_ϕ to a scalar multiplet ϕ^I with momenta P_J suitable for instance for the Higgs field. While we will consider only single-scalar models in our specific examples, there is an additional nontrivial property of multiplets given by global symmetries that can be used to formulate physical conditions on admissible modified theories. For purposes such as quantum field theory on a curved background, it is important to know the gauge current as a space-time vector, which is not directly related to general covariance but implies additional conditions from the Poisson brackets of the gauge generator with the hypersurface-deformation generators. There is a remnant of this important property in models with a single scalar field, which we will make use of in some of our explicit constructions.

Consider a scalar field multiplet ϕ^I with internal indices $I = 1, 2, \ldots, n$. The scalar field's indices denote its components as a vector in the representation $\mathcal{R}$ of some Lie group $\mathcal{G} = \text{SU}(N)$ of dimension n. Its Lie algebra $\mathfrak{g}$ then has $\dim(\mathfrak{g}) = N^2 - 1$ generators τ_i with $i = 1, \ldots, \dim(\mathfrak{g})$ satisfying the algebra $[\tau_i, \tau_j] = f_{ijk}\tau_k$, where $f_{ijk} = f_{[ijk]}$ are the structure constants. Given a Lie-algebra generator $\tau_i \in \mathfrak{g}$, the associated Lie-group element $g = \exp(\alpha^i\tau_i) \in \mathcal{G}$, $\alpha^i \in \mathbb{R}$ acts on the scalar field by

$$\phi^I \to (e^{\alpha^i\tau_i})^I{}_J\phi^J. \tag{13}$$

The classical Higgs-type action in curved space-time with metric $g_{\mu\nu}$ and its canonical decomposition are given by

$$\begin{aligned}S_{\text{scalar}}[\phi] &= -\int \mathrm{d}^4x\sqrt{-\det g}\left(\frac{1}{2}\delta_{IJ}g^{\mu\nu}(\nabla_\mu\phi^I)(\nabla_\nu\phi^J) + V(\delta_{IJ}\phi^I\phi^J)\right) \\ &= \int \mathrm{d}^4x\left[P_I\dot\phi^I - N^a(P_I\partial_a\phi^I) - N\left(\frac{1}{2}\frac{\delta^{IJ}P_IP_J}{\sqrt{\det q}} + \frac{1}{2}\delta_{IJ}\sqrt{\det q}\,q^{ab}(\partial_a\phi^I)(\partial_b\phi^J) + \sqrt{\det q}\,V(\delta_{IJ}\phi^I\phi^J)\right)\right],\end{aligned} \tag{14}$$

where $V(\delta_{IJ}\phi^I\phi^J)$ is the potential and the momenta are given by

$$P_I = \frac{\delta S_{\rm scalar}[\phi]}{\delta\dot{\phi}^I} = \delta_{IJ}\sqrt{\det q}\, n^\mu\partial_\mu\phi^J. \tag{15}$$

The scalar field therefore implies a contribution

$$\vec{H}_{\rm scalar}[\vec{N}] = \int d^3x N^a P_I \partial_a\phi^I \tag{16}$$

to the diffeomorphism constraint $\vec{H}[\vec{N}]$, and a contribution

$$H_{\rm scalar}[N] = \int d^3x N\left(\frac{1}{2}\frac{\delta^{IJ}P_IP_J}{\sqrt{\det q}} + \frac{1}{2}\delta_{IJ}\sqrt{\det q}\, q^{ab}(\partial_a\phi^I)(\partial_b\phi^J) + \sqrt{\det q}\, V(\delta_{IJ}\phi^I\phi^I)\right) \tag{17}$$

to the Hamiltonian constraint $H[N]$.

Elements of the Lie group and Lie algebra act on the momentum and field values as

$$\begin{aligned} P_I &\to P_J(e^{-\alpha^i\tau_i})^J{}_I \approx P_J(\delta^J{}_I - \alpha^i(\tau_i)^J{}_I), \\ \phi^I &\to (e^{\alpha^i\tau_i})^I{}_J\phi_J \approx (\delta^I{}_J + \alpha^i(\tau_i)^I{}_J)\phi^J, \\ \phi_I = \delta_{IJ}\phi^J &\to \phi_J(e^{-\alpha^i\tau_i})^J{}_I \approx \phi_J(\delta^J{}_I - \alpha^i(\tau_i)^J{}_I), \end{aligned} \tag{18}$$

where we used $\tau_i^{\rm T} = \tau_i^{-1} = -\tau_i$. Thus, the action (14) is invariant under transformations generated by the Lie group $\mathcal{G}$ and, thus, also under infinitesimal transformations generated by the Lie algebra $\mathfrak{g}$, leading to a Noether current. For later applications, we derive this conserved current from the Hamiltonian perspective with due attention to applications of nontrivial covariance conditions that are required for a meaningful space-time current.

In canonical terms, the transformation (18) is generated by the phase-space function,

$$G[\alpha] = \int d^3x\, \alpha^i P_I(\tau_i)^I{}_J\phi^J, \tag{19}$$

smeared with a $\mathfrak{g}$-valued constant α^i. Thus, $G[\alpha]$ generates a global symmetry, which could be generalized to a local one by the usual introduction of gauge fields but we leave this step for future treatments as it would complicate our analysis. The global symmetry generator commutes, up to possible boundary terms, with the Hamiltonian and diffeomorphism constraints,

$$\{H[N], G[\alpha]\} = \{\vec{H}[\vec{N}], G[\alpha]\} = 0, \tag{20}$$

and it reproduces brackets of the Lie algebra it is based on,

$$\{G[\alpha_1], G[\alpha_2]\} = \int d^3x\, \alpha_1^i\alpha_2^j f_{ijk}G_k = G[[\alpha_1,\alpha_2]] \tag{21}$$

with the Lie commutator $[\alpha_1, \alpha_2]$. The brackets (20) imply $\mathcal{G}$-gauge invariance of the theory. Therefore, the nonlocal phase-space function $G[\alpha]$ is conserved during evolution, and the smearing constant transforms in the adjoint representation $\alpha_1^i \to \alpha_1^i + f_{jk}{}^i\alpha_2^j\alpha_1^k$. The local phase-space function $G_i = \tau_i P_I\phi^I$ then evolves according to an equation of the form $\dot{G}_i = -\partial_a J_i^a$ where J^a are obtained from possible boundary terms in (20). In a covariant theory, the spatial vector J_i^a must be part of a space-time current J_i^μ with density weight one, satisfying the covariant conservation equation $\partial_\mu J_i^\mu = \nabla_\mu J_i^\mu = 0$. The completion of J_i^a to a space-time vector allows us to identify the charge density J_i^t (which turns out to equal G_i) as a function of the canonical fields.

An explicit computation with the classical constraints yields,

$$\begin{aligned} &\{G_i, H[N] + H_a[N^a]\} \\ &= -(\tau_i)^I{}_J\partial_a\left(N\sqrt{\det q}\left(\delta_{IK}q^{ab}\phi^J\partial_b\phi^K - \phi^J\frac{N^a}{N}\frac{P_I}{\sqrt{\det q}}\right)\right) \\ &= -\partial_a J_i^a \end{aligned} \tag{22}$$

with

$$J_i^a = (\tau_i)^I{}_J N\sqrt{\det q}\left(\delta_{IK}q^{ab}\phi^J\partial_b\phi^K - \phi^J\frac{N^a}{N}\frac{P_I}{\sqrt{\det q}}\right). \tag{23}$$

If we consider $H[N] + H_a[N^a]$ as a gauge transformations, N and N^a approach zero at any boundary, and therefore the smeared $\int d^3x G_i\alpha^i$ Poisson commutes with any gauge generator of hypersurface deformations. The system is therefore first class. If N or N^a do not approach zero at the boundary, they generate gravitational symmetries, such as a time translation $H[1]$ in an asymptotically flat space-time, that are not gauge.

The canonical equations of motion for the scalar field allow us to relate the momenta P_I in the spatial current (23) to time derivatives $\partial_t\phi^J$, and an emergent space-time metric $\tilde{g}_{\mu\nu}$ derived from the covariance condition of a modified gravitational theory expresses q^{ab} and N^a through spatial and space-time components of the metric. The components $g^{t\mu}$ of the inverse emergent space-time metric then imply a unique expression for the time component J_i^t, and we have the full 4-current with space-time density weight $N\sqrt{\det q}$ as $\sqrt{-\det g}$ in Lorentzian signature. The resulting covariant and conserved current J_i^μ is of fundamental importance in quantum field theory in curved space-time because it provides a well-defined inner product. We will thus try to preserve the existence of a symmetry generator (19) or, equivalently, the $\mathcal{G}$-invariance in the modified theory.

We illustrate this procedure for the case of a single complex scalar field ϕ, corresponding to the $\mathcal{G} = \mathrm{U}(1)$ case. Starting with the Klein–Gordon action in curved space-time,

$$S_{\rm scalar}[\phi] = -\int \mathrm{d}^4x\sqrt{-\det g}(g^{\mu\nu}(\nabla_\mu\phi^*)(\nabla_\nu\phi) + V(\phi^*\phi)) \tag{24}$$

with a potential $V(\phi^*\phi)$. Using the inverse metric

$$g^{\mu\nu} = q^{ab}s_a^\mu s_a^\nu - \frac{1}{N^2}(t^\mu - N^a s_a^\mu)(t^\nu - N^b s_b^\nu) \tag{25}$$

in canonical form, the decomposition of the action is given by

$$S_{\rm scalar}[\phi] = \int \mathrm{d}^4xN\sqrt{\det q}\left(-\frac{1}{N^2}\dot{\phi}^*\dot{\phi} + \frac{N^a}{N^2}\dot{\phi}^*(\partial_a\phi) + \frac{N^a}{N^2}(\partial_a\phi^*)\dot{\phi} + \left(q^{ab} - \frac{N^aN^b}{N^2}\right)(\partial_a\phi^*)(\partial_b\phi) + V(\phi^*\phi)\right). \tag{26}$$

The momenta are

$$P_\phi = \frac{\delta S_{\rm scalar}[\phi]}{\delta\dot{\phi}} = -\frac{\sqrt{\det q}}{N}(\dot{\phi}^* - N^a(\partial_a\phi^*)), \tag{27}$$

$$P_\phi^* = \frac{\delta S_{\rm scalar}[\phi]}{\delta\dot{\phi}^*} = -\frac{\sqrt{\det q}}{N}(\dot{\phi} - N^a(\partial_a\phi)), \tag{28}$$

and therefore we can use

$$N^aP_\phi\partial_a\phi = -N^a\frac{\sqrt{\det q}}{N}(\dot{\phi}^* - N^b(\partial_b\phi^*))\partial_a\phi, \tag{29}$$

$$N^aP_\phi^*\partial_a\phi^* = -N^a\frac{\sqrt{\det q}}{N}(\dot{\phi} - N^b(\partial_b\phi))\partial_a\phi^*, \tag{30}$$

and

$$\begin{aligned}\frac{N}{\sqrt{\det q}}P_\phi^*P_\phi &= \frac{\sqrt{\det q}}{N}(\dot{\phi}^*\dot{\phi} - N^a\dot{\phi}^*(\partial_a\phi) - N^a(\partial_a\phi^*)\dot{\phi} + N^aN^b(\partial_a\phi)(\partial_b\phi^*))\\ &= \frac{\sqrt{\det q}}{N}\dot{\phi}^*\dot{\phi} - N^a\frac{\sqrt{\det q}}{N}(\dot{\phi}^*(\partial_a\phi) + (\partial_a\phi^*)\dot{\phi} - N^b(\partial_a\phi)(\partial_b\phi^*))\\ &= \frac{\sqrt{\det q}}{N}(\dot{\phi}^*\dot{\phi} - N^aN^b(\partial_a\phi)(\partial_b\phi^*)) + N^a(P_\phi\partial_a\phi + P_\phi^*\partial_a\phi^*)\end{aligned} \tag{31}$$

in order to replace some of the time derivatives of ϕ and ϕ^* in the action by momenta,

$$S_{\rm scalar}[\phi] = \int \mathrm{d}^4x\left[P_\phi\dot{\phi} + P_\phi^*\dot{\phi}^* - N^a(P_\phi\partial_a\phi + P_\phi^*\partial_a\phi^*) + N\left(\frac{P_\phi^*P_\phi}{\sqrt{\det q}} + \sqrt{\det q}\,q^{ab}(\partial_a\phi^*)(\partial_b\phi) + \sqrt{\det q}\,V(\phi^*\phi)\right)\right]. \tag{32}$$

In this form, we immediately read off the Hamiltonian and diffeomorphism constraints,

$$H=\frac{P_\phi^* P_\phi}{\sqrt{\det q}}+\sqrt{\det q}\,q^{ab}(\partial_a\phi^*)(\partial_b\phi)+\sqrt{\det q}\,V(\phi^*\phi), \tag{33}$$

$$H_a = P_\phi\partial_a\phi + P_\phi^*\partial_a\phi^*, \tag{34}$$

which are both real.

The global symmetry transformation $\phi\to\phi e^{i\alpha}$ for constant α, which is manifest in the original action, is still present in Hamiltonian form. It is completed by a canonical transformation,

$$\phi\to\phi e^{i\alpha}, \qquad P_\phi\to P_\phi e^{-i\alpha}, \tag{35}$$

by including the momenta, and an analogous version for their complex conjugate counterparts. The infinitesimal version,

$$\phi\to\phi+i\alpha\phi, \qquad P_\phi\to P_\phi-i\alpha P_\phi, \tag{36}$$

is generated by the phase-space function,

$$G[\alpha]=\int \mathrm{d}^3x\,\alpha i(\phi P_\phi-\phi^* P_\phi^*), \tag{37}$$

which we have smeared with the infinitesimal, real constant α. (There is a single global-gauge generator $G[\alpha]$ rather than local transformations.) This generator obeys the relations,

$$\{H[N],G[\alpha]\}=\{\vec{H}[\vec{N}],G[\alpha]\}=\{G[\alpha_1],G[\alpha_2]\}=0, \tag{38}$$

to first order in the constant α and up to possible boundary terms according to (22). It therefore provides a global first-class constraint in addition to the local ones, H and H_a, and implies U(1)-invariance.

The physical meaning of this function can be seen by replacing momenta with time derivatives of the scalar field, using (28),

$$\begin{aligned}G&=-\frac{i}{N}\sqrt{\det q}(\phi\dot{\phi}^*-\phi^*\dot{\phi}+N^a(\phi^*(\partial_a\phi)-\phi(\partial_a\phi^*)))\\&=-i\sqrt{-\det g}(g^{tt}(\phi^*\dot{\phi}-\phi\dot{\phi}^*)+g^{ta}(\phi^*(\partial_a\phi)-\phi(\partial_a\phi^*)))\\&=:g^{tt}J_t+g^{ta}J_a=J^t,\end{aligned} \tag{39}$$

using standard expressions of the scalar-field current J_μ. The metric factors identify the global gauge generator $G=J^t$ with the time component of the densitized space-time current of the Klein-Gordon field.

The usual space-time formulation tells us that the current is conserved in the sense that $\partial_\mu J^\mu=\nabla_\mu J^\mu=0$, using the space-time density weight of J^μ. If we include boundary terms in (38) according to (22), we reproduce this conservation law of the space-time current at the canonical level,

$$\begin{aligned}\partial_t J^t&=\{G,H[N]+H_a[N^a]\}\\&=-i\partial_a\left(\sqrt{-\det g}\left(q^{ab}(\phi\partial_b\phi^*-\phi^*\partial_b\phi)-\frac{N^a}{N}\left(\phi\frac{P_\phi}{\sqrt{\det q}}-\phi^*\frac{P_\phi^*}{\sqrt{\det q}}\right)\right)\right)\\&=-i\partial_a(\sqrt{-\det g}(g^{ab}(\phi\partial_b\phi^*-\phi^*\partial_b\phi)+g^{ta}(\phi\dot{\phi}^*-\phi^*\dot{\phi})))\\&=-\partial_a(g^{ab}J_b+g^{at}J_t)=-\partial_aJ^a,\end{aligned} \tag{40}$$

where we used (28) in the third line. This result has several implications: (i) The spatial component of the Klein–Gordon current with space-time density weight one is given by the boundary terms of (38), derived after smearing G with a constant α; (ii) The unsmeared symmetry generator equals the time component J^t of the densitized space-time current; and (iii) We need the space-time metric, including g^{ta} and not just the spatial part, in order to combine the correct terms in $\partial_t J^t$ and derive the conservation law, equating this term to $-\partial_a J^a$. The conservation law is therefore related to covariance in the sense that a well-defined emergent space-time metric must exist in the modified case.

For the scalar field, our results show that the symmetry generator (37) is the Noether charge density, the integration of which is a conserved charge. This may be generalized to other systems for a Hamiltonian version of Noether's theorem, and also applied to a local symmetry by the introduction of gauge fields. In canonical terms, the symmetry generator (37) is a Dirac observable.

C. Spherically symmetric sector

We evaluate the full covariance conditions within a viewpoint of effective field theory, starting with a generic Hamiltonian constraint with terms up to a fixed number of spatial derivatives. It is easier to perform the required calculations after a reduction to spherical symmetry, which is able to provide new interesting models for nonvacuum black holes as well as inhomogeneous cosmological models.

1. Classical theory

Using spherical symmetry, the space-time line element can be written as

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + q_{xx}(\mathrm{d}x + N^r\mathrm{d}t)^2 + q_{\vartheta\vartheta}\mathrm{d}\Omega^2. \quad (41)$$

As initially developed for models of loop quantum gravity [18–20], it is convenient to parametrize the metric components q_{xx} and $q_{\vartheta\vartheta}$ as

$$q_{xx} = \frac{(E^\varphi)^2}{E^x}, \qquad q_{\vartheta\vartheta} = E^x, \quad (42)$$

where E^x and E^φ are the radial and angular densitized-triad components, respectively. We assume $E^x > 0$, fixing the orientation of space.

The canonical pairs for classical gravity are given by (K_φ, E^φ) and (K_x, E^x), where $2K_x$ and K_φ are components of extrinsic curvature. We have the canonical pair (ϕ, P_ϕ) for scalar matter. The basic Poisson brackets are given by

$$\{K_x(x), E^x(y)\} = \{K_\varphi(x), E^\varphi(y)\} = \{\phi(x), P_\phi(y)\} = \delta(x-y). \quad (43)$$

(Compared with other conventions, our scalar phase-space variables are divided by $\sqrt{4\pi}$, absorbing the remnant of a spherical integration. We use units in which Newton's constant equals one.)

The Hamiltonian constraint has the vacuum gravitational contribution depending only on (K_φ, E^φ) and (K_x, E^x), as well as a matter contribution that depends also on (ϕ, P_ϕ). To be specific, we consider a minimally coupled scalar field in this section. The Hamiltonian and diffeomorpshism constraints in the spherically symmetric theory are then given by

$$H = -\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(-V(\phi) + \frac{1}{E^x} + \frac{K_\varphi^2}{E^x} + 4\frac{K_x}{E^\varphi}K_\varphi - \frac{1}{E^x}\frac{P_\phi^2}{(E^\varphi)^2}\right) - E^x\frac{(\phi')^2}{E^\varphi} - \frac{1}{4E^x}\frac{((E^x)')^2}{E^\varphi} + \frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right], \quad (44)$$

with a scalar potential $V(\phi)$ (or $\frac{1}{2}V(\phi)$, depending on conventions), and

$$H_r = E^\varphi K_\varphi' - K_x(E^x)' + P_\phi\phi'. \quad (45)$$

These constraints are first class and have Poisson brackets of hypersurface-deformation form,

$$\{H_r[N^r], H_r[M^r]\} = H_r[N^r M^{r\prime} - N^{r\prime} M^r], \quad (46a)$$

$$\{H[N], H_r[M^r]\} = -H[M^r N'], \quad (46b)$$

$$\{H[N], H[M]\} = H_r[q^{xx}(NM' - N'M)], \quad (46c)$$

with the structure function $q^{xx} = E^x/(E^\varphi)^2$ equal to the inverse radial component of the space-time metric. The covariance conditions

$$\left.\frac{\partial(\{q^{\theta\theta}, H[\epsilon^0]\})}{\partial(\epsilon^0)'}\right|_{\text{O.S.}} = \left.\frac{\partial(\{q^{\theta\theta}, H[\epsilon^0]\})}{\partial(\epsilon^0)''}\right|_{\text{O.S.}} = \cdots = 0, \quad (47a)$$

and

$$\left.\frac{\partial(\{q^{xx}, H[\epsilon^0]\})}{\partial(\epsilon^0)'}\right|_{\text{O.S.}} = \left.\frac{\partial(\{q^{xx}, H[\epsilon^0]\})}{\partial(\epsilon^0)''}\right|_{\text{O.S.}} = \cdots = 0, \quad (47b)$$

derived in [5] are clearly satisfied.

The off shell gauge transformations for lapse and shift,

$$\delta_\epsilon N = \dot{\epsilon}^0 + \epsilon^r N' - N^r(\epsilon^0)', \quad (48a)$$

$$\delta_\epsilon N^r = \dot{\epsilon}^r + \epsilon^r(N^r)' - N^r(\epsilon^r)' + q^{xx}(\epsilon^0 N' - N(\epsilon^0)'), \quad (48b)$$

together with the realization of covariance conditions ensures that the line element (41) is invariant, with a covariant metric tensor in the sense that its canonical gauge transformations reproduce space-time diffeomorphisms on shell,

$$\delta_\epsilon g_{\mu\nu}|_{\text{O.S.}} = \mathcal{L}_\xi g_{\mu\nu}. \quad (49)$$

The gauge functions (ϵ^0, ϵ^r) on the left-hand side are related to the 2-component vector generator $\xi^\mu = (\xi^t, \xi^r)$ of the diffeomorphism on the right-hand side by

$$\xi^\mu = \epsilon^0 n^\mu + \epsilon^r s^\mu = \xi^t t^\mu + \xi^r s^\mu \quad (50)$$

with

$$\xi^t = \frac{\epsilon^0}{N}, \qquad \xi^r = \epsilon^r - \frac{\epsilon^0}{N}N^r. \quad (51)$$

2. Covariance in emergent modified gravity

We now consider modifications to the spherically symmetric theory with canonical variables (K_φ, E^φ) and (K_x, E^x). Neither (E^φ, E^x) nor (K_φ, K_x) then have a direct relationship with a spatial metric or extrinsic curvature on spacelike hypersurfaces, but we continue to use these symbols to denote the gravitational configuration and momentum variables.

If we modify the Hamiltonian constraint such that the first-class nature is maintained, the constraint brackets (46) in general imply a modified structure function, $\tilde{q}^{xx} \neq q^{xx}$. There is no indication that the angular component of the spatial metric should be modified because it does not appear as a structure function in spherically symmetric hypersurface-deformation brackets. The emergent space-time metric then equals

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + \tilde{q}_{xx}(\mathrm{d}x + N^r\mathrm{d}t)^2 + E^x\mathrm{d}\Omega^2, \quad (52)$$

where $\tilde{q}_{xx} = 1/\tilde{q}^{xx}$ (as long as $\tilde{q}^{xx} > 0$).

The covariance condition (47) for the angular component of the emergent spatial metric implies, using $\delta_{\epsilon^0}E^x = -\delta\tilde{H}[\epsilon^0]/\delta K_x$,

$$\left.\frac{\partial\tilde{H}}{\partial K_x'}\right|_{\mathrm{O.S.}} = \left.\frac{\partial\tilde{H}}{\partial K_x''}\right|_{\mathrm{O.S.}} = \cdots = 0, \quad (53)$$

which restricts possible modified Hamiltonian constraints to those that do not contain radial derivatives of K_x. The radial component of the covariance condition becomes

$$\left.\frac{\partial(\delta_{\epsilon^0}\tilde{q}^{xx})}{\partial(\epsilon^0)'}\right|_{\mathrm{O.S.}} = \left.\frac{\partial(\delta_{\epsilon^0}\tilde{q}^{xx})}{\partial(\epsilon^0)''}\right|_{\mathrm{O.S.}} = \cdots = 0 \quad (54)$$

and has important implications that cannot simply be summarized as independence of the Hamiltonian constraint on certain spatial derivatives. This condition will therefore be analyzed in more detail below. The covariance condition (12) for the scalar field in spherical symmetry reduces to

$$\left.\frac{\partial\tilde{H}}{\partial P_\phi'}\right|_{\mathrm{O.S.}} = \left.\frac{\partial\tilde{H}}{\partial P_\phi''}\right|_{\mathrm{O.S.}} = \cdots = 0, \quad (55)$$

which restricts the possible modified Hamiltonian constraints to those that do not contain radial derivatives of P_ϕ.

Given a modified structure function $\tilde{q}^{xx}$ obtained from the vacuum theory, and thus an emergent metric, one may postulate that a massive scalar field obeys the Klein-Gordon equation,

$$g^{\mu\nu}\nabla_\mu\nabla_\nu\phi - m^2\phi = 0, \quad (56)$$

where one uses the emergent metric instead of the classical one. This equation of motion is derived from the invariant action functional,

$$S[\phi] = \frac{1}{2}\int \mathrm{d}^4x\sqrt{-\det g}(g^{\mu\nu}(\nabla_\mu\phi)(\nabla_\nu\phi) + m^2\phi^2), \quad (57)$$

by varying with respect to the scalar field for a given background metric. However, in the modified case, this proposal assumes that the emergent space-time metric depends only on the gravitational matter variables and not on the scalar field itself. The emergent nature of the space-time geometry means that the canonical variables no longer have a close relationship with their emergent geometrical roles, and any phase-space degree of freedom, including a matter field, could possibly contribute to the geometry. Moreover, previous studies of emergent modified gravity have shown that more general equations of motion not necessarily derivable from an invariant action functional such as (57) may still be covariant. The following sections extend this conclusion to gravity-scalar systems in spherical symmetry, deriving several large classes of new models that go even beyond nonminimal coupling terms in the standard action formalism. They also provide explicit examples in which the emergent space-time metric depends on a scalar field.

Nevertheless, a specific and potentially interesting version of emergent modified gravity coupled to a scalar field is given by minimal coupling of the scalar field to an emergent space-time metric. Since the emergent space-time metric is not one of the fundamental fields, it cannot be implemented by an action principle of the form (57) because $g_{\mu\nu}$ remains unknown until the constraint brackets and equations of motion have been analyzed. Such a theory requires a canonical formulation with due attention to covariance conditions. The spatial part $\tilde{q}_{xx}$ of the emergent space-time metric (in spherical symmetry) can then be used to replace the classical q_{xx} in the Hamiltonian constraint of the scalar field, amounting to minimal coupling as suggested in [6]. Given the nonfundamental nature of $\tilde{q}_{xx}$ and its potential dependence on momentum variables, which can complicate constraint brackets, it is not obvious that minimal coupling is always possible in emergent modified gravity. The existence of such minimally coupled emergent gravity-scalar theories therefore requires a proof, which we present here as a specific application of our covariance conditions.

3. Proof of minimal coupling in emergent modified gravity

Minimal coupling of the scalar field, expressed in canonical form, amounts to using a matter contribution to the constraint in which the phase-space function $q_{xx} = (E^\varphi)^2/E^x$ has been replaced by $\tilde{q}_{xx}$, provided the latter depends only on the gravitational phase-space variables. Otherwise, it would be impossible to have the correct hypersurface-deformation terms for the gravitational contribution to the Hamiltonian constraint, $\{H_{\mathrm{grav}}[N_1], H_{\mathrm{grav}}[N_2]\} = H_x^{\mathrm{grav}}[\tilde{q}^{xx}(N_1'N_2 - N_1N_2')]$, where all terms other than $\tilde{q}^{xx}$ by definition do not depend on matter fields. As we will see later, polymerization of the scalar field, a modification common in models of loop quantum gravity, requires a scalar-dependent $\tilde{q}^{xx}$ and therefore cannot be minimally coupled. Nevertheless, in cases of scalar independent $\tilde{q}^{xx}$, minimal coupling might be a useful model to analyze certain matter properties. Specifically, the matter contribution to the Hamiltonian constraint is then given by

$$H_{\mathrm{matter}} = E^x\sqrt{\tilde{q}_{xx}}\left(\frac{1}{2}\frac{P_\phi^2}{(E^x)^2\tilde{q}_{xx}} + \frac{1}{2}\frac{(\phi')^2}{\tilde{q}_{xx}} + V(\phi)\right), \quad (58)$$

generalizing the matter contribution in the classical (44). In this form, the postulated emergent gravity-scalar theories with minimal coupling have been introduced in [6].

Anomaly freedom of the vacuum constraints implies that $\tilde{q}_{xx}$ transforms just as the classical q_{xx} under spatial coordinate changes, such that these two expressions have the same Poisson bracket with the full diffeomorphism constraint. Minimal coupling using the emergent metric is therefore compatible with the Poisson bracket $\{H[N], D[M]\}$ where $H[N] = H_{\rm grav}[N] + H_{\rm matter}[N]$ and $D[M] = D_{\rm grav}[M] + D_{\rm matter}[M]$ contain both gravitational and scalar contributions, the former with minimal coupling using $\tilde{q}_{xx}$.

The Poisson bracket of two Hamiltonian constraints, $\{H[N_1], H[N_2]\}$ is more restrictive. If the vacuum theory is anomaly free and covariant, and $\tilde{q}^{xx}$ is independent of ϕ, the gravitational contribution $H_{\rm grav}$ by construction has a Poisson bracket $\{H_{\rm grav}[N_1], H_{\rm grav}[N_2]\}$ of the correct form required for hypersurface deformations, with structure function $\tilde{q}^{xx}$. Similarly, $\{H_{\rm matter}[N_1], H_{\rm matter}[N_2]\}$ is of the same form, with the same structure function, because antisymmetry of the Poisson bracket implies that only derivative terms of momenta lead to nonzero contributions to this bracket proportional to $N_1 N_2' - N_1' N_2$ after integrating by parts. The functional form of $\tilde{q}_{xx}$ does not matter for this conclusion. For the gravitational variables, the terms in (58) only depend on E^x and $\tilde{q}_{xx}$, and since the latter cannot depend on spatial derivatives of K_x according to (53), there are no nonzero contributions to the matter Poisson bracket $\{H_{\rm matter}[N_1], H_{\rm matter}[N_2]\}$ from the gravitational dependence. The only nonzero contributions are from the ϕ'-term with the P_ϕ-term using the Poisson bracket for matter variables, and these contributions produce the correct diffeomorphism constraint with structure function $\tilde{q}^{xx}$. Without the covariance condition, this part of the bracket would not necessarily be correct.

The gravity-matter cross-terms of the form $\{\tilde{H}_{\rm grav}[N_1], \tilde{H}_{\rm matter}[N_2]\}$ in the Poisson bracket of two full modified Hamiltonian constraints, given by

$$\{\tilde{H}[N_1], \tilde{H}[N_2]\} = \{\tilde{H}_{\rm grav}[N_1] + \tilde{H}_{\rm matter}[N_1], \tilde{H}_{\rm grav}[N_2] + \tilde{H}_{\rm matter}[N_2]\}, \tag{59}$$

are also nontrivial. They have to vanish for an anomaly-free bracket of hypersurface-deformation form. However, if $\tilde{q}_{xx}$ depends on K_φ, as it does in many interesting examples of emergent modified gravity, there are nontrivial Poisson brackets that result from $(E^\varphi)'$-terms in $H_{\rm grav}$ with the K_φ-dependence of $\tilde{q}_{xx}$ in the minimally coupled scalar Hamiltonian (58). Since there is a sum of two cross-terms, $\{\tilde{H}_{\rm grav}[N_1], \tilde{H}_{\rm matter}[N_2]\} + \{\tilde{H}_{\rm matter}[N_1], \tilde{H}_{\rm grav}[N_2]\}$, these contributions are still antisymmetric under flipping N_1 and N_2. Any nonzero contribution must therefore contain a derivative of one of the lapse functions obtained after integrating by parts, resulting in the nonzero antisymmetric combination $N_1 N_2' - N_1' N_2$, as opposed to the vanishing $N_1 N_2 - N_2 N_1$. Since the gravitational Hamiltonian does not contain any matter variables, the only relevant derivative terms are obtained from the Poisson bracket of $H_{\rm grav}[N]$ with the emergent spatial metric $\tilde{q}_{xx}$ in the minimally coupled scalar term. There are nonzero cross-terms, implying anomalies in the constraint brackets, if and only if $\{\tilde{q}_{xx}, H[N]\}$ depends on spatial derivatives of N. However, this possibility is ruled out (on shell) by the second gravitational covariance condition, (54).

Minimal coupling of a scalar field is therefore consistent in spherically symmetric emergent modified gravity, but only with a rather nontrivial application of the covariance conditions. The arguments used rely on the form of these conditions in spherical symmetry together with the assumption that the structure function does not depend on the scalar field kinematically, and they do not guarantee the consistency of minimal coupling beyond these models.

III. CONDITIONS ON THE MODIFIED THEORY

We are now ready to begin our systematic derivation of covariance and symmetry conditions for scalar fields coupled to gravity. The resulting class of allowed theories is vast and requires several restrictions not only from basic physical principles but also to help organize different versions of these theories. We therefore impose a variety of conditions, some of which are necessary for consistency or based on fundamental principles, others are useful for follow-up constructions, and there is yet another set that may be used to classify different theories.

It is important to keep in mind that emergent modified gravity may be used in different ways, and the necessity or desirability of some of our conditions depends on the viewpoint taken toward this class of theories. One general attitude toward modified gravity is as a collection of possible effective theories that may be obtained in a semiclassical regime of quantum gravity. In this case, we would only use the classical-type equations of a modified theory for solutions, for instance in a phenomenological analysis, but we would not use them as a starting point for quantization toward quantum gravity, or for quantized matter fields on a curved classical background described by an emergent space-time metric. Some of our conditions are then void.

However, since, as it turns out, there are nontrivial modifications of general relativity within emergent modified gravity that retain the second-order nature of field equations for both gravity and matter, emergent modified gravity may well be an alternative to general relativity in a broader sense. In particular, it would be meaningful to apply quantization procedures to emergent modified gravity, both to the gravitational sector and to the matter fields, the former resulting in a theory of quantum gravity and the latter resulting in quantum field theory on a curved emergent space-time. Since these may be viewed as fundamental constructions, we would not be requantizing fields of an effective theory of some other fundamental theory. The consistency of such quantization procedures then necessitates additional conditions on allowed theories of emergent modified gravity.

A. Required conditions

Several conditions are necessary for the consistency of emergent modified gravity itself and not just for possible quantizations, related mainly to their gauge, symmetry and space-time structures.

1. Anomaly freedom

Modifications to canonical gravity are usually encoded in a modified Hamiltonian constraint, $\tilde{H}$. A modified Hamiltonian constraint would generally change the Poisson brackets with itself and with the diffeomorphism constraint, risking a violation not only of covariance but also of their consistency as gauge generators. Thus, we need to restrict admissible canonical theories to those given by modified constraints that preserve the hypersurface deformation form (1) of their Poisson brackets,

$$\{\vec{H}[\vec{N}], \vec{H}[\vec{M}]\} = -\vec{H}[\mathcal{L}_{\vec{M}}\vec{N}], \tag{60a}$$

$$\{\tilde{H}[N], \vec{H}[\vec{M}]\} = -\tilde{H}[M^b\partial_b N], \tag{60b}$$

$$\{\tilde{H}[N], \tilde{H}[M]\} = -\vec{H}[\tilde{q}^{ab}(M\partial_b N - N\partial_b M)], \tag{60c}$$

where the structure function, $\tilde{q}^{ab}$, is modified and determined by $\tilde{H}$. In an explicit calculation of Poisson bracket, this statement contains several consistency conditions: The Poisson brackets must be closed in the sense that they vanish when evaluated on the constraint surface (anomaly freedom as a gauge theory). And for a relationship between gauge transformations and hypersurface deformations to be possible, they must maintain the specific form (1) as seen in the classical theory where the structure function may be modified in its dependence on phase-space degrees of freedom, but no additional constraint terms appear such as a Hamiltonian constraint in the Poisson bracket $\{\tilde{H}[N], \tilde{H}[M]\}$. If this condition is satisfied, the theory has off shell gauge transformations that may be compared with hypersurface deformations. As already discussed, further restrictions beyond anomaly freedom are required for off shell hypersurface deformations to be equivalent to on shell coordinate transformations in an emergent space-time geometry, but anomaly-freedom is an important first step.

In their role as gauge functions labeling hypersurface-deformation generators $\tilde{H}[N]$ and $\vec{H}[\vec{N}]$, the lapse function N and shift vector $\vec{N}$ are subject to gauge transformations that follow from consistency of gauge transformations and evolution on phase space, generated by the same constraints $\tilde{H}$ and $\vec{H}$. For constraint brackets of hypersurface-deformation type, these gauge transformations are given by [16,17]

$$\delta_\epsilon N = \dot{\epsilon}^0 + \epsilon^a\partial_a N - N^a\partial_a\epsilon^0, \tag{61}$$

$$\delta_\epsilon N^a = \dot{\epsilon}^a + \epsilon^b\partial_b N^a - N^b\partial_b\epsilon^a + \tilde{q}^{ab}(\epsilon^0\partial_b N - N\partial_b\epsilon^0), \tag{62}$$

where the only change with respect to the original theory is the use of the modified structure function. If new terms would appear in modified constraint brackets, such as a Hamiltonian constraint in the Poisson bracket of two Hamiltonian constraints, there would also be extra terms in (61) and (62) that could not be reconciled with coordinate transformations of lapse and shift in a space-time line element. It is therefore required that the constraints not only remain first class, with Poisson brackets vanishing on the constraint surface, but also model the classical form (60) with the only option of having a modified structure function. If the inverse of this modified function is used as the spatial part of an emergent space-time metric, (62) is compatible with coordinate transformations as shown in [15], provided that $\tilde{q}_{ab}$ indeed transforms like the spatial part of a space-time metric.

2. Covariance

A comparison between gauge transformations of lapse and shift with space-time coordinate changes suggests that the lapse function and shift vector may play the role of time components of a space-time metric, such that gauge transformations are on shell equivalent to coordinate transformations in space-time. If this step is still possible in the modified theory, the corresponding space-time line element is given by

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + \tilde{q}_{ab}(\mathrm{d}x^a + N^a\mathrm{d}t)(\mathrm{d}x^b + N^b\mathrm{d}t), \tag{63}$$

where the spatial metric, $\tilde{q}_{ab}$, is the inverse of the structure function, $\tilde{q}^{ab}$. This conclusion is again obtained from the geometrical behavior of hypersurface deformations, which have generators with brackets (60) provided $\tilde{q}_{ab}$ is the induced metric on an embedded spacelike hypersurface. In a modified theory, however, it is not guaranteed that the inverse of the structure function (depending on the phase-space degrees of freedom) indeed gauge transforms in a way equivalent to infinitesimal coordinate changes of a spatial metric. The space-time interpretation therefore implies a new consistency condition, in addition to anomaly freedom of the underlying gauge theory.

We say that there is a covariant space-time with line element (63) if

$$\delta_\epsilon\tilde{g}_{\mu\nu}|_{\mathrm{O.S.}} = \mathcal{L}_\xi\tilde{g}_{\mu\nu}, \tag{64}$$

that is, if the canonical gauge transformations with gauge functions (ϵ^0, ϵ^a) reproduce infinitesimal diffeomorphisms on shell with a space-time vector field ξ related to the gauge functions by

$$\xi^\mu = \epsilon^0 n^\mu + \epsilon^a s_a^\mu = \xi^t t^\mu + \xi^a s_a^\mu, \qquad (65a)$$

$$\xi^t = \frac{\epsilon^0}{N}, \qquad \xi^a = \epsilon^a - \frac{\epsilon^0}{N} N^a. \qquad (65b)$$

At this point, the on shell condition requires that the constraints be solved and equations of motion hold, which allows us to replace momenta with time derivatives of the configuration variables on phase space.

The timelike components of the covariance condition are automatically satisfied by virtue of the hypersurface-deformation brackets, (1), via the gauge transformation of the lapse function and shift vector, (61) and (62), provided the covariance condition of the spatial metric, $\delta_\epsilon q_{ab}|_{\text{O.S.}} = \mathcal{L}_\xi q_{ab}$, is satisfied [15]. The latter does not automatically hold for any anomaly-free constraint algebra of hypersurface-deformation form. It can be simplified to the conditions [5],

$$\left.\frac{\partial(\delta_{\epsilon^0}\tilde{q}^{ab})}{\partial(\partial_c\epsilon^0)}\right|_{\text{O.S.}} = \left.\frac{\partial(\delta_{\epsilon^0}\tilde{q}^{ab})}{\partial(\partial_c\partial_d\epsilon^0)}\right|_{\text{O.S.}} = \cdots = 0 \qquad (66)$$

already shown in (6), where $\delta_{\epsilon^0}\tilde{q}^{ab} = \{\tilde{q}^{ab}, H[\epsilon^0]\}$ without a spatial shift.

We now extend the covariance condition to the scalar multiplet ϕ^I. For a canonical theory with hypersurface-deformation brackets (60), we say that the scalar field is covariant if its amplitude obeys

$$\delta_\epsilon|\phi|^2|_{\text{O.S.}} = \mathcal{L}_\xi|\phi|^2|_{\text{O.S.}}. \qquad (67)$$

As in the case of a single-component scalar field, shown in Sec. II B 1, this equation implies the conditions

$$\phi^I \frac{\partial H}{\partial(\partial_c P_I)} = \phi^I \frac{\partial H}{\partial(\partial_c\partial_d P_I)} = \cdots = 0. \qquad (68)$$

Unlike the single scalar field, the Hamiltonian constraint of a multiplet allows derivatives of the conjugate momenta P_I through the dependence,

$$H(\phi^{\bar{I}}\partial_c P_{\bar{I}} - \phi^{\bar{J}}\partial_c P_{\bar{J}}, \phi^{\bar{I}}\partial_{c_1}\partial_{c_2}P_{\bar{I}} - \phi^{\bar{J}}\partial_{c_1}\partial_{c_2}P_{\bar{J}}, \ldots), \qquad (69)$$

where $\bar{I} \neq \bar{J}$ are understood as noncontracted.

Anomaly freedom of the constraints and general covariance of space-time as well as matter are non-negotiable conditions to be placed on a modified theory of space-time. In the following, we formulate a series of further conditions that we may require for a modified theory, but as we will find out, not all of them are mutually inclusive.

3. $\mathcal{G}$-invariance and conservation of the scalar current

In quantum field theory on a curved space-time, the generator (19) plays a role in the definition of the Klein-Gordon inner product because of its many useful properties, in particular its being preserved under time evolution. If we require a well-defined field quantization of matter in emergent modified gravity, we should preserve the existence of the conserved current. The imposition of this condition depends on the specific application of emergent modified gravity. If it is used as an alternative to general relativity on which quantization may be built, we must impose the condition of a conserved matter current. This condition may be relaxed if emergent modified gravity is viewed as a possible effective theory of some quantum theory of gravity constructed by other means. If the underlying fundamental theory contains matter fields, it provides quantized gravity and matter, and we do not need to requantize a scalar field on an effective space-time geometry. The condition that there be a conserved scalar current could then be relaxed. In practice, however, even in this case one would usually desire an intermediate regime of quantized matter coupled to classical gravity. If the gravitational sector of this quantum-gravity theory is emergent, the intermediate regime would still need a conserved scalar current for meaningful quantum fields on the emergent background to exist. We are not requantizing the scalar field in this case, but rather assume that it retains its quantum properties while gravity is close to its classical limit.

The requirement that the theory is $\mathcal{G}$-invariant implies that the brackets (20) hold, which in turn implies that (19) is a conserved charge associated with a Noether current. The equivalence between $\mathcal{G}$-invariance and the existence of a conserved current in general does not apply to the single scalar field. However, in the classical single-scalar theory, there is a well-known conserved current for the *free* field, obtained when the potential vanishes. In what follows, we will assume that conservation of the single-scalar current in the free limit (or, equivalently, $\mathcal{G}$-invariance in the case of a scalar multiplet) is a necessary condition because it covers a more useful set of interesting applications than a non-conserved effective current.

Therefore, we postulate that the modified theory contains a conserved current. In order to formulate this condition in a specific way, we make use of the generator (19), which does not depend on the structure function or on any other phase-space function except for the scalar field and its conjugate momentum, and demand that the Hamiltonian and diffeomorphism constraints of the modified theory commute with it up to possible boundary terms. That is, given a lapse function N and shift vector N^a, the modified constraints H and H_a must commute with the generator G up to boundary terms such that, at least on shell,

$$\{G_i, H[N] + H[N^a]\}|_{\text{O.S.}} = -\partial_a J_i^a|_{\text{O.S.}}. \qquad (70)$$

If this condition is satisfied, we identify $J_i^t = G_i$ as the charge density associated to the ith generator of the Lie algebra, as in (39), and the boundary term J_i^a as the spatial current density associated with the observer's frame (defined via N and N^a in the Hamiltonian and diffeomorphism constraints).

Using the matter covariance condition (12), Eq. (70) can be written as

$$\partial_a J_i^a = -(\tau_i)^I{}_J \left[\partial_a\left(\frac{\partial H}{\partial(\partial_a\phi^I)}\phi^J N + P_I\phi^J N^a\right) - \left(\frac{\partial H}{\partial\phi^I}\phi^J + \frac{\partial H}{\partial(\partial_b\phi^I)}\partial_b\phi^J - P_I\frac{\partial H}{\partial P_J} - \partial_b P_I\frac{\partial H}{\partial(\partial_b P_J)} - \partial_{b_1}\partial_{b_2}P_I\frac{\partial H}{\partial(\partial_{b_1}\partial_{b_2}P_J)} - \cdots\right)N\right], \tag{71}$$

where we have assumed the constraints depend on derivatives of the field up to first order (while derivatives of the momentum are allowed to be of higher finite order) and neglected boundary terms of the constraints. For the symmetry generator to be preserved under time evolution, the second term in the parenthesis on the right-hand side must vanish. Using antisymmetry of the Lie-algebra generators τ_i, this condition implies the usual dependence,

$$H = H(\delta^{IJ}P_IP_J, \delta_{IJ}\phi^I\phi^J, \delta^{IJ}\partial_aP_I\partial_bP_J, \times\delta_{IJ}\partial_a\phi^I\partial_b\phi^J, P_I\phi^I, P_I\partial_a\phi^I, \phi^I\partial_aP_I), \tag{72}$$

of a possible modified Hamiltonian constraint on scalar fields and momenta. (Higher-order spatial derivatives of P_I are allowed as long as its $\mathcal{G}$-index is contracted.) Combining this dependence with the one allowed by covariance, (69), we conclude that the Hamiltonian constraint cannot depend on derivatives of the momenta, and is reduced to the dependence

$$H = H(P_IP^I, \phi_I\phi^I, \partial_a\phi_I\partial_b\phi^I, P_I\phi^I, P_I\partial_a\phi^I). \tag{73}$$

This form is compatible with, but is not limited to, the dependence of the classical constraint (14). The spatial component of the conserved current is then,

$$J_i^a = -(\tau_i)^I{}_J\left(\frac{\partial H}{\partial(\partial_a\phi^I)}\phi^J N + P_I\phi^J N^a\right), \tag{74}$$

read off from the boundary term in (71).

4. Gravitational mass as an observable

A Dirac observable is a phase-space function that weakly Poisson-commutes with all the constraints, such that the Poisson brackets vanish when the constraints are satisfied. Dirac observables are thus preserved under time evolution if the system is fully constrained. The smeared symmetry generator of the scalar field discussed above is an example of a Dirac observable associated to the matter field. However, general relativity in its four-dimensional form does not have such observables associated to the gravitational field in any obvious way. The construction of gravitational Dirac observables is simplified in the presence of boundaries or asymptotic fall-off conditions, in which case boundary terms of the constraints can often be related to Dirac observables with physical meaning [21]. In vacuum spherical symmetry, which we will discuss in detail in the next section, a Dirac observable exists which has the physical meaning of mass. The existence of such an observable is desirable for various reasons, and therefore we postulate that the modified theory must preserve the existence of a mass observable, at least in vacuum. If this condition is violated, there is no unambiguous definition of the gravitational mass, a questionable outcome in a supposedly gravitational theory.

We conclude that the existence of both the matter and gravitational observables is important. They will play a crucial role in restricting the class of anomaly-free, covariant constraints even further.

5. Factoring out canonical transformations

The canonical formulation of a specific theory in general is uniquely defined only up to an application of canonical transformations. In a classification of new versions of canonical theories it is therefore essential to eliminate the freedom of performing canonical transformations by imposing suitable relationships between the canonical variables or other phase-space functions. If this step is omitted, a canonical transformation of the classical theory might be misclassified as a new modified theory, even though it would not imply new physics, or two equivalent modified theories might be misclassified as different ones. A careful treatment of canonical transformations also makes it possible to clarify whether specific modifications are required by a certain quantization approach, such as polymerization in models of loop quantum gravity, or merely appear because a fixed set of canonical variables has been used.

Some canonical transformations can easily be eliminated because they would not preserve the diffeomorphism constraint, which we always assume to be unmodified but the condition of preserving the diffeomorphism constraint still leaves a large class of possible canonical transformations. We will therefore impose additional conditions, guided for instance by how certain modification terms appear in the Hamiltonian constraint that can sometimes be eliminated by a canonical transformation, simplifying follow-up calculations. While the general condition that canonical transformations be factored out is essential, the specific implementation therefore depends on detailed steps of our constructions and, to some degree, is subject to preferences in the solution procedure. (For instance, the vacuum models of [6] are based on different but canonically equivalent choices compared with those of [5].)

B. Desirable properties

The structure of hypersurface-deformation brackets as well as general properties of space-time solutions related to singularities suggest additional conditions that may not be strictly necessary (as always, depending on how emergent modified gravity is used) but are strongly desirable for common applications.

1. Absence of singularities

One motivation to pursue general physical theories beyond the standard model and general relativity rests on the expectation that new physics may tame some of the divergences present in standard dynamical solutions. In the case of general relativity, the most well-known divergences are singularities at the center of black holes and at the big bang. In some cases, coupling matter to gravity can have a significant effect on the structure of singularities.

Emergent modified gravity may be viewed as a novel class of fundamental theories that grant us access to new geometrical models of space-time beyond general relativity. It is therefore important to ask what this class of theories may tell us about divergences and singularities. In vacuum, it has been shown [7,8] that some of the modifications in emergent modified gravity may resolve the classical singularity of a static black hole. In the presence of matter, the resolution of the singularity is not guaranteed. For instance, by coupling a perfect fluid in a covariant way, it was shown that the gravitational collapse of dust develops a singularity once again, although in a more harmless way compared to the classical case [22]. (The case of a perfect fluid differs from the scalar field in that the conditions of anomaly-freedom and covariance determine the theory almost uniquely, except for a free function in the pressure term. A perfect fluid is therefore always close to minimal coupling. Moreover, in this case the structure function does not depend on the matter variables.) Given this partial evidence, we expect that a certain class of modified constraints coupled to the scalar field within emergent modified gravity will still develop singularities, but there is a chance that some modifications imply dynamical solutions free of this dynamical divergence.

The matter case in spherical symmetry differs qualitatively from vacuum solutions because the presence of scalar field implies a new local degree of freedom. Different initial conditions chosen for the scalar field represent different physical scenarios, which may have an effect on the nature of the singularity (or its absence). Furthermore, the equations of motion we will obtain are complicated to work with analytically in general scenarios, for instance because the matter field may contribute to the emergent space-time metric. Emergent gravity-matter theories are usually more strongly coupled than their classical counterparts. In our explicit examples, we will focus on a specific and simplified physical scenario, given by a spatially constant scalar field on a collapsing homogeneous space with a topology suitable for a region within spherically symmetric space-time. This scenario is intended to model the interior of a black hole, which in the static vacuum case is indeed homogeneous. While it is limited, it does allow us to observe interesting and nontrivial distinctions between different outcomes, depending on the class of scalar coupling in emergent modified gravity.

The resolution of singularities is a strongly desired fundamental property and may therefore be used to rule out versions of emergent modified gravity that do not lead to this outcome. However, emergent modified gravity presents a classical setting of space-time physics, and additional quantum effects that cannot be modeled by some of the modification functions in an effective way could contribute to the resolution of singularities even if a version of emergent modified gravity, by itself, does not do so. For this reason, we do not consider singularity freedom as a strict condition to be imposed on emergent modified gravity, in contrast to conditions such as covariance or conservation laws that are required for internal consistency of a given space-time theory coupled to matter.

2. Absence of kinematical divergences in the Hamiltonian constraint

As a phase-space function, the classical Hamiltonian constraint always takes finite values provided it is evaluated for nondegenerate spatial metrics and bounded extrinsic curvature as well as finite matter variables. The equations of motion it generates then contain only finite terms under these conditions. The nondegeneracy condition on the spatial metric and boundedness of extrinsic curvature may not always be satisfied in certain regions of explicit solutions of the equations of motion, for instance at a horizon or a physical singularity. However, these divergences are properties of solutions in regions where the canonical fields reach boundaries of phase space.

It turns out that some versions of emergent modified gravity imply stronger divergences of the Hamiltonian constraint as a phase-space function, for instance at values of some of the gravitational phase-space fields in the interior of phase space, such as finite momenta with nondegenerate configuration degrees of freedom. Such divergences then also appear in equations of motion generated by the constraint, and not only in their solutions. Similarly, it is possible to have divergences of the Hamiltonian constraint at certain values of a matter field even if the gravitational degrees of freedom are in well-defined interior regions of phase-space. When this happens, the interpretation of the Hamiltonian constraint as a well-defined generator of gauge transformations or evolution breaks down, even though we have not reached a boundary of phase space where we may have to look for a reparametrization of solutions for instance by a coordinate transformation in the covariant space-time picture.

Depending on the solution procedures to be applied, it may therefore be desirable to restrict modified theories to those cases in which the Hamiltonian constraint does not have divergences in the phase-space interior. This kind of divergences is sometimes related to, but usually not identical with, the concept of space-time singularities. It does not make use of the emergent space-time metric but only of the constraint functions and their equations of motion.

3. Partial Abelianization

Partial Abelianization was proposed in [23,24] to simplify common quantization procedures that are often untractable in the presence of structure functions. The general idea of this proposal is to define a new phase-space function as a linear combination of the constraints, $H^{(\mathrm{A})} = BH + A^a H_a$, such that the Poisson brackets of $H^{(\mathrm{A})}$ together with the classical diffeomorphism constraint take the form of hypersurface-deformation brackets, but with a vanishing structure function. The geometrical space-time interpretation is then lost because there is no non-vanishing candidate for a spatial metric, but the resulting partially Abelian algebra is free of structure functions and may be quantized more easily through operator versions of the equations $H^{(\mathrm{A})} = 0$ and $H_a = 0$. The condition of partial Abelianization requires that A^a and B are phase-space functions, such that the off shell behavior of the resulting theory is different from the original version. For this reason, it may be considered a modified theory, but not directly of space-time or gravity because a compatible space-time geometry must be recovered in a more indirect way than in emergent modified gravity.

A useful property of a partial Abelianization is that the phase-space submanifold given by $H^{(\mathrm{A})} = 0$ and $H_a = 0$ is identical with the classical constraint surface. Classical solutions to the constraints can therefore be used, but their gauge behavior and equations of motion are not necessarily classical. Moreover, $H^{(\mathrm{A})}$ is preserved under time evolution in the normal direction in the absence of a spatial shift.

In [23,24], a partial Abelianization for spherical symmetry was constructed in two steps, first combining the classical diffeomorphism and Hamiltonian constraints in order to remove K_x from the resulting expression, and then integrating by parts. The second step removes spatial derivatives from the remaining terms of K_φ and E^φ, which implies a vanishing $\{H^{(\mathrm{A})}[N], H^{(\mathrm{A})}[M]\}$ based only on antisymmetry of the Poisson bracket: the bracket produces only the vanishing $NM - MN$ and no term of the form $NM' - N'M$. However, integrating the original local constraint functions turns them into global expressions that require a careful analysis of boundary terms, and it obscures any possible relationship of the resulting gauge theory with space-time geometry, and the new lapse function becomes explicitly phase-space dependent. There is an intrinsic consistency problem in this version of partial Abelianization because boundary terms in a theory of gravitational variables require concepts such as mass observables or asymptotically flat regions, but they are available only if the theory has a consistent space-time interpretation. As shown in [5], an emergent space-time metric does exist in some partially Abelianized theories, but its spatial part is not necessarily identical with the classical $(E^\varphi)^2/E^x$ that had been implicitly assumed in [23,24].

A new method that manages to obtain a local off shell partial Abelianization with a compatible space-time interpretation has been given in [5]. Moreover, in vacuum spherical symmetry, it was shown that a partial Abelianization of this kind, if it exists, is always unique up to an overall factor multiplying the new constraint, both for the classical H and for a general covariantly modified $\tilde{H}$ as the initial expression of the Hamiltonian constraint. In the latter case, partial Abelianization is possible only if a specific modification function vanishes. Therefore, the possibility of a partial Abelianization can be used as another condition in a classification of modified canonical theories. The importance of this condition depends on the specific application of emergent modified gravity, viewing it as a potential effective description of some quantum theory of gravity, or a new and more general starting point for a quantization of gravity not necessarily based on general relativity. In the former case, the existence of a partial Abelianization may simplify some calculations but is not necessary because we would not re-quantize the underlying phase-space degrees of freedom and constraints. In the latter case, the existence of a partial Abelianization is strongly desired because it may help to construct consistent quantizations of the constraints. As shown in [25], a fundamental origin of MOdified Newtonian Dynamics (MOND, [26–28]) may then be obtained because the conditions on partial Abelianization may require logarithmic terms in modification functions that can be relevant on intermediate scales.

4. Polymerization of the scalar field

An example of modified scalar theories is given by so-called polymerization, motivated by mathematical constructions in loop quantum gravity. An ongoing challenge in this field is whether bounded phase-space functions such as holonomies, used for a well-defined kinematical quantization scheme, can be introduced and studied effectively as modifications of the constraints in a way that preserves covariance. In the example of a single real scalar field, the general scheme requires that the Hamiltonian constraint be modified such that it depends on the scalar field only via point holonomies [29], defined as bounded and pointwise periodic functions,

$$h_\phi(x) = \exp(i\nu\phi(x)), \tag{75}$$

with a constant ν. In what follows, we will refer to ν simply as the holonomy parameter, which is usually considered a quantization ambiguity to be fixed by phenomenological considerations. More generally in the context of modified theories, ν may also be a phase-space function depending on the gravitational variables of the canonical theory. A polymerized theory is a modified scalar theory, possibly coupled to gravity, in which any ϕ-dependence of the constraints can be written through a dependence on h_ϕ.

Most scalar potentials of interest are not of a polymerized form and must therefore be modified if a polymerized theory is desired. Moreover, the spatial current (23) is not of the required form and must be adjusted to a polymerized theory, or be derived anew from a consistent modified constraint if it is to comply with the principle of point holonomies. Without systematic derivations, it is then unclear how a compatible time component J^t for a space-time current can be found.

Polymerization may also be applied to the gravitational dependence, in which case it usually appears for K_φ in spherically symmetric theories because this component appears in the Ashtekar-Barbero connection [30,31] used in loop quantum gravity and, unlike K_x, has spatial density weight zero and can therefore be exponentiated. If the gravitational variables are polymerized in this way, general covariance is a major question that can be addressed by emergent modified gravity. If gravity is coupled to scalar matter, an important question is whether both kinds of polymerization can be applied consistently, maintaining covariance and the existence of a conserved current.

In this work we explore modified theories much more general than those proposed by spherically symmetric models of loop quantum gravity. Polymerization will therefore not play a central role in the modifications we are seeking. However, owing to the great interest enjoyed by polymerization in loop quantum gravity and its critical covariance issues, which have rarely been addressed in a successful manner, we will discuss possible ways in which polymerization can be accommodated in emergent modified gravity. The consistent versions turn out to be highly restricted and nontrivial, shedding light on the important question of whether and how loop quantum gravity may be compatible with space-time covariance even on a semiclassical level of effective space-time line elements.

C. Organizational principles

Finally, we formulate several further conditions that may be used to classify mutually distinct classes of emergent modified gravity. Most of these conditions take the form of requiring the existence of certain limits, which also help us to interpret possible physical effects in general terms.

1. Classical constraint surface in a limit

A modified constraint will inevitably change the dynamics of the system via the equations of motion. However, modified constraints may preserve the classical constraint surface in some cases. One example is given by the spherically symmetric modified constraint first obtained in [7]. A simple way to arrive at a modified Hamiltonian constraint obeying this condition is by postulating a new constraint as an invertible linear combination of the classical Hamiltonian constraint and the diffeomorphism constraint, $H^{(\text{new})} = BH^{(\text{cl})} + AH_x$, where A and $B \neq 0$ are initially free phase-space functions.

One usually does not expect modifications of physical solutions if they are derived from invertible linear combinations of the original constraints and gauge generators. However, while such linear combinations preserve the constraint surface, they can change the off shell behavior of gauge transformations and, for the gravitational constraints, possibly the structure function as well. These two ingredients are crucial in relating constraint brackets first to hypersurface deformations, and then to a compatible space-time geometry obeying general covariance such that infinitesimal coordinate changes are equivalent to gauge transformations on shell. If we start with a modified canonical theory, a potential geometrical space-time interpretation of its solutions is yet to be derived. Using the well-known relationship $g^{\mu\nu} = q^{\mu\nu} - n^\mu n^\nu$ between the inverse space-time metric $g^{\mu\nu}$, the inverse spatial metric $q^{\mu\nu}$, and the unit normal n^μ on spacelike hypersurfaces of a foliation, we must be able to identify both $q^{\mu\nu}$ and n^μ in order to find a candidate for the space-time metric.

The inverse spatial metric is determined by the structure function of modified but anomaly-free constraint brackets, using the known brackets of hypersurface deformations. The unit normal does not appear explicitly as another structure function, but it is implicitly determined by what we consider the Hamiltonian constraint to be among all the constraints. This property again follows from the known brackets of hypersurface deformations, in which $H[N]$ is the generator of normal deformations, singled out among the constraints by the condition that it be the only one with a structure function in $\{H[N], H[M]\}$. Replacing the classical constraint $H^{(\text{cl})}$ by a linear combination $H^{(\text{new})}$ with the diffeomorphism constraint changes the identification of the normal direction compared with the classical theory, provided the linear combination is done in an anomaly-free way that preserves the hypersurface-deformation property of $\{H^{(\text{new})}[N], H^{(\text{new})}\}$ depending only on the diffeomorphism constraint off shell. Therefore, both $q^{\mu\nu}$ and n^μ can be derived from anomaly-free constraint brackets, the former from the structure function and the latter (implicitly) from how the Hamiltonian constraint is singled out among all the constraints. The covariant space-time interpretation of solutions of the theory is therefore not invariant under taking linear combinations of the constraints. It also follows that we cannot replace the diffeomorphism constraint by a linear combination with $H^{(\mathrm{cl})}$ because doing so would introduce structure functions in Poisson brackets of the diffeomorphism constraint, which is not compatible with hypersurface-deformation commutators.

This discussion demonstrates the importance of two requirements to be imposed on the new constraint $H^{(\mathrm{new})}$. Together with the classical diffeomorphism constraint, the new Hamiltonian constraint must still satisfy the hypersurface-deformation brackets, perhaps with a modified structure function. And the emergent space-time metric obtained from this modified structure function must be covariant according to the general conditions derived in [5] and reviewed earlier in the present paper. In vacuum, it turns out that these two requirements uniquely determine the general form of the phase-space functions A and B (up to an overall factor multiplying the new constraint), which in turn determine the general form of the modified structure function.

If the new Hamiltonian constraint is a linear combination of the classical constraints, the new constraint surface is the same as determined by the classical constraints. However, gauge transformations and the dynamics generated by the modified constraints are in general nonclassical, and so is the emergent space-time metric. The most general modified constraint in vacuum for spherically symmetric systems [5] allows further modifications that can make the modified constraint surface nonclassical. But given the existence of modified theories with a classical constraint surface, there is a limit of any further free functions in the general modification such that the classical constraint surface is recovered, without having to take the full classical limit. We refer to this nontrivial limit as a limit of reaching the classical constraint surface. The dynamics and emergent space-time may remain modified in this limit.

We are not aware of a fundamental argument that would require us to preserve the classical constraint surface in a modified theory. However, one may use this condition as a way of keeping the modifications as minimal as possible, which is often useful in novel classes of theories that possess a large number of free functions and possible modifications. For example, a standard modification of general relativity may have an infinite number of independent curvature scalars in the action. But the simplest nontrivial model is given by the classical choice of simply using the Ricci scalar R, which can be used to motivate $f(R)$ theories as a large class of tractable modifications. In the same vein, we postulate the existence of a nontrivial limit of reaching the classical constraint surface imposed as a condition on certain modified theories as a principle that we can follow to differentiate between two classes of modified constraints, those that do possess such a limit and those that do not. Unlike the conditions of anomaly freedom and covariance, or the existence of observables, we do not consider the existence of a nontrivial limit of reaching the classical constraint surface as non-negotiable or strongly desired. We use it only in order to define these two distinct sets of modified constraints, thereby organizing a larger class of possible modifications.

2. Classical matter in a limit

We expect, and show below, that the coupling of matter to a modified theory will allow modifications with additional free functions beyond those obtained in vacuum, in particular functions depending on the canonical matter field. With this result in mind, there is another limit of interest, which we call the classical-matter limit. In this limit, by definition, the equations of motion of the matter fields take their classical form, except for the appearance of the emergent space-time metric instead of the classical one. This limit is therefore closely related to a choice of minimal coupling.

Since we are focusing on the scalar field here, the classical-matter limit will manifest itself as the condition that the Klein-Gordon equation be reproduced in a curved, emergent spacetime. This condition is similar to the limit of reaching the classical constraint surface, in that it is neither non-negotiable nor strongly desired, but it can be used to differentiate between two classes of modified constraints, depending on whether the limit exists.

3. Classical geometry in a limit

We define the classical-geometry limit such that it leads to a space-time picture of solutions with a classical, nonemergent space-time line element. If the space-time is nonemergent, the spatial metric (or a triad) used as a configuration degree of freedom on phase space is then equivalent to the gravitational field, as in general relativity. However, equations of motion for the gravitational field obtained in this limit may still be nonclassical due to residual freedom in modifications functions that do not affect the emergent metric.

4. Classical gravity in a limit

Applying a further restriction or limit on the modification functions that lead to the classical constraint surface, we may require that the equations of motion have a limit equivalent to Einstein's equation with the classical space-time metric. In the presence of matter, the stress-energy tensor may retain nonclassical features in this limit, depending on some of the remaining modification functions.

5. Summary of classical limits

After identifying the above conditions that may be imposed on a modified theory, we conclude that there is more than one kind of limit that may be considered classical:

(i) *Classical constraint surface in a limit:* Defined as the limit in which the modified constraints define the same constraint surface in phase space as the classical constraints, this property is possible even when the constraints and their emergent space-time are nonclassical.

(ii) *Classical-matter limit:* This limit is defined such that the equations of motion of matter take the classical form, except for an appearance of the emergent rather than classical space-time metric. In the explicit example of the scalar field in spherical symmetry given below, the classical-matter limit means that the equation of motion for the matter field is the Klein–Gordon equation on a curved, emergent space-time.

(iii) *Classical-geometry limit:* Defined as the limit in which the structure function in hypersurface-deformation brackets takes the classical form, it retains a possibility of modified dynamics on a space-time of classical type.

(iv) *Classical-gravity limit:* Defined as the limit in which the gravitational equations of motion take the form of Einstein's equation, it includes the classical-geometry limit but is more restrictive because the latter does not require classical equations of motion. While Einstein's equation is recovered in this limit, the stress-energy tensor may be nonclassical.

(v) *Vacuum limit:* One other limit we may be interested in is the vacuum limit, although it is not necessarily classical. From [5], we know the most general modified Hamiltonian constraint for the vacuum case in an expansion to second order in spatial derivative terms. Thus, we can use this expression as a limiting case to be recovered when we remove the matter field.

D. *A priori* and *a posteriori* principles

We finish this section by noting the nontrivial nature of any application of the conditions discussed above. In applying these conditions we are implicitly using them as guiding principles. In particular, we will distinguish between *a priori* and *a posteriori* principles based on how they can be applied to restrict or classify the modified theories. This dinstinction is different from the three sets of conditions, given by necessary requirements, desirable properties, and the existence of certain limits. In the following we classify the principles into *a priori* and *a posteriori* based on the procedures we followed for the spherically symmetric system, the details of which are given in the following sections.

The *a priori* principles are those that we can apply as conditions on the modified theory before obtaining an explicit expression of the constraint. The two archetypal *a priori* principles here are anomaly-freedom and general covariance. Because they are required for internal consistency of a space-time theory, we must apply both conditions from the very beginning. They will provide us with a system of differential equations that the constraints and their modification functions must satisfy. However, the full system of equations is complicated, and we will not be able to solve it exactly. In order to simplify these equations, we will apply a few additional conditions in various combinations, which we will refer to as *a priori* too. One such condition is the existence of the classical-matter limit and another is the existence of a limit in which the classical constraint surface is reached. As it will turn out, these two conditions are not mutually inclusive. The condition of the existence of the classical-matter limit will be restrictive enough to simplify the conditions for anomaly-freedom and covariance such that they can all be solved exactly. We then obtain an explicit expression of the Hamiltonian constraint with some ambiguities in the modifications that manifest themselves as undetermined functions of some of the phase-space variables. On the other hand, the limit of a classical constraint surface, while simplifying the anomaly-freedom and covariance conditions, is still too complicated to be solved exactly. We will find that a specific ambiguity in the modification functions can be chosen in two distinct versions. The first one complies with the classical constraint surface as a limit, and the other one does not, giving rise to the two classes of modified theories.

The *a posteriori* principles are the remaining ones listed in this section. This includes the important ones given by conditions of being free of singularities and divergences, as they cannot be checked until one has obtained the dynamical solutions. The conditions of the existence of the matter and gravitational observables, and the partial Abelianization, as well as the existence of the vacuum limit, and of scalar-field polymerization, can be applied directly to the explicit expressions of the constraints obtained from the a-priori principles, restricting (or classifying) their modification ambiguities to comply with these conditions.

As an example, we may pick the simplest, but nonclassical, constraint version of each class, solve for the dynamical solutions it implies in the homogeneous case, and check whether a singularity develops as expected classically. The outcome determines whether these constraints belong to the class of singularity-free ones. Surprisingly, we find that neither the class of constraints compatible with the classical-matter limit nor with the limit of a classical constraint surface are singularity free. Singularity freedom is allowed only by the remaining class, following just the *a priori* principles of anomaly freedom and covariance and some weaker conditions. We also find that scalar-field polymerization does not play a crucial role in the taming of a spatially homogeneous singularity, but all classes can, in fact, be polymerized.

IV. SPHERICALLY SYMMETRIC THEORY WITH A SCALAR FIELD

We now present detailed derivations of theories of emergent modified gravity subject to our conditions from the preceding section.

A. Classical theory

From Sec. II C we recall the following elements of the spherically symmetric classical theory in vacuum. The spacetime metric is

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + q_{xx}(\mathrm{d}x + N^r\mathrm{d}t)^2 + q_{\vartheta\vartheta}\mathrm{d}\Omega^2 \quad (76)$$

with

$$q_{xx} = \frac{(E^\varphi)^2}{E^x}, \qquad q_{\vartheta\vartheta} = E^x, \quad (77)$$

where E^x and E^φ are the radial and angular components of a densitized triad, respectively, assuming $E^x > 0$ in order to fix spatial parity. The canonical pairs are (K_φ, E^φ) and (K_x, E^x) for gravity and (ϕ, P_ϕ) for a single scalar field, such that,

$$\{K_x(x), E^x(y)\} = \{K_\varphi, E^\varphi(y)\} = \{\phi(x), P_\phi(y)\} = \delta(x-y). \quad (78)$$

The diffeomorpshism and Hamiltonian constraints are given by

$$H_x = E^\varphi K_\varphi' - K_x(E^x)' + P_\phi\phi' \quad (79)$$

and

$$H = H_{\mathrm{grav}} + H_\phi, \quad (80)$$

where H_{grav} and H_ϕ are the gravitational and matter contributions to the Hamiltonian constraint. In the classical theory with a cosmological constant Λ and minimal coupling of the scalar field, they are given by

$$H_{\mathrm{grav}} = -\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(-\Lambda + \frac{1}{E^x} + \frac{K_\varphi^2}{E^x} + 4K_\varphi\frac{K_x}{E^\varphi}\right) - \frac{1}{4E^x}\frac{((E^x)')^2}{E^\varphi} + \frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right] \quad (81)$$

and

$$H_\phi = \frac{1}{2}\left(\frac{\sqrt{q^{xx}}}{E^x}{P_\phi}^2 + E^x\sqrt{q^{xx}}(\phi')^2 + \sqrt{q_{xx}}E^xV(\phi)\right). \quad (82)$$

(A factor of 2 may be absorbed in the scalar potential.) These constraints have Poisson brackets of hypersurface-deformation form,

$$\{H_x[N^x], H_x[M^x]\} = -H_x[M^x(N^x)' - N^x(M^x)'], \quad (83a)$$

$$\{H[N], H_x[M^x]\} = -H[M^xN'], \quad (83b)$$

$$\{H[N], H[M]\} = -H_x[q^{xx}(MN' - NM')], \quad (83c)$$

with the structure function $q^{xx} = E^x/(E^\varphi)^2$.

The off shell gauge transformations for the lapse function and shift vector are

$$\delta_\epsilon N = \dot\epsilon^0 + \epsilon^x N' - N^x(\epsilon^0)',$$
$$\delta_\epsilon N^x = \dot\epsilon^x + \epsilon^x(N^x)' - N^x(\epsilon^x)' + q^{xx}(\epsilon^0N' - N(\epsilon^0)'). \quad (84)$$

The condition (6) for space-time covariance simplifies in spherical symmetry to two sets of equations,

$$\left.\frac{\partial(\{q^{\theta\theta}, H[\epsilon^0]\})}{\partial(\epsilon^0)'}\right|_{\mathrm{O.S.}} = \left.\frac{\partial(\{q^{\theta\theta}, H[\epsilon^0]\})}{\partial(\epsilon^0)''}\right|_{\mathrm{O.S.}} = \cdots = 0 \quad (85a)$$

and

$$\left.\frac{\partial(\{q^{xx}, H[\epsilon^0]\})}{\partial(\epsilon^0)'}\right|_{\mathrm{O.S.}} = \left.\frac{\partial(\{q^{xx}, H[\epsilon^0]\})}{\partial(\epsilon^0)''}\right|_{\mathrm{O.S.}} = \cdots = 0. \quad (85b)$$

These conditions are clearly satisfied in the classical case because the Hamiltonian constraint does not depend on spatial derivatives of the momenta canonically conjugate to spatial metric components. The matter covariance condition (68) in spherical symmetry takes the simplified form,

$$\frac{\partial H}{\partial P_\phi'} = \frac{\partial H}{\partial P_\phi''} = \cdots = 0, \quad (86)$$

and is satisfied too.

The gauge transformations of the lapse function and shift vector, (84), and the realization of the covariance condition (85) ensure that the space-time metric (76) is covariant in the sense that canonical gauge transformations applied to the metric reproduce diffeomorphisms when on shell. The gauge functions (ϵ^0, ϵ^x) are related to the 2-component vector $\xi^\mu = (\xi^t, \xi^x)$ generating a radial space-time diffeomorphism by

$$\xi^\mu = \epsilon^0 n^\mu + \epsilon^x s^\mu = \xi^t t^\mu + \xi^x s^\mu,$$
$$\xi^t = \frac{\epsilon^0}{N}, \qquad \xi^x = \epsilon^x - \frac{\epsilon^0}{N}N^x. \quad (87)$$

The global symmetry generator of the real scalar field is

$$G[\alpha] = \int \mathrm{d}x\, \alpha P_\phi, \tag{88}$$

with constant α. However, unlike the scalar field multiplets with values in some Lie group, the symmetry of the real scalar field holds only for the free field, $V = 0$. Its Poisson brackets with the constraints is given by

$$\{G, H_x[N^x]\} = (N^x G)', \qquad \{G, H[N]\} = 0, \tag{89}$$

which is a boundary term. This gives rise to the conserved current with components

$$J^t = P_\phi, \qquad J^x = -N^x P_\phi. \tag{90}$$

The gravitational mass observable is

$$m = \frac{\sqrt{E^x}}{2}\left(1 + K_\varphi^2 - \left(\frac{(E^x)'}{2E^\varphi}\right)^2 - \frac{\Lambda}{3}E^x\right). \tag{91}$$

B. Covariance in the modified theory

We consider modifications of the spherically symmetric theory with canonical variables (K_φ, E^φ) and (K_x, E^x). If we modify the Hamiltonian constraint, then the constraint brackets (83) imply a modified structure function, $\tilde{q}^{xx}$, which then determines the emergent spatial metric. The angular component of the metric, which does not independently appear in the structure functions, remains unmodified. The emergent space-time metric is then

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + \tilde{q}_{xx}(\mathrm{d}x + N^x\mathrm{d}t)^2 + E^x\mathrm{d}\Omega^2, \tag{92}$$

where $\tilde{q}_{xx} = 1/\tilde{q}^{xx}$, provided $\tilde{q}^{xx} > 0$. (More generally, we can allow for a modified angular component $\tilde{E}^x \neq E^x$, but we will show that it can always be mapped back to E^x by a canonical transformation. This function does not affect the covariance condition.) There is no direct correspondence between the phase-space variable E^φ and the spatial metric or a densitized triad. And since modified constraints generate nonclassical equations of motion, K_x and K_φ do not have a direct relationship with extrinsic curvature of spacelike hypersurfaces in the emergent space-time. We will therefore refer to E^φ and E^x simply as the gravitational configuration variables, and to K_φ and K_x as the gravitational momenta. (As usual, the roles of configuration variables and momenta could be reversed.)

The space-time covariance condition (6) for the angular component of the emergent spatial metric implies, using $\delta_{\epsilon^0} E^x = -\delta\tilde{H}[\epsilon^0]/\delta K_x$,

$$\frac{\partial \tilde{H}}{\partial K_x'}\bigg|_{\mathrm{O.S.}} = \frac{\partial \tilde{H}}{\partial K_x''}\bigg|_{\mathrm{O.S.}} = \cdots = 0, \tag{93}$$

which restricts the possible modified Hamiltonian constraints to those that do not contain radial derivatives of K_x. The radial component of the space-time covariance condition becomes

$$\frac{\partial(\delta_{\epsilon^0}\tilde{q}^{xx})}{\partial(\epsilon^0)'}\bigg|_{\mathrm{O.S.}} = \frac{\partial(\delta_{\epsilon^0}\tilde{q}^{xx})}{\partial(\epsilon^0)''}\bigg|_{\mathrm{O.S.}} = \cdots = 0 \tag{94}$$

and does not have simple solutions. The covariance condition for the scalar field, (68), is reduced in spherical symmetry to

$$\frac{\partial \tilde{H}}{\partial P_\phi'}\bigg|_{\mathrm{O.S.}} = \frac{\partial \tilde{H}}{\partial P_\phi''}\bigg|_{\mathrm{O.S.}} = \cdots = 0, \tag{95}$$

which restricts possible modified Hamiltonian constraints to those that do not contain radial derivatives of P_ϕ.

C. Linear combinations of the constraints and the limit of reaching the classical constraint surface

The aim of this section is to obtain a covariant modified constraint from a linear combination of the classical constraints. We will use these results later on when we compute more general modified constraints because the class of modified constraints that comply with the limit of reaching the classical constraint surface is closely related to modified theories obtained from linear combinations of the classical constraints. Such linear combinations also provide a useful and tractable example of the general analysis.

1. Anomaly-free linear combination

Consider the following linear combination of the classical constraints,

$$H^{(\mathrm{new})} = BH^{(\mathrm{old})} + AH_x, \tag{96}$$

where A and $B \neq 0$ are, at this point, undetermined phase-space functions. We restrict ourselves to the dependence $B = B(K_\varphi, E^x, \phi)$ including only phase-space fields of spatial density weight zero. Unlike B, the function A must have density weight minus one and may therefore depend on the remaining fields as well, for instance through $(E^x)'/(E^\varphi)^2$. Given these density weights, the bracket $\{H^{(\mathrm{new})}[N], H_x[M]\}$ is then of the required form, and only the bracket of two new Hamiltonian constraints must be checked. The derivation here follows the method of [5] almost line by line, with the only major difference given by the inclusion of a scalar field.

We begin by defining the quantities $\mathcal{B}$ and $\mathcal{B}^x$ according to

$$\{B, H^{(\mathrm{old})}[\epsilon^0]\}|_{\mathrm{O.S.}} =: (\mathcal{B}\epsilon^0 + \mathcal{B}^x(\epsilon^0)')|_{\mathrm{O.S.}}. \tag{97}$$

In this equation, no second-order derivative of ϵ^0 can appear because we assumed that B does not depend on the momentum K_x conjugate to the only variable, E^x, that appears with a second-order derivative in the Hamiltonian constraint. An explicit application of the classical Hamiltonian constraint $H^{(\mathrm{old})}$ shows that

$$\mathcal{B}^x = \sqrt{E^x}\frac{(E^x)'}{2(E^\varphi)^2}\frac{\partial B}{\partial K_\varphi}. \tag{98}$$

Anomaly freedom of

$$\begin{aligned}\{H^{(\mathrm{new})}[N_1], H^{(\mathrm{new})}[N_2]\} = {} & -H_x[B^2 q^{xx}(N_2N_1' - N_1N_2')] + H^{(\mathrm{old})}[BN_2\{H^{(\mathrm{old})}[N_1], B\}] - H^{(\mathrm{old})}[BN_1\{H^{(\mathrm{old})}[N_2], B\}] \\ & + H_x[BN_2\{H^{(\mathrm{old})}[N_1], A\}] - H_x[BN_1\{BH^{(\mathrm{old})}[N_2], A\}] - H^{(\mathrm{old})}[ABN_2N_1'] + H^{(\mathrm{old})}[ABN_1'N_2] \\ & - H_x[A^2(N_2N_1' - N_1N_2')] + H_x[A(N_1A)'N_2] - H_x[AN_1(N_2A)']\end{aligned} \tag{99}$$

in hypersurface-deformation form implies that all terms proportional to $H^{(\mathrm{old})}$ must cancel out. (We have used the density weight minus one of A in the last line, which then vanishes identically.) This is the case only if

$$A = -\mathcal{B}^x = -\sqrt{E^x}\frac{(E^x)'}{2(E^\varphi)^2}\frac{\partial B}{\partial K_\varphi} \tag{100}$$

from the second and fourth line, which indeed has density weight minus one. (As usual, antisymmetry means that only terms with derivatives of N need be checked.)

Given this expression for A, we now write

$$\{A, H^{(\mathrm{old})}[\epsilon^0]\} =: \mathcal{A}\epsilon^0 + \mathcal{A}^x(\epsilon^0)', \tag{101}$$

where

$$\mathcal{A}^x = -\frac{E^x}{(E^\varphi)^2}\left(K_\varphi\frac{\partial B}{\partial K_\varphi} + \left(\frac{(E^x)'}{2E^\varphi}\right)^2\frac{\partial^2 B}{(\partial K_\varphi)^2}\right). \tag{102}$$

This Poisson bracket, together with $B^2\{H^{(\mathrm{old})}[N_1], H^{(\mathrm{old})}[N_2]\}$ in (99), contributes a term proportional to the diffeomorphism constraint which is allowed for brackets in hypersurface-deformation form. The combined coefficient of all terms of this form determines the new structure function

$$\tilde{q}^{xx} = B^2 q^{xx} + B\mathcal{A}^x, \tag{103}$$

implementing anomaly freedom.

2. Covariant modified theory

In order to impose the covariance condition (85), applied to the new structure function (103) and using the new constraint (96), we now write,

$$\{\mathcal{A}^x, H[\bar{\epsilon}^0]\} =: \Lambda^0\bar{\epsilon}^0 + \Lambda^x(\bar{\epsilon}^0)', \tag{104}$$

defining Λ^0 and Λ^x. The covariance condition then implies that

$$0 = (\Lambda^x - B^{-1}\mathcal{B}^x\mathcal{A}^x)|_{\mathrm{O.S.}} = \mathcal{C} = \mathcal{C}_\varepsilon (E^x)' + \mathcal{C}_{\varepsilon\varepsilon\varepsilon}((E^x)')^3 \tag{105}$$

must vanish, defining two new coefficients $\mathcal{C}_\varepsilon$ and $\mathcal{C}_{\varepsilon\varepsilon\varepsilon}$ which must vanish independently if $\mathcal{C}$ is to vanish for all functions $E^x(x)$. The equation $\mathcal{C}_\varepsilon = 0$ implies,

$$K_\varphi\left(\frac{\partial B}{\partial K_\varphi}\right)^2 + B\left(K_\varphi\frac{\partial^2 B}{(\partial K_\varphi)^2} - \frac{\partial B}{\partial K_\varphi}\right) = 0, \tag{106}$$

solved by

$$B = c_1\sqrt{c_2 \pm K_\varphi^2}, \tag{107}$$

where c_1 and c_2 are free functions of E^x and ϕ. The equation $\mathcal{C}_{\varepsilon\varepsilon\varepsilon} = 0$ implies

$$B\frac{\partial^3 B}{(\partial K_\varphi)^3} + 3\frac{\partial B}{\partial K_\varphi}\frac{\partial^2 B}{(\partial K_\varphi)^2} = 0, \tag{108}$$

solved by

$$B = \tilde{c}_1\sqrt{\tilde{c}_2 \pm K_\varphi^2 + \tilde{c}_3 K_\varphi} \tag{109}$$

with additional free functions of E^x and ϕ, $\tilde{c}_1$, $\tilde{c}_2$, and $\tilde{c}_3$. Consistency between the two solutions requires $\tilde{c}_3 = 0$ while $\tilde{c}_1 = c_1$ and $\tilde{c}_2 = c_2$, leaving two free functions of E^x and ϕ which we write in a form such that,

$$B_s(K_\varphi, E^x, \phi) = \lambda_0\sqrt{1 - s\lambda^2 K_\varphi^2}, \tag{110}$$

where $\lambda_0 = \lambda_0(E^x, \phi), \lambda = \lambda(E^x, \phi)$, and we have split off an explicit sign choice by $s = \pm 1$. For nonzero λ, this solution restricts the phase space to a range of K_φ such that $1 - s\lambda^2 K_\varphi^2 \geq 0$, which is a nontrivial condition only if $s = +1$.

Inserting this solution in (100), we derive

$$A_s = \lambda_0 \frac{\sqrt{E^x}}{2} \frac{(E^x)'}{(E^\varphi)^2} \frac{s\lambda^2 K_\varphi}{\sqrt{1 - s\lambda^2 K_\varphi^2}} \tag{111}$$

and the new structure function

$$q^{xx}_{(\mathrm{new})} = \lambda_0^2 \left(1 + \frac{s\lambda^2}{1 - s\lambda^2 K_\varphi^2} \left(\frac{(E^x)'}{2E^\varphi}\right)^2\right) \frac{E^x}{(E^\varphi)^2} \tag{112}$$

from (103). With these results, the modified Hamiltonian constraint is

$$H^{(\mathrm{new})} = -\lambda_0 \frac{\sqrt{E^x}}{2} \sqrt{1 - s\lambda^2 K_\varphi^2} \left[E^\varphi \left(-V(\phi) + \frac{1}{E^x} + \frac{K_\varphi^2}{E^x} + 4K_x \frac{K_\varphi}{E^\varphi} - \frac{1}{E^x} \frac{P_\phi^2}{(E^\varphi)^2}\right) - E^x \frac{(\phi')^2}{E^\varphi} - \frac{1}{4E^x} \frac{((E^x)')^2}{E^\varphi} \right.$$
$$\left. + \frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi} - \frac{(E^x)'}{(E^\varphi)^2} \frac{s\lambda^2 K_\varphi}{1 - s\lambda^2 K_\varphi^2} (E^\varphi K_\varphi' + P_\phi \phi' - K_x (E^x)')\right], \tag{113}$$

parametrized by the same two functions, λ_0 and λ, and the sign parameter s.

It is interesting to note that the two sign choices for s suggest physically distinct new phenomena. The case $s = 1$, together with a reality condition imposed on the constraint, implies a curvature bound $K_\varphi < 1/\lambda$. In this case, $q^{xx}_{(\mathrm{new})}$ is guaranteed to be positive within the allowed range of K_φ. The case $s = -1$ is compatible with the classical range of K_φ, but the structure function $q^{xx}_{(\mathrm{new})}$ may become negative. In this case, as discussed in more detail in [5], we have to separate the sign of this function before we can define the spatial metric. The emergent space-time line element then reads,

$$\mathrm{d}s^2 = -\mathrm{sgn}(q^{xx}_{(\mathrm{new})}) N^2 \mathrm{d}t^2 + \frac{1}{|q^{xx}_{(\mathrm{new})}|} (\mathrm{d}x + N^x \mathrm{d}t)^2 + E^x \mathrm{d}\Omega^2. \tag{114}$$

This case therefore implies a possibility of signature change.

In the case of $s = 1$, a natural canonical transformation is given by

$$K_\varphi \to \frac{\sin(\lambda K_\varphi)}{\lambda}, \quad E^\varphi \to \frac{E^\varphi}{\cos(\lambda K_\varphi)},$$
$$\phi \to \phi, \quad P_\phi \to P_\phi - \frac{E^\varphi}{\cos(\lambda K_\varphi)} \frac{\partial}{\partial\phi} \left(\frac{\sin(\lambda K_\varphi)}{\lambda}\right),$$
$$E^x \to E^x, \quad K_x \to K_x + \frac{E^\varphi}{\cos(\lambda K_\varphi)} \frac{\partial}{\partial E^x} \left(\frac{\sin(\lambda K_\varphi)}{\lambda}\right), \tag{115}$$

which makes the bound on K_φ explicit by replacing this variable with the bounded sine function. (When checking the canonical transformation, note that λ is a function only of E^x and ϕ, but not of E^φ.) After the canonical transformation, the previous modified Hamiltonian constraint becomes

$$H^{(\mathrm{c})} = -\lambda_0 \frac{\sqrt{E^x}}{2} \left[E^\varphi \left(-V(\phi) + \frac{1}{E^x} + \frac{1}{E^x} \frac{\sin^2(\lambda K_\varphi)}{\lambda^2} + 4\left(K_x + E^\varphi \left(K_\varphi - \frac{\tan(\lambda K_\varphi)}{\lambda}\right) \frac{\partial \ln\lambda}{\partial E^x}\right) \frac{1}{E^\varphi} \frac{\sin(2\lambda K_\varphi)}{2\lambda} - \frac{1}{E^x} \frac{\cos^2(\lambda K_\varphi)}{(E^\varphi)^2} \right.\right.$$
$$\times \left.\left(P_\phi - E^\varphi \left(K_\varphi - \frac{\tan(\lambda K_\varphi)}{\lambda}\right) \frac{\partial \ln\lambda}{\partial\phi}\right)^2\right) - \left(\frac{\cos^2(\lambda K_\varphi)}{4E^x} - \lambda^2 \frac{\sin(2\lambda K_\varphi)}{2\lambda} \frac{1}{E^\varphi} \left(K_x + E^\varphi K_\varphi \frac{\partial \ln\lambda}{\partial E^x}\right)\right) \frac{((E^x)')^2}{E^\varphi}$$
$$\left. - \lambda^2 \frac{\sin(2\lambda K_\varphi)}{2\lambda} \left(P_\phi + E^\varphi K_\varphi \frac{\partial \ln\lambda}{\partial\phi}\right) \frac{(E^x)'(\phi)'}{(E^\varphi)^2} - E^x \cos^2(\lambda K_\varphi) \frac{(\phi')^2}{E^\varphi} + \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right) \cos^2(\lambda K_\varphi)\right] \tag{116}$$

with structure function

$$q_c^{xx} = \lambda_0^2 \cos^2(\lambda K_\varphi) \left(1 + \lambda^2 \left(\frac{(E^x)'}{2E^\varphi}\right)^2\right) \frac{E^x}{(E^\varphi)^2}. \tag{117}$$

A second canonical transformation

$$K_\varphi \to \frac{\bar\lambda}{\lambda} K_\varphi, \qquad E^\varphi \to \frac{\lambda}{\bar\lambda} E^\varphi,$$
$$\phi \to \phi, \qquad P_\phi \to P_\phi + E^\varphi K_\varphi \frac{\partial \ln\lambda}{\partial\phi},$$
$$E^x \to E^x, \qquad K_x \to K_x - E^\varphi K_\varphi \frac{\partial \ln\lambda}{\partial E^x}, \tag{118}$$

with constant $\bar\lambda$ renders the modified Hamiltonian constraint periodic in K_φ,

$$H^{(\mathrm{cc})} = -\frac{\bar{\lambda}}{\lambda}\lambda_0 \frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-V(\phi)+\frac{1}{E^x}\right)+\frac{1}{E^x}\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+4\left(\frac{K_x}{E^\varphi}-\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right.\right.$$
$$\left.-\frac{\cos^2(\bar{\lambda}K_\varphi)}{E^x}\left(\frac{P_\phi}{E^\varphi}+\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial\phi}\right)^2\right)+\left(\left(\frac{\partial\ln\lambda}{\partial E^x}-\frac{1}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi)+\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\frac{K_x}{E^\varphi}\right)\frac{((E^x)')^2}{E^\varphi}$$
$$\left.+\left(\frac{\partial\ln\lambda}{\partial\phi}\cos^2(\bar{\lambda}K_\varphi)-\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\frac{P_\phi}{E^\varphi}\right)\frac{(E^x)'\phi'}{E^\varphi}-E^x\cos^2(\bar{\lambda}K_\varphi)\frac{(\phi')^2}{E^\varphi}+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right], \tag{119}$$

with structure function

$$q^{xx}_{(cc)} = \frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\cos^2(\bar{\lambda}K_\varphi)\left(1+\bar{\lambda}^2\left(\frac{(E^x)'}{2E^\varphi}\right)^2\right)\frac{E^x}{(E^\varphi)^2}. \tag{120}$$

One can then redefine $\lambda_0 \to \lambda_0\lambda/\bar{\lambda}$ to absorb the overall factor in the Hamiltonian constraint and in the structure function. Unlike the expression in (113), which contains a term of $1/\sqrt{1-s\lambda^2K_\varphi^2}$ that diverges at maximum K_φ for $s=1$, the holonomylike coordinates of (119) maintain a finite constraint even at the curvature bound. [There are two coefficients of $\tan(\bar{\lambda}K_\varphi)$ in the latter expression, but they are both multiplied by at least one factor of $\cos(\bar{\lambda}K_\varphi)$ which removes the divergence.] The divergence-free version, which in the vacuum case had been obtained by different means in [7,8], allows crossing this maximum-curvature hypersurface at least in the absence of matter, as explicitly shown in these papers.

The modified constraint (119) represents the nontrivial limit of reaching the classical constraint surface, to be used for the more general modified constraints we will obtain in the next subsections.

3. Matter and gravitational observables

The system with modified Hamiltonian constraint (113), obtained from a linear combination of the classical constraints, retains the global symmetry generated by (88) on shell when $V=0$. Thus, the constraints (116) and (119) retain the same symmetry generator, but only if the proper canonical transformations (115) and (118), respectively, are applied to the symmetry generator. Therefore, the symmetry generator of (116) is given by

$$G[\alpha] = \int \mathrm{d}x\,\alpha\left(P_\phi - E^\varphi\left(K_\varphi - \frac{\tan(\lambda K_\varphi)}{\lambda}\right)\frac{\partial\ln\lambda}{\partial\phi}\right). \tag{121}$$

while the symmetry generator of (119) is given by

$$G[\alpha] = \int \mathrm{d}x\,\alpha\left(P_\phi + E^\varphi\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial\phi}\right). \tag{122}$$

Similarly, the gravitational observable (91) is also preserved by the new constraint (113), but only in the vacuum limit where $\phi, P_\phi \to 0$. Also in this case, its form changes because of the application of canonical transformations. In particular, the observable associated with (116) is given by

$$m = \frac{\sqrt{E^x}}{2}\left(1+\frac{\sin^2(\lambda K_\varphi)}{\lambda^2}-\left(\frac{(E^x)'}{2E^\varphi}\right)^2\cos^2(\lambda K_\varphi)-\frac{\Lambda}{3}E^x\right), \tag{123}$$

while that of (118) is given by

$$m = \frac{\sqrt{E^x}}{2}\left(1+\frac{\bar{\lambda}^2}{\lambda^2}\left(\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}-\left(\frac{(E^x)'}{2E^\varphi}\right)^2\cos^2(\bar{\lambda}K_\varphi)\right)-\frac{\Lambda}{3}E^x\right). \tag{124}$$

D. General modified constraint

We will now derive a general modified constraint in spherical symmetry that depends on the canonical fields for gravity and scalar matter with up to second order in spatial derivatives. There are no additional phase-space degrees of freedom that could represent higher time derivatives. We are therefore working at the classical order of derivatives, seen from a viewpoint of effective field theory, and yet we will find that general relativity minimally coupled to a scalar field is not the only solution of our conditions. Within spherical symmetry, there is therefore a difference between manifestly covariant space-time actions of gravity and scalar matter, and the larger class of covariant canonical theories. Moreover, the uniqueness results of [32] in vacuum and their extensions to matter fields in [33–36], derived like ours in a Hamiltonian formulation, are based on implicit assumptions, in particular that the spatial part of a space-time metric is one of the canonical configuration fields. In our analysis, we have eliminated these assumptions and obtain a larger class of admissible theories.

1. Second-order constraints

Based on past models considered for instance in [5,13,14], we consider the following ansatz for a Hamiltonian constraint that, together with the classical diffeomorphism constraint, (79), has anomaly-free hypersurface-deformation brackets for the spherically symmetric theory with scalar field coupling,

$$
\begin{aligned}
H = a &+ ((E^x)')^2 e_{xx} + (E^x)'(E^\varphi)' e_{x\varphi} + (E^x)'' e_{2x} \\
&+ (E^x)' K_\varphi' c_{x\varphi} + (E^\varphi)' K_\varphi' c_{\varphi\varphi} + ((E^\varphi)')^2 e_{\varphi\varphi} \\
&+ e_{2\varphi}(E^\varphi)'' + c_{2\varphi} K_\varphi'' + (\phi')^2 f_{\phi\phi} + (E^x)'\phi' f_{x\phi} \\
&+ (E^\varphi)'\phi' f_{\varphi\phi}. \qquad (125)
\end{aligned}
$$

The free functions a, e_i, c_i, and f_i have spatial density weight zero and depend on the basic phase-space degrees of freedom. The covariance conditions (93) and (95) have already ruled out spatial derivatives of K_x and P_ϕ in the Hamiltonian constraint. For second-order field equations, the constraint must be linear in any second-order derivative terms of the remaining fields, E^x, E^φ, K_φ.

We do not include a term with ϕ'', also here modeling the classical derivative order of standard scalar field theories, and we do not include coupling terms between spatial derivatives of the scalar field and those of K_φ. There may be covariant theories that include such terms, but the relevant equations become rather intractable. One conceptual difficulty of including a ϕ''-term is that this variable then becomes indistinguishable from E^x in the general second-order constraint and in the covariance conditions that prohibit derivatives of their momenta (in contrast to K_φ). Omitting this term allows us to have a well-defined distinction between gravitational and matter degrees of freedom in a modified theory.

The dependence on first-order derivatives may in principle be higher-order or even nonpolynomial, but the specific form is restricted by the condition that H have density weight zero. The main higher-order or nonpolynomial dependence on spatial derivatives to be expected is a dependence on the ratio $(E^x)'/E^\varphi$, which has density weight zero. The free functions in (125) may therefore depend on this ratio. Since previous results in vacuum showed that the modified structure function in nonclassical models depends on this expression, it turns out to be convenient to parametrize a dependence on $(E^x)'/E^\varphi$ as a dependence on the future structure function q^{xx}, or alternatively as a dependence on the quantity $\sqrt{q_{xx}} = 1/\sqrt{q^{xx}}$ which is required to have spatial density weight one. We will therefore include $\sqrt{q_{xx}}$ among the canonical fields K_x, E^φ and P_ϕ of density weight one. For now, a dependence on $\sqrt{q_{xx}}$ parametrizes a dependence on first-order spatial derivatives, but by evaluating the consistency conditions we will simultaneously be solving for $\sqrt{q_{xx}}$ as a phase-space function.

2. Anomaly-freedom of the bracket $\{H, H_x\}$

We first compute the bracket $\{H[N], H_x[N^x]\}$ where, as we recall,

$$H_x = E^\varphi K_\varphi' - K_x (E^x)' + P_\phi \phi' \qquad (126)$$

remains classical, and put it in the form

$$\{H[N], H_x[N^x]\} = \int \mathrm{d}x\, N^x [N\mathcal{F}_0 + N'\mathcal{F}_1 + N''\mathcal{F}_2 + N'''\mathcal{F}_3], \qquad (127)$$

using integration by parts to avoid derivatives of N^x. For this expression to match (83b) we set $\mathcal{F}_0 = \mathcal{F}_2 = \mathcal{F}_3 = 0$ and $\mathcal{F}_1 + H = 0$. Since all the functions in the Hamiltonian constraint (125) are independent of spatial derivatives of the phase-space variables, each term in these equations multiplying derivatives must vanish independently.

The term $\mathcal{F}_3 = 0$ implies

$$e_{2\varphi} = 0. \qquad (128)$$

The term $\mathcal{F}_2 = 0$ can be separated into the following derivative terms, which must vanish independently:

$$K_\varphi' :\ c_{2\varepsilon} = 0, \qquad (129)$$

$$\phi' :\ f_{\varphi\phi} = 0, \qquad (130)$$

$$(E^x)' e_{2x} = -E^\varphi e_{x\varphi}, \qquad (131)$$

$$(E^\varphi)' :\ e_{\varphi\varphi} = 0. \qquad (132)$$

Using these results, the term $\mathcal{F}_1 + H = 0$ can be separated into derivatives, each of which must again vanish independently (where $0^{\rm th}$ means no derivatives):

$$0^{\rm th} :\ a = \sqrt{q_{xx}} \frac{\partial a}{\partial \sqrt{q_{xx}}} + P_\phi \frac{\partial a}{\partial P_\phi} + K_x \frac{\partial a}{\partial K_x} + E^\varphi \frac{\partial a}{\partial E^\varphi}, \qquad (133)$$

$$(E^x)' K_\varphi' :\ c_{x\varphi} = -\sqrt{q_{xx}} \frac{\partial c_{x\varphi}}{\partial \sqrt{q_{xx}}} - P_\phi \frac{\partial c_{x\varphi}}{\partial P_\phi} - K_x \frac{\partial c_{x\varphi}}{\partial K_x} - E^\varphi \frac{\partial c_{x\varphi}}{\partial E^\varphi}, \qquad (134)$$

$$((E^x)')^2\colon\ e_{xx} = -\sqrt{q_{xx}}\frac{\partial e_{xx}}{\partial\sqrt{q_{xx}}} - P_\phi\frac{\partial e_{xx}}{\partial P_\phi} - K_x\frac{\partial e_{xx}}{\partial K_x} - E^\varphi\frac{\partial e_{xx}}{\partial E^\varphi}, \tag{135}$$

$$(E^x)'(E^\varphi)'\colon\ 2e_{x\varphi} = -\sqrt{q_{xx}}\frac{\partial c_{x\varphi}}{\partial\sqrt{q_{xx}}} - P_\phi\frac{\partial c_{x\varphi}}{\partial P_\phi} - K_x\frac{\partial c_{x\varphi}}{\partial K_x} - E^\varphi\frac{\partial c_{x\varphi}}{\partial E^\varphi}, \tag{136}$$

$$(E^x)'\phi'\colon\ f_{x\phi} = -\sqrt{q_{xx}}\frac{\partial f_{x\phi}}{\partial\sqrt{q_{xx}}} - P_\phi\frac{\partial f_{x\phi}}{\partial P_\phi} - K_x\frac{\partial f_{x\phi}}{\partial K_x} - E^\varphi\frac{\partial f_{x\phi}}{\partial E^\varphi}, \tag{137}$$

$$(E^x)'\phi'\colon\ f_{\phi\phi} = -\sqrt{q_{xx}}\frac{\partial f_{\phi\phi}}{\partial\sqrt{q_{xx}}} - P_\phi\frac{\partial f_{\phi\phi}}{\partial P_\phi} - K_x\frac{\partial f_{\phi\phi}}{\partial K_x} - E^\varphi\frac{\partial f_{\phi\phi}}{\partial E^\varphi}, \tag{138}$$

$$K_\varphi''\colon\ 2c_{\varphi\varphi} = -\sqrt{q_{xx}}\frac{\partial c_{\varphi\varphi}}{\partial\sqrt{q_{xx}}} - P_\phi\frac{\partial c_{\varphi\varphi}}{\partial P_\phi} - K_x\frac{\partial c_{\varphi\varphi}}{\partial K_x} - E^\varphi\frac{\partial c_{\varphi\varphi}}{\partial E^\varphi}. \tag{139}$$

These equations are derived from Poisson brackets, separating terms according to derivative orders. We do not know the phase-space function $\sqrt{q_{xx}}$ at this point, and it does not have an obvious momentum. Derivatives by $\sqrt{q_{xx}}$ therefore do not follow from basic Poisson brackets, but they are nevertheless uniquely determined because we are computing a Poisson bracket with the diffeomorphism constraint. The fact that $\sqrt{q_{xx}}$ has spatial density weight one, as determined by its geometrical role in hypersurface deformations, then implies the Poisson-bracket terms as used here, where $\sqrt{q_{xx}}$ appears in the same way as the basic phase-space variables of density weight one.

Thus,

$$a = -\frac{\sqrt{E^x}}{2}E^\varphi g A\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{140}$$

$$e_{xx} = -\frac{\sqrt{E^x}}{2}\frac{1}{E^\varphi}gE_{xx}\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{141}$$

$$e_{x\varphi} = -\frac{\sqrt{E^x}}{2}\frac{1}{(E^\varphi)^2}g\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{142}$$

$$c_{x\varphi} = -\frac{\sqrt{E^x}}{2}\frac{1}{E^\varphi}gC_{x\varphi}\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{143}$$

$$f_{\phi\phi} = -\frac{\sqrt{E^x}}{2}\frac{1}{E^\varphi}gF_{\phi\phi}\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{144}$$

$$f_{x\phi} = -\frac{\sqrt{E^x}}{2}\frac{1}{E^\varphi}gF_{x\phi}\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P^*_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right), \tag{145}$$

$$c_{\varphi\varphi} = -\frac{\sqrt{E^x}}{2}\frac{1}{(E^\varphi)^2}gC_{\varphi\varphi}\left(\frac{\sqrt{E^x q_{xx}}}{E^\varphi}, \frac{P_\phi}{E^\varphi}, \frac{K_x}{E^\varphi}\right). \tag{146}$$

For later convenience, it turns out to be useful to include a factor of the function g from $e_{x\varphi}$ in the remaining functions, which all have the same general dependence. In addition to the dependence on phase-space variables with density weight one, all free functions are at this point allowed to have an unrestricted dependence on the variables E^x, K_φ and ϕ with density weight zero. A factor of $-\sqrt{E^x}/2$, matching the classical limit, has been extracted in each function for later convenience. Using this, the term $\mathcal{F}_0 = 0$ is satisfied automatically.

3. Anomaly freedom of the bracket $\{H, H\}$

The analysis of the bracket of two Hamiltonian constraints can be split into parts, first removing any term that does not obey the hypersurface-deformation form and would therefore be anomalous, and then analyzing the remaining terms in order to derive the structure function. We begin with the removal of anomalous terms, but already at this stage the covariance condition is useful because it implies that $\{q_{xx}, H[N]\}$ does not depend on derivatives of N and therefore does not contrinute to $\{H[N], H[M]\}$ thanks to antisymmetry in (N, M). (The combination $\sqrt{E^x q_{xx}}/E^\varphi$ in some of our modification functions does contribute to the Poisson bracket, but only because it depends on E^φ and there may be terms in the modified Hamiltonian with derivatives of K_φ.)

Computing the bracket $\{H[N], H[M]\}$, it can be put in the form

$$\begin{aligned}\{H[N], H[M]\} &= \int \mathrm{d}x[(NM' - MN')\mathcal{G}_0 \\ &\quad + (NM'' - MN'')\mathcal{G}_1 + (NM''' - MN''')\mathcal{G}_2] \\ &= \int \mathrm{d}x[(NM' - MN')(\mathcal{G}_0 - \mathcal{G}_1' + (NM''' \\ &\quad - MN''')\mathcal{G}_2)],\end{aligned} \tag{147}$$

where we used several integrations by parts. For this to match (83c) we must set $\mathcal{G}_2 = 0$ and $\mathcal{G} \equiv \mathcal{G}_0 - \mathcal{G}_1' = H_r q^{xx}$ for some function q^{xx} of density weight -2.

The equation $\mathcal{G}_2 = 0$ implies $C_{\varphi\varphi} = 0$. Any terms in $\mathcal{G}$ that do not contain K'_φ, $(E^x)'$, or ϕ' cannot contribute to reproducing H_x. These terms are

$$\mathcal{G} \supset G_0 + G^\phi P'_\phi + G^x K'_x + G_\varphi (E^\varphi)' + G_{2x}(E^x)'' + G_{3x}(E^x)''' + G_{2x\varphi}(E^x)''(E^\varphi)' + G^\phi_{2x}(E^x)'' P'_\phi + G^x_{2x}(E^x)'' K'_x, \tag{148}$$

which must all vanish in order to obtain an anomaly-free bracket of hypersurface-deformation form. It turns out that the equations implied by each of these terms being zero are not all independent, and only four independent ones remain,

$$G_{3x} = 0\colon\ \frac{\partial g}{\partial(K_x/E^\varphi)} = 0, \tag{149}$$

$$G^x = 0\colon\ -\frac{\partial A}{\partial(K_x/E^\varphi)}\frac{\partial g}{\partial(K_x/E^\varphi)} + g\frac{\partial^2 A}{(\partial(K_x/E^\varphi))^2} = 0, \tag{150}$$

$$G^\phi = 0\colon\ -\frac{\partial A}{\partial(K_x/E^\varphi)}\frac{\partial g}{\partial(P_\phi/E^\varphi)} + \frac{\partial A^x}{\partial(P_\phi/E^\varphi)} = 0, \tag{151}$$

$$G_\varphi = 0\colon\ \frac{\partial A^x}{\partial(\sqrt{q_{xx}}E^x/E^\varphi)} = 0. \tag{152}$$

Their solution is given by

$$g = g\left(E^x, \phi, K_\varphi, \frac{\sqrt{E^x}}{E^\varphi}\sqrt{q_{xx}}, \frac{P_\phi}{E^\varphi}\right), \tag{153}$$

$$A = A_0\left(E^x, \phi, K_\varphi, \frac{\sqrt{E^x}}{E^\varphi}\sqrt{q_{xx}}, \frac{P_\phi}{E^\varphi}\right) + \frac{K_x}{E^\varphi} f_1(E^x, \phi, K_\varphi), \tag{154}$$

with a new function $f_1(E^x, \phi, K_\varphi)$ defined as the coefficient of K_x/E^φ in A. With these results, the remaining anomalous terms vanish automatically, and we can continue with the analysis of structure-function terms.

The remaining nonzero terms in $\mathcal{G}$ contain either K'_φ, $(E^x)'$, or ϕ', but they must be of the right form in order to contribute to reproducing the diffeomorphism constraint. They are

$$\begin{aligned}
\mathcal{G} = {}& (G^\varphi E^\varphi K'_\varphi - G_x K_x (E^x)' + G_\phi P_\phi \phi')\frac{1}{(E^\varphi)^2} + (G_{(xx)}{}^\varphi E^\varphi K'_\varphi - G_{(xx)}{}_x K_x (E^x)' + G_{(xx)}{}^\phi P_\phi \phi')\frac{((E^x)')^2}{(E^\varphi)^4}\\
&+ (G_{(\phi\phi)}{}^\varphi E^\varphi K'_\varphi - G_{(\phi\phi)}{}_x K_x (E^x)' + G_{(\phi\phi)}{}^\phi P_\phi \phi')\frac{(\phi')^2}{(E^\varphi)^4} + (G_{(2x)}{}^\varphi E^\varphi (K_\varphi)' - G_{(2x)}{}_x K_x (E^x)'\\
&+ G_{(2x)}{}_\phi P_\phi \phi')\frac{(E^x)''}{(E^\varphi)^4} + (-G_{(2\phi)}{}_x K_x (E^x)' + G_{(2\phi)}{}_\phi P_\phi \phi')\frac{\phi''}{(E^\varphi)^4}\\
&- G^{(2\varphi)}{}_x K_x (E^x)'\frac{K''_\varphi}{(E^\varphi)^4} + (G^{(\varphi\varphi)}{}_x E^\varphi K'_\varphi + G^\varphi_{x\phi} P_\phi \phi')\frac{(E^x)' K'_\varphi}{(E^\varphi)^6}\\
&+ [(G^{(\phi)}{}_{\varphi x} K'_\varphi + G^{(\phi)}{}_{\phi x}\phi' + G^{(\phi)}{}_{xx}(E^x)')(E^x)' + G^{(\phi)}{}_{\phi\phi}(\phi')^2]\frac{P'_\phi}{(E^\varphi)^6}\\
&+ [(G_{(\varphi)}{}^\varphi_x K'_\varphi + G_{(\varphi)}{}_{\phi x}\phi' + G_{(\varphi)}{}_{xx}(E^x)')(E^x)' + G_{(\varphi)}{}_{\phi\phi}(\phi')^2]\frac{(E^\varphi)'}{(E^\varphi)^6}\\
&+ [(G^{(x)}{}_{\varphi x} K'_\varphi + G^{(x)}{}_{\phi x}\phi' + G^{(x)}{}_{xx}(E^x)')(E^x)' + G^{(x)}{}_{\phi\phi}(\phi')^2]\frac{K'_x}{(E^\varphi)^6}\\
&+ ((G_{(q)}{}^\varphi_x K'_\varphi + G_{(q)}{}_{\phi x}\phi' + G_{(q)}{}_{xx}(E^x)')(E^x)' + G_{(q)}{}_{\phi\phi}(\phi')^2)(\sqrt{q_{xx}})'.
\end{aligned} \tag{155}$$

Any terms multiplying K''_φ and ϕ'', given by

$$G^{(2\varphi)}{}_x = \frac{E^x}{4} g^2 \frac{E^\varphi}{K_x}\frac{\partial C_{x\varphi}}{\partial(K_x/E^\varphi)}, \tag{156}$$

$$G_{(2\phi)}{}_x = \frac{E^x}{4} g^2 \frac{E^\varphi}{K_x}\frac{\partial F_{x\phi}}{\partial(K_x/E^\varphi)}, \tag{157}$$

$$G_{(2\phi)\phi} = -\frac{E^x}{4} g^2 \frac{E^\varphi}{P_\phi} \frac{\partial F_{\phi\phi}}{\partial(K_x/E^\varphi)}, \tag{158}$$

must each vanish independently, implying that $C_{x\varphi}$, $F_{x\phi}$, and $F_{\phi\phi}$ are independent of K_x/E^φ. The only nontrivial term multiplying P'_ϕ is then $G^{(\phi)}{}_{xx}$, and it must vanish,

$$\frac{\partial C_{x\varphi}}{\partial(P_\phi/E^\varphi)} + \frac{\partial^2 E_{xx}}{\partial(K_x/E^\varphi)\partial(P_\phi/E^\varphi)} = 0. \tag{159}$$

Using all the above results, we obtain the following conditions. All the terms multiplying K'_x trivialize, except for $G^{(x)}{}_{xx}$ which must vanish and implies.

$$\frac{\partial^2 E_{xx}}{\partial(K_x/E^\varphi)^2} = 0. \tag{160}$$

All the terms multiplying $(E^\varphi)'$ then trivialize, except for $G_{(\varphi)x\phi}$ and $G_{(\varphi)xx}$, which now must vanish. The former implies

$$0 = \frac{\partial g}{\partial(P_\phi/E^\varphi)} \tag{161}$$

and we will soon return to the latter. The term $G^{(\varphi\varphi)}{}_\phi$ then trivializes, while the nontrivial equation $G^{(\varphi\varphi)}{}_x = 0$ implies

$$\frac{\partial^2 E_{xx}}{\partial(K_x/E^\varphi)\partial(P_\phi/E^\varphi)} = 0. \tag{162}$$

Using this result in (159) we obtain that $C_{x\varphi}$ is independent of P_ϕ.

Continuing using these results in the remaining equations, all terms multiplying $(\sqrt{q_{xx}})'$ trivialize, except for $G_{(q)xx}$ which must vanish and implies

$$\frac{\partial C_{x\varphi}}{\partial(\sqrt{q_{xx}E^x}/E^\varphi)} + \frac{\partial^2 E_{xx}}{\partial(K_x/E^\varphi)\partial(\sqrt{q_{xx}E^x}/E^\varphi)} = 0. \tag{163}$$

All terms multiplying $(E^x)''$ and $(E^\varphi)'$ then trivialize, except for $G_{(2x)x}$ and $G_{(\varphi)xx}$ which must both vanish but imply the same equation,

$$C_{x\varphi} \frac{\sqrt{q_{xx}E^x}}{E^\varphi} \frac{\partial \ln g}{\partial(\sqrt{q_{xx}}E^x/E^\varphi)} + C_{x\varphi} + \frac{\partial \ln g}{\partial K_\varphi} + 2\frac{\partial E_{xx}}{\partial(K_x/E^\varphi)} = 0. \tag{164}$$

Finally, the term $G_{(\phi\phi)}{}^\varphi$ trivializes, while the nontrivial equations from $G_{(\phi\phi)}{}^\phi$ and $G_{(\phi\phi)x}$ now imply

$$\frac{\partial F_{\phi\phi}}{\partial(P_\phi/E^\varphi)} = 0, \tag{165}$$

and

$$0 = C_{x\varphi} \frac{\sqrt{q_{xx}E^x}}{E^\varphi} \frac{\partial F_{\phi\phi}}{\partial(\sqrt{q_{xx}}E^x/E^\varphi)} - 2F_{\phi\phi} \frac{\partial F_{x\phi}}{\partial(P_\phi/E^\varphi)} - 2F_{\phi\phi} \frac{\partial E_{xx}}{\partial(K_x/E^\varphi)} + \frac{\partial F_{\phi\phi}}{\partial K_\varphi}, \tag{166}$$

respectively.

The structure function can now be obtained from

$$\begin{aligned} q^{xx} &= \frac{G^\varphi}{(E^\varphi)^2} + G_{(\phi\phi)}{}^\varphi \frac{((E^x)')^2}{(E^\varphi)^4} \\ &= \frac{E^x}{4(E^\varphi)^2} g^2 \left(\frac{\partial f_1}{\partial K_\varphi} - C_{x\varphi} f_1 + \frac{((E^x)')^2}{(E^\varphi)^2} \left(-C_{x\varphi}{}^2 \left(1 + \sqrt{q_{xx}} \frac{\sqrt{E^x}}{E^\varphi} \frac{\partial \ln g}{\partial(\sqrt{q_{xx}E^x}/E^\varphi)} \right) \right.\right. \\ &\quad \left.\left. - C_{x\varphi} \left(\sqrt{q_{xx}} \frac{\sqrt{E^x}}{E^\varphi} \frac{\partial C_{x\varphi}}{\partial(\sqrt{q_{xx}E^x}/E^\varphi)} + \frac{\partial \ln g}{\partial K_\varphi} + \frac{\partial E_{xx}}{\partial(K_x/E^\varphi)} \right) + \frac{\partial^2 E_{xx}}{\partial K_\varphi \partial(K_x/E^\varphi)} \right) \right). \end{aligned} \tag{167}$$

This function is composed of the free functions g, $C_{x\varphi}$, f_1, and $\partial E_{xx}/\partial(K_x/E^\varphi)$. Its inverse q_{xx} appeared in some of the original dependences allowed for free functions, except for f_1 which was introduced in (154) as a function independent of q_{xx} as a consequence of anomaly-freedom. For the sake of simplicity, we will assume that the remaining functions that determine q^{xx}, given by g, $C_{x\varphi}$, and $\partial E_{xx}/\partial(K_x/E^\varphi)$, cannot independently depend on the structure function itself or its inverse.

This assumption turns (167) into an explicit equation for the structure function, which simplifies to

$$q^{xx} = \frac{G^{\varphi}}{(E^{\varphi})^2} + G_{(\phi\phi)}{}^{\varphi}\frac{((E^x)')^2}{(E^{\varphi})^4}$$
$$= \frac{E^x g^2}{4(E^{\varphi})^2}\left(\frac{\partial f_1}{\partial K_{\varphi}} - C_{x\varphi} f_1 + \frac{((E^x)')^2}{(E^{\varphi})^2}\left(\frac{\partial^2 E_{xx}}{\partial K_{\varphi}\partial(K_x/E^{\varphi})} - C_{x\varphi}\left(C_{x\varphi} + \frac{\partial \ln g}{\partial K_{\varphi}} + \frac{\partial E_{xx}}{\partial(K_x/E^{\varphi})}\right)\right)\right). \tag{168}$$

Equation (163) for anomaly freedom now trivializes, while (164) simplifies to

$$0 = C_{x\varphi} + \frac{\partial \ln g}{\partial K_{\varphi}} + 2\frac{\partial E_{xx}}{\partial(K_x/E^{\varphi})}. \tag{169}$$

Combining the latter with (162) and (165), we find that

$$\frac{\partial^2 F_{x\phi}}{\partial(P_{\phi}/E^{\varphi})^2} = 0. \tag{170}$$

As a summary so far, the Hamiltonian constraint is of the form

$$H = -\frac{\sqrt{E^x}}{2}\bar{g}\left[E^{\varphi}\left(A_0 + \frac{K_x}{E^{\varphi}}\bar{f}_1\right) + \frac{((E^x)')^2}{E^{\varphi}}E_{xx} + \frac{(E^x)'(E^{\varphi})'}{(E^{\varphi})^2} - \frac{(E^x)''}{E^{\varphi}} + \frac{(E^x)'K_{\varphi}'}{E^{\varphi}}\bar{C}_{x\varphi} + \frac{(\phi')^2}{E^{\varphi}}F_{\phi\phi} + \frac{(E^x)'\phi'}{E^{\varphi}}F_{x\phi}\right], \tag{171}$$

where we use a bar on $\bar{g} = g$, $\bar{f}_1 = f_1$, $\bar{E}_{xx} = E_{xx}$, and $\bar{C}_{x\varphi} = C_{x\varphi}$ in order to indicate that these functions (and any other free function with a bar) may depend on E^x, ϕ, and K_{φ} but not on $\sqrt{q_{xx}E^x}/E^{\varphi}$. Any unbarred free function is allowed to depend also on $\sqrt{q_{xx}E^x}/E^{\varphi}$. We use the same convention in the expansions

$$A_0 = f_0 + \frac{P_{\phi}}{E^{\varphi}}h_0 + \frac{P_{\phi}{}^2}{(E^{\varphi})^2}f_3, \tag{172}$$

$$E_{xx} = f_2 + \frac{K_x}{E^{\varphi}}\bar{h} + \frac{P_{\phi}}{E^{\varphi}}h_1 + \frac{P_{\phi}{}^2}{(E^{\varphi})^2}h_2, \tag{173}$$

$$F_{\phi\phi} = f_4, \tag{174}$$

$$F_{x\phi} = h_3 + \frac{P_{\phi}}{E^{\varphi}}h_4, \tag{175}$$

of some of the coefficient functions in the Hamiltonian constraint, observing conditions implied by anomaly freedom. (While A_0 and E_{xx} are so far allowed to have higher powers of P_{ϕ}/E^{φ}, the remaining equations for anomaly freedom, to be analyzed in the following section, imply that they must vanish.) With these expansions, we have four functions, $\bar{g}$, $\bar{C}_{x\varphi}$, $\bar{f}_1$, and $\bar{h}$, depending only on E^x, ϕ, and K_{φ}, and nine functions, f_0, f_2, f_3, f_4, and h_i, $i = 0, \ldots, 4$, depending on E^x, ϕ, K_{φ}, and $\sqrt{q_{xx}E^x}/E^{\varphi}$. Anomaly freedom requires that these functions satisfy the equations,

$$0 = \bar{C}_{x\varphi}\frac{\sqrt{E^x}}{E^{\varphi}}\sqrt{q_{xx}}\frac{\partial f_4}{\partial(\sqrt{q_{xx}E^x}/E^{\varphi})} - 2f_4(h_4 + \bar{h}) + \frac{\partial f_4}{\partial K_{\varphi}}, \tag{176}$$

$$0 = \bar{C}_{x\varphi} + \frac{\partial \ln \bar{g}}{\partial K_{\varphi}} + 2\bar{h}. \tag{177}$$

In order to proceed, it is convenient to apply suitable canonical transformations in order to eliminate some of the free functions.

4. Canonical transformations I

The constraint (171) was shown in [5] to fully determine the vacuum theory by completely factoring out canonical transformations that preserve the diffeomorphism constraint. Here, we generalize the set of diffeomorphism-preserving canonical transformations to include the scalar field,

$$\phi = f_c^{\phi}(E^x, \tilde{\phi}), \quad P_{\phi} = \tilde{P}_{\phi}\left(\frac{\partial f_c^{\phi}}{\partial\tilde{\phi}}\right)^{-1} - \tilde{E}^{\varphi}\frac{\partial f_c^{\varphi}}{\partial\tilde{\phi}}\left(\frac{\partial f_c^{\varphi}}{\partial\tilde{K}_{\varphi}}\right)^{-1}, \tag{178a}$$

$$K_{\varphi} = f_c^{\varphi}(E^x, \tilde{\phi}, \tilde{K}_{\varphi}), \qquad E^{\varphi} = \tilde{E}^{\varphi}\left(\frac{\partial f_c^{\varphi}}{\partial\tilde{K}_{\varphi}}\right)^{-1}, \tag{178b}$$

$$K_x = \frac{\partial(\alpha_c^2 E^x)}{\partial E^x}\tilde{K}_x + \tilde{E}^\varphi \frac{\partial f_c^\varphi}{\partial E^x}\left(\frac{\partial f_c^\varphi}{\partial \tilde{K}_\varphi}\right)^{-1} + \tilde{P}_\phi \frac{\partial f_c^\phi}{\partial E^x}\left(\frac{\partial f_c^\phi}{\partial \tilde{\phi}}\right)^{-1},$$

$$\tilde{E}^x = \alpha_c^2(E^x)E^x, \tag{178c}$$

where the new phase-space variables are written with a tilde. A transformation with $f_c^\phi = \tilde{\phi}$, $f_c^\varphi = \tilde{K}_\varphi$, and $\alpha_c = \alpha_c(E^x)$ can always be used to transform the angular component of the metric from a potentially modified $q_{\vartheta\vartheta}(E^x)$ to its classical expression $\tilde{E}^x$. If we fix the classical form for this component, the residual canonical transformations are given by (178) with $\alpha_c = 1$. Following [5], we can use a canonical transformation with $f_c^\phi = \tilde{\phi}$, and a function $f_c^\varphi(E^x, \tilde{\phi}, \tilde{K}_\varphi)$ such that the transformed $\bar{C}_{x\varphi}(E^x, \tilde{\phi}, \tilde{K}_\varphi)$ vanishes. In the following, we will assume that we have applied this canonical transformation, setting $\bar{C}_{x\varphi} = 0$. Equations (176) and (177) for anomaly freedom then simplify to

$$\frac{\partial f_4}{\partial K_\varphi} = -2f_4(h_4 + \bar{h}), \tag{179}$$

$$\bar{h} = -\frac{1}{2}\frac{\partial \ln \bar{g}}{\partial K_\varphi}, \tag{180}$$

and the structure function turns into

$$q^{xx} = \left(\frac{1}{4}\frac{\partial \bar{f}_1}{\partial K_\varphi} - \frac{1}{2}\left(\frac{(E^x)'}{2E^\varphi}\right)^2 \frac{\partial \ln \bar{g}}{\partial K_\varphi^2}\right)\bar{g}^2 \frac{E^x}{(E^\varphi)^2}. \tag{181}$$

The residual canonical transformations that preserve both $q_{\vartheta\vartheta} = E^x$ and $\bar{C}_{x\varphi} = 0$ are

$$\phi = f_c^\phi(E^x, \tilde{\phi}), \qquad P_\phi = \tilde{P}_\phi\left(\frac{\partial f_c^\phi}{\partial \tilde{\phi}}\right)^{-1} - \frac{\tilde{E}^\varphi}{f_x^\varphi}\left(\frac{\partial f_x^\varphi}{\partial \tilde{\phi}}\tilde{K}_\varphi - \frac{\partial \tilde{\mu}_\varphi}{\partial \tilde{\phi}}\right), \tag{182a}$$

$$K_\varphi = f_x^\varphi(E^x, \phi)\tilde{K}_\varphi - \tilde{\mu}_\varphi(E^x, \phi), \qquad E^\varphi = \tilde{E}^\varphi / f_x^\varphi, \tag{182b}$$

$$K_x = \tilde{K}_x + \frac{\tilde{E}^\varphi}{f_x^\varphi}\left(\frac{\partial f_x^\varphi}{\partial E^x}\tilde{K}_\varphi - \frac{\partial \tilde{\mu}_\varphi}{\partial E^x}\right) + \tilde{P}_\phi \frac{\partial f_c^\phi}{\partial E^x}\left(\frac{\partial f_c^\phi}{\partial \tilde{\phi}}\right)^{-1}, \qquad \tilde{E}^x = E^x. \tag{182c}$$

5. Expansion by the scalar momentum

In order to complete the conditions for anomaly-freedom, the remaining undetermined functions must reproduce all terms in the diffeomorphism constraint,

$$\begin{aligned}\mathcal{G} &= (G^\varphi + G_{(xx)}{}^\varphi((E^x)')^2)K_\varphi' + (G_x + G_{(xx)}{}_x((E^x)')^2)(E^x)' + (G_\phi + G_{(xx)}{}_\phi((E^x)')^2)\phi' \\ &=: \mathcal{G}^\varphi E^\varphi K_\varphi' - \mathcal{G}_x K_x (E^x)' + \mathcal{G}_\phi P_\phi \phi' \\ &=: q^{xx} H_r.\end{aligned} \tag{183}$$

Thus, the undetermined functions must satisfy the equations $\mathcal{G}^\varphi = \mathcal{G}_x$ and $\mathcal{G}^\varphi = \mathcal{G}_\phi$. Because they are all independent of P_ϕ, an expansion of the relevant equations in this variable will be useful, in which each power P_ϕ must vanish independently.

We first note that the nontrivial terms in the expansion are $\mathcal{G} = Q^0 + Q^\phi P_\phi + Q^{\phi\phi} {P_\phi}^2/(E^\varphi)^2$, where

$${P_\phi}^2 Q^{\phi\phi} = {P_\phi}^2 \frac{E^x}{2}\frac{(E^x)'}{E^\varphi}\left[\bar{g}\frac{\partial(\bar{g}f_3)}{\partial K_\varphi} - 2\bar{g}f_3\bar{g}h_4 + 2\bar{g}\bar{f}_1\bar{g}h_2 + \frac{((E^x)')^2}{(E^\varphi)^2}\left(\bar{g}\frac{\partial(\bar{g}h_2)}{\partial K_\varphi} - \bar{g}h_2\left(2\bar{g}h_4 + \frac{\partial \bar{g}}{\partial K_\varphi}\right)\right)\right] = 0, \tag{184}$$

must vanish, as it cannot contribute to the diffeomorphism constraint.

The expansion of the condition $\mathcal{G}^\varphi = \mathcal{G}_x$ gives the equations,

$$\begin{aligned}0 = {}& \bar{g}h_0\bar{g}h_3 - \bar{g}\bar{f}_1\left(2\bar{g}f_2 + \frac{\partial \bar{g}}{\partial E^x}\right) + g\left(\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x} - \frac{\partial(\bar{g}f_0)}{\partial K_\varphi}\right) \\ &+ \frac{((E^x)')^2}{(E^\varphi)^2}\left(-\bar{g}\frac{\partial(\bar{g}f_2)}{\partial K_\varphi} + \bar{g}f_2\frac{\partial \bar{g}}{\partial K_\varphi} + \bar{g}h_1\bar{g}h_3 - \bar{g}^2\frac{1}{2}\frac{\partial}{\partial E^x}\frac{\partial \ln \bar{g}}{\partial K_\varphi}\right)\end{aligned} \tag{185}$$

and

$$0 = P_\phi \left[-\bar{g} \frac{\partial(\bar{g}h_0)}{\partial K_\varphi} - 2\bar{g}\bar{f}_1\bar{g}h_1 + 2\bar{g}f_3\bar{g}h_3 + \bar{g}h_0\bar{g}h_4 + \frac{((E^x)')^2}{(E^\varphi)^2} \left(-\bar{g} \frac{\partial(\bar{g}h_1)}{\partial K_\varphi} + 2\bar{g}h_2\bar{g}h_3 + \bar{g}h_1 \left(\bar{g}h_4 + \frac{\partial \bar{g}}{\partial K_\varphi} \right) \right) \right]. \tag{186}$$

The expansion of the condition $\mathcal{G}^\varphi = \mathcal{G}_\phi$ gives the equations,

$$0 = 2\bar{g}f_4\bar{g}h_0 - \bar{g}\bar{f}_1 \left(\bar{g}h_3 + \frac{\partial \bar{g}}{\partial \phi} \right) + \bar{g} \frac{\partial(\bar{g}\bar{f}_1)}{\partial \phi} + \frac{((E^x)')^2}{(E^\varphi)^2} \left(-\bar{g} \frac{\partial(\bar{g}h_3)}{\partial K_\varphi} + 2\bar{g}f_4\bar{g}h_1 + \bar{g}h_3 \left(\bar{g}h_4 + \frac{1}{2} \frac{\partial \bar{g}}{\partial K_\varphi} \right) - \bar{g}^2 \frac{1}{2} \frac{\partial^2 \ln \bar{g}}{\partial \phi \partial K_\varphi} \right) \tag{187}$$

and

$$\begin{aligned} 0 = P_\phi \Bigg[& -\bar{g} \frac{\partial(\bar{g}\bar{f}_1)}{\partial K_\varphi} + 4\bar{g}f_3\bar{g}f_4 + \bar{g}\bar{f}_1 \left(-\bar{g}h_4 + \frac{\partial \bar{g}}{\partial K_\varphi} \right) \\ & + \frac{((E^x)')^2}{(E^\varphi)^2} \left(-\bar{g} \frac{\partial(\bar{g}h_4)}{\partial K_\varphi} + \bar{g}h_4 \left(\bar{g}h_4 + \frac{1}{2} \frac{\partial \bar{g}}{\partial K_\varphi} \right) + 4\bar{g}f_4\bar{g}h_2 + \frac{1}{2}\bar{g}^2 \frac{\partial^2 \ln \bar{g}}{\partial K_\varphi^2} \right) \Bigg]. \end{aligned} \tag{188}$$

We keep the P_ϕ factor in the previous equations because it helps us to identify which equations must be neglected in the vacuum limit, $\phi, P_\phi \to 0$. Anomaly-freedom is then ensured by Eqs. (179), (180), and (184)–(188).

6. Expansion by the structure function

In order to implement the classical-matter limit in the modified constraint, we will use an expansion by the structure function in the coefficients f_3 and f_4 relevant to the scalar equations of motion,

$$f_3 = \bar{f}_3 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{f}_3^q, \tag{189}$$

$$f_4 = \bar{f}_4 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{f}_4^q, \tag{190}$$

where, as before, we write a bar on some functions to indicate that they are independent of q^{xx}. We use the structure function rather than its inverse that appeared in previous equations, such that $E^\varphi \sqrt{q^{xx}}$ has spatial density weight zero. This expansion is useful because $\bar{f}_3^q$ and $\bar{f}_4^q$ will be responsible for obtaining the classical-matter limit, while $\bar{f}_3$ and $\bar{f}_4$ allow us to explore alternative theories. There can be no higher-order terms in $\sqrt{q^{xx}}$ because the product of two such functions, one from $H[N]$ and one from $H[M]$ in a Poisson bracket of two Hamiltonian constraints, must give us a single factor of q^{xx} in the hypersurface-deformation bracket.

We perform the same expansion by the structure function for the remaining functions,

$$f_0 = \frac{\sqrt{q_{xx}E^x}}{E^\varphi} \bar{f}_{0q} + \bar{f}_0 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{f}_0^q, \tag{191}$$

$$f_2 = \bar{f}_2 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{f}_2^q, \tag{192}$$

$$h_0 = \bar{h}_0 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{h}_0^q, \tag{193}$$

$$h_1 = \bar{h}_1 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{h}_1^q, \tag{194}$$

$$h_2 = \bar{h}_2 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{h}_2^q, \tag{195}$$

$$h_3 = \bar{h}_3 + E^\varphi \frac{\sqrt{q^{xx}}}{\sqrt{E^x}} \bar{h}_3^q, \tag{196}$$

$$h_4 = \bar{h}_4, \tag{197}$$

where we have chosen the expansion coefficients according to what they multiply in the constraints. The function f_0 is the only one with a $\sqrt{q_{xx}}$ term, suitable for a measure of radial integration, because no other function can reproduce the potential term of the Klein–Gordon constraint in the classical-matter limit. The function h_2 contains a $\sqrt{q^{xx}}$ term because it multiplies P_ϕ^2, just as f_3 and f_4. Equation (179) implies that h_4 cannot have any structure-function term, hence $h_4 = \bar{h}_4$: The left-hand side is linear in a derivative of f_4 by K_φ and is therefore at most linear in $\sqrt{q^{xx}}$. The right-hand side multiplies f_4 by h_4, which can be at most linear in $\sqrt{q^{xx}}$ only if h_4 does not depend on $\sqrt{q^{xx}}$. (The same equation shows that $\bar{f}_4^q$ must depend on K_φ if it is nonzero.) For the sake of generality, we have expanded the remaining functions f_2, h_0, h_1, and h_3 by including a zeroth-order term and a linear term in $\sqrt{q^{xx}}$.

We will proceed by substituting these expansions into the conditions (179) and (184)–(188) for anomaly-freedom, taking into account that cross-terms multiplying q^{xx} may mix the zeroth-order terms and linear terms in $((E^x)')^2$, and that the functions f_i must be nonzero because they are responsible for reproducing the complete classical limit.

Condition (179) can be rewritten as a combination of two equations,

$$\frac{\partial(\bar{g}\bar{f}_4)}{\partial K_\varphi} = 2\bar{g}\bar{f}_4\bar{h}_4, \tag{198}$$

$$\frac{\partial(\bar{g}\bar{f}_4^q)}{\partial K_\varphi} = 2\bar{g}\bar{f}_4^q\bar{h}_4. \tag{199}$$

Condition (184) becomes

$$0 = \bar{g}\left(\frac{\partial(\bar{g}\bar{f}_3)}{\partial K_\varphi} - 2\bar{g}\bar{f}_3\bar{h}_4 + 2\bar{g}\bar{f}_1\bar{h}_2\right) + \bar{g}E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(\frac{\partial(\bar{g}\bar{f}_3^q)}{\partial K_\varphi} - 2\bar{g}\bar{f}_3^q\bar{h}_4 + 2\bar{g}\bar{f}_1\bar{h}_2^q\right)$$
$$+ \bar{g}^2\frac{((E^x)')^2}{(E^\varphi)^2}\left(\frac{\partial\bar{h}_2}{\partial K_\varphi} - 2\bar{h}_2\bar{h}_4 + E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(\frac{\partial\bar{h}_2^q}{\partial K_\varphi} - 2\bar{g}\bar{h}_2^q\bar{h}_4\right)\right) \tag{200}$$

and Eq. (185) is turned into

$$0 = -\bar{g}\frac{\sqrt{q_{xx}E^x}}{E^\varphi}\frac{\partial(\bar{g}\bar{f}_{0q})}{\partial K_\varphi} - \bar{g}\frac{\partial(\bar{g}\bar{f}_0)}{\partial K_\varphi} + \bar{g}\bar{h}_0\bar{g}\bar{h}_3 - 2\bar{g}\bar{f}_1\bar{g}\bar{f}_2 - \bar{g}\bar{f}_1\frac{\partial\bar{g}}{\partial E^x} + \bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x} + \frac{1}{4}\bar{g}^2\frac{\partial\bar{f}_1}{\partial K_\varphi}\bar{g}\bar{h}_0^q\bar{g}\bar{h}_3^q$$
$$+ E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(-\bar{g}\frac{\partial(\bar{g}\bar{f}_0^q)}{\partial K_\varphi} - 2\bar{g}\bar{f}_1\bar{g}\bar{f}_2^q + \bar{g}\bar{h}_0^q\bar{g}\bar{h}_3 + \bar{g}\bar{h}_0\bar{g}\bar{h}_3^q\right)$$
$$+ \frac{((E^x)')^2}{(E^\varphi)^2}\left(-\bar{g}\frac{\partial(\bar{g}\bar{f}_2)}{\partial K_\varphi} + \bar{g}\bar{f}_2\frac{\partial\bar{g}}{\partial K_\varphi} - \bar{g}^2\frac{1}{2}\frac{\partial}{\partial E^x}\frac{\partial\ln\bar{g}}{\partial K_\varphi} + \bar{g}\bar{h}_1\bar{g}\bar{h}_3 - \frac{1}{8}\bar{g}^2\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2}\bar{g}\bar{h}_0^q\bar{g}\bar{h}_3^q\right.$$
$$\left. + E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(-\bar{g}\frac{\partial(\bar{g}\bar{f}_2^q)}{\partial K_\varphi} + \bar{g}\bar{f}_2^q\frac{\partial\bar{g}}{\partial K_\varphi} + \bar{g}\bar{h}_1^q\bar{g}\bar{h}_3 + \bar{g}\bar{h}_1\bar{g}\bar{h}_3^q\right) + \frac{(E^\varphi)^2}{E^x}q^{xx}\bar{g}\bar{h}_1^q\bar{g}\bar{h}_3^q\right), \tag{201}$$

where we have used (181).

Equation (186) now reads

$$0 = P_\phi\left[-\bar{g}\frac{\partial(\bar{g}\bar{h}_0)}{\partial K_\varphi} - 2\bar{g}\bar{f}_1\bar{g}\bar{h}_1 + \bar{g}\bar{h}_0\bar{g}\bar{h}_4 + 2\bar{g}\bar{f}_3\bar{g}\bar{h}_3 + \frac{1}{2}\bar{g}^2\frac{\partial\bar{f}_1}{\partial K_\varphi}\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3^q\right.$$
$$+ E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(-\bar{g}\frac{\partial(\bar{g}\bar{h}_0^q)}{\partial K_\varphi} - 2\bar{g}\bar{f}_1\bar{g}\bar{h}_1^q + \bar{g}\bar{h}_0^q\bar{g}\bar{h}_4 + 2\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3 + 2\bar{g}\bar{f}_3\bar{g}\bar{h}_3^q\right)$$
$$+ \frac{((E^x)')^2}{(E^\varphi)^2}\left(-\bar{g}\frac{\partial(\bar{g}\bar{h}_1)}{\partial K_\varphi} + 2\bar{g}\bar{h}_2\bar{g}\bar{h}_3 + \bar{g}\bar{h}_1\left(\bar{g}\bar{h}_4 + \frac{\partial\bar{g}}{\partial K_\varphi}\right) - \frac{1}{4}\bar{g}^2\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2}\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3^q\right.$$
$$\left.\left. + E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(-\bar{g}\frac{\partial(\bar{g}\bar{h}_1^q)}{\partial K_\varphi} + 2\bar{g}\bar{h}_2^q\bar{g}\bar{h}_3 + 2\bar{g}\bar{h}_2\bar{g}\bar{h}_3^q + \bar{g}\bar{h}_1^q\left(\bar{g}\bar{h}_4 + \frac{\partial\bar{g}}{\partial K_\varphi}\right)\right) + \frac{(E^\varphi)^2}{E^x}q^{xx}2\bar{g}\bar{h}_2^q\bar{g}\bar{h}_3^q\right)\right], \tag{202}$$

where we have used (181), and Eq. (187) becomes

$$0 = \bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial\phi} - \bar{g}\bar{f}_1\left(\bar{g}\bar{h}_3 + \frac{\partial\bar{g}}{\partial\phi}\right) + 2\bar{g}\bar{h}_0\bar{g}\bar{f}_4 + \frac{1}{2}\bar{g}^2\frac{\partial\bar{f}_1}{\partial K_\varphi}\bar{g}\bar{h}_0^q\bar{g}\bar{f}_4^q + E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}(2\bar{g}\bar{h}_0\bar{g}\bar{f}_4^q + 2\bar{g}\bar{h}_0^q\bar{g}\bar{f}_4 - \bar{g}\bar{f}_1\bar{g}\bar{h}_3^q)$$
$$+ \frac{((E^x)')^2}{(E^\varphi)^2}\left(-\bar{g}\frac{\partial(\bar{g}\bar{h}_3)}{\partial K_\varphi} + \bar{g}\bar{h}_3\left(\bar{g}\bar{h}_4 + \frac{1}{2}\frac{\partial\bar{g}}{\partial K_\varphi}\right) + 2\bar{g}\bar{h}_1\bar{g}\bar{f}_4 - \bar{g}^2\frac{1}{2}\frac{\partial^2\ln\bar{g}}{\partial\phi\partial K_\varphi} - \frac{1}{4}\bar{g}^2\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2}\bar{g}\bar{h}_0^q\bar{g}\bar{f}_4^q\right.$$
$$\left. + E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}\left(-\bar{g}\frac{\partial(\bar{g}\bar{h}_3^q)}{\partial K_\varphi} + \bar{g}\bar{h}_3^q\left(\bar{g}\bar{h}_4 + \frac{1}{2}\frac{\partial\bar{g}}{\partial K_\varphi}\right) + 2\bar{g}\bar{h}_1\bar{g}\bar{f}_4^q + 2\bar{g}\bar{h}_1^q\bar{g}\bar{f}_4\right) + (E^\varphi)^2\frac{q^{xx}}{E^x}2\bar{g}\bar{h}_1^q\bar{g}\bar{f}_4^q\right), \tag{203}$$

where we have used (181). Finally, Eq. (188) appears as

$$
\begin{aligned}
0 = P_\phi\Bigg[&-\bar{g}^2\frac{\partial\bar{f}_1}{\partial K_\varphi}(1-\bar{g}\bar{f}_3^q\bar{g}\bar{f}_4^q)+4\bar{g}\bar{f}_3\bar{g}\bar{f}_4-\bar{g}\bar{f}_1\bar{g}\bar{h}_4+4E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}(\bar{g}\bar{f}_3\bar{g}\bar{f}_4^q+\bar{g}\bar{f}_3^q\bar{g}\bar{f}_4)\\
&+\frac{((E^x)')^2}{(E^\varphi)^2}\Bigg(-\bar{g}\frac{\partial(\bar{g}\bar{h}_4)}{\partial K_\varphi}+\bar{g}\bar{h}_4\left(\bar{g}\bar{h}_4+\frac{1}{2}\frac{\partial\bar{g}}{\partial K_\varphi}\right)+4\bar{g}\bar{h}_2\bar{g}\bar{f}_4+\frac{1}{2}\bar{g}^2\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2}(1-\bar{g}\bar{f}_3^q\bar{g}\bar{f}_4^q)\\
&+4E^\varphi\frac{\sqrt{q^{xx}}}{\sqrt{E^x}}(\bar{g}\bar{h}_2\bar{g}\bar{f}_4^q+\bar{g}\bar{h}_2^q\bar{g}\bar{f}_4)+4\frac{(E^\varphi)^2}{E^x}q^{xx}\bar{g}\bar{h}_2^q\bar{g}\bar{f}_4^q\Bigg)\Bigg],
\end{aligned}
\tag{204}
$$

where we have used (181).

Only the $\sqrt{q_{xx}E^x}$ term in (201) can be readily solved at this stage,

$$\bar{g}\bar{f}_{0q} = -\lambda_0^2 V_q, \tag{205}$$

where V_q and λ_0 are undetermined functions of E^x and ϕ. This function represents the freedom to choose a potential for a scalar field on an emergent spacetime.

Equations (198)–(204) are the whole anomaly-freedom equations left, and their zeroth orders as well as linear orders in $\sqrt{q^{xx}}$, $((E^x)')^2$, $((E^x)')^2\sqrt{q^{xx}}$, and $((E^x)')^2 q^{xx}$ must all vanish separately. Due to the complexity of these equations, they cannot be solved exactly, and we must rely on a number of principles to simplify them further. The first and primary such principle is covariance.

7. Covariance

The covariance condition imposed on the structure function (181) is trivial, except for the first-order derivative term in the gauge function. This condition has one term independent of spatial derivatives of the phase-space variables, and another term multiplying $((E^x)')^2$. Because the on shell condition cannot mix these two terms, they must vanish independently, such that the covariance condition is satisfied off the constraint surface (while the equations of motion are still being used in order to compare time-derivative terms). The two equations implied by the covariance condition are

$$0 = \frac{\partial^3\ln\bar{g}}{\partial K_\varphi^3}+\frac{\partial\ln\bar{g}}{\partial K_\varphi}\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2} \tag{206}$$

and

$$0 = \frac{\partial^2\ln g}{\partial K_\varphi^2}f_1-2\frac{\partial\ln g}{\partial K_\varphi}\frac{\partial f_1}{\partial K_\varphi}-\frac{\partial^2 f_1}{\partial K_\varphi^2}. \tag{207}$$

They have the general solutions,

$$
\begin{aligned}
\bar{g} &= \lambda_0\cos^2(\lambda(K_\varphi+\mu_\varphi)),\\
\bar{g}\bar{f}_1 &= 4\lambda_0\left(c_f\frac{\sin(2\lambda(K_\varphi+\mu_\varphi))}{2\lambda}+q\cos(2\lambda(K_\varphi+\mu_\varphi))\right),
\end{aligned}
\tag{208}
$$

recovering the classical limit for $\lambda,\mu_\varphi,q\to 0$, and $\lambda_0, c_f\to 1$.

8. Canonical transformations II

It is now convenient to employ the residual canonical transformation (182). To simplify the anomaly-freedom equations we will perform the canonical transformation,

$$
\begin{aligned}
&\phi\to\phi,\quad P_\phi\to P_\phi+E^\varphi\left(\frac{\partial\ln\lambda}{\partial\phi}K_\varphi+\frac{\lambda}{\bar{\lambda}}\frac{\partial\mu_\varphi}{\partial\phi}\right),\\
&K_\varphi\to\frac{\bar{\lambda}}{\lambda}K_\varphi-\mu_\varphi,\quad E^\varphi\to\frac{\lambda}{\bar{\lambda}}E^\varphi,\\
&K_x\to K_x-E^\varphi\left(\frac{\partial\ln\lambda}{\partial E^x}K_\varphi+\frac{\lambda}{\bar{\lambda}}\frac{\partial\mu_\varphi}{\partial E^x}\right),\quad E^x\to E^x,
\end{aligned}
\tag{209}
$$

with constant $\bar{\lambda}$, and we redefine the undetermined functions so as to absorb the λ and μ_φ factors. As was shown in [5], this particular canonical transformations renders the constraint periodic in K_φ. Any nonperiodic modification and the freedom of nonconstant λ as coefficient of K_φ in trigonometric functions can then be recovered by inverting the canonical transformation once the anomaly-freedom equations have been solved.

Thus, in the new phase-space coordinates we have

$$\bar{g} = \lambda_0\cos^2(\bar{\lambda}K_\varphi), \tag{210}$$

$$\bar{g}\bar{f}_1 = 4\lambda_0\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+q\cos(2\bar{\lambda}K_\varphi)\right), \tag{211}$$

recovering the classical limit for $\bar{\lambda}, q\to 0$, and $\lambda_0, c_f\to 1$. The structure function (181) can now be explicitly obtained,

$$
\begin{aligned}
q^{xx} = &\left(\left(c_f+\left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi)-2q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\lambda_0^2\\
&\times\frac{E^x}{(E^\varphi)^2}.
\end{aligned}
\tag{212}
$$

This still leaves the freedom of a final residual canonical transformation preserving periodicity, which takes the form

$$\phi = f_c^{\phi}(E^x, \tilde{\phi}), \qquad P_\phi = \tilde{P}_\phi \left(\frac{\partial f_c^{\phi}}{\partial \tilde{\phi}}\right)^{-1},$$
$$K_\varphi = \tilde{K}_\varphi, \qquad E^\varphi = \tilde{E}^\varphi,$$
$$K_x = \tilde{K}_x + \tilde{P}_\phi \frac{\partial f_c^{\phi}}{\partial E^x}\left(\frac{\partial f_c^{\phi}}{\partial \tilde{\phi}}\right)^{-1}, \qquad \tilde{E}^x = E^x. \tag{213}$$

Unlike the effects of the previous canonical transformations, which had already been understood in the vacuum case [5], this last residual canonical transformation of the matter variable remains to be factored out and fully interpreted. We will do so after solving the anomaly-freedom equations in the remainder of this section.

Equations (198)–(204) for anomaly-freedom are hard to solve exactly. We will thus rely on the principles described in Sec. III to simplify their solutions. These principles will differentiate between three classes of constraints which we will obtain in the following subsections. The first class of constraints is given by those compatible with the classical-matter limit, the second class by those compatible with the limit of reaching the classical constraint surface, and the third one by having a dynamical solution free of singularities. For now, we will look for possible restrictions from the remaining principles.

9. Vacuum limit

The vacuum limit is given by $\phi, P_\phi \to 0$, and in the anomaly-freedom equations one has to further take $\partial_\phi g, \partial_\phi f_1, h_i, f_3, f_4 \to 0$ wherever such terms survive. Equations (198)–(204) for anomaly-freedom then reduce to

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_0)}{\partial K_\varphi} = -2\bar{g}\bar{f}_1\bar{g}\bar{f}_2 - \bar{g}\bar{f}_1\frac{\partial \bar{g}}{\partial E^x} + \bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x}, \tag{214}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_0^q)}{\partial K_\varphi} = -2\bar{g}\bar{f}_1\bar{g}\bar{f}_2^q, \tag{215}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_2)}{\partial K_\varphi} = \bar{g}\bar{f}_2\frac{\partial \bar{g}}{\partial K_\varphi} - \bar{g}^2\frac{1}{2}\frac{\partial}{\partial E^x}\frac{\partial \ln \bar{g}}{\partial K_\varphi}, \tag{216}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_2^q)}{\partial K_\varphi} = \bar{g}\bar{f}_2^q\frac{\partial \bar{g}}{\partial K_\varphi}, \tag{217}$$

which can all be solved exactly,

$$\bar{g}\bar{f}_0 = \lambda_0\left(\frac{\alpha_0}{E^x} + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(c_f\frac{\alpha_2}{E^x} + 2\frac{\partial c_f}{\partial E^x}\right) + 2\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(q\frac{\alpha_2}{E^x} + 2\frac{\partial q}{\partial E^x}\right)\right), \tag{218}$$

$$\bar{g}\bar{f}_0^q = \frac{\alpha_{0q}}{E^x} + \frac{\alpha_{2q}}{E^x}\left(c_f\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + 2q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right), \tag{219}$$

$$\bar{g}\bar{f}_2 = -\frac{\alpha_2}{4E^x}\lambda_0\cos^2(\bar{\lambda}K_\varphi), \tag{220}$$

$$\bar{g}\bar{f}_2^q = -\frac{\alpha_{2q}}{4E^x}\cos^2(\bar{\lambda}K_\varphi). \tag{221}$$

The general vacuum Hamiltonian constraint is

$$\begin{aligned} H = {}& \lambda_0^2\frac{E^x}{2}\sqrt{q_{xx}}V_q - \frac{E^\varphi}{2}\sqrt{q^{xx}}\left[E^\varphi\left(\frac{\alpha_{0q}}{E^x} + \frac{\alpha_{2q}}{E^x}\left(c_f\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + 2q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\right) - \frac{((E^x)')^2}{E^\varphi}\frac{\alpha_{2q}}{4E^x}\cos^2(\bar{\lambda}K_\varphi)\right] \\ & - \lambda_0\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\alpha_0}{E^x} + \left(c_f\frac{\alpha_2}{E^x} + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + 2\left(q\frac{\alpha_2}{E^x} + 2\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + 4\frac{K_x}{E^\varphi}\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + q\cos(2\bar{\lambda}K_\varphi)\right)\right)\right. \\ & \left. + \frac{((E^x)')^2}{E^\varphi}\left(-\frac{\alpha_2}{4E^x}\cos^2(\bar{\lambda}K_\varphi) + \bar{\lambda}^2\frac{K_x}{E^\varphi}\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) + \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right], \end{aligned} \tag{222}$$

with structure function

$$q^{xx} = \left(\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi) - 2q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\lambda_0^2\frac{E^x}{(E^\varphi)^2}, \tag{223}$$

where V_q, α_i, and α_{iq} are undetermined functions of E^x.

10. Existence of a gravitational observable

The vacuum constraint (222) admits a Dirac observable $\mathcal{D}$ only if $\delta_\epsilon \mathcal{D} = \mathcal{D}_H H + \mathcal{D}_x H_x$, where $\mathcal{D}_H$ and $\mathcal{D}_x$ depend on the phase-space variables and on the gauge function ϵ. We consider the dependence $\mathcal{D}(E^x, K_\varphi, (E^x)'/E^\varphi, (E^\varphi)^2 q^{xx}/E^x)$ and require that this expression has the classical mass observable as a limit.

The condition for a Dirac observable can then be rewritten as

$$\begin{aligned}\mathcal{O} &= \frac{\partial\mathcal{D}}{\partial E^x}\delta_\epsilon E^x + \frac{\partial\mathcal{D}}{\partial K_\varphi}\delta_\epsilon K_\varphi + \frac{\partial\mathcal{D}}{\partial z}\delta_\epsilon z + \frac{\partial\mathcal{D}}{\partial\beta}\delta_\epsilon\beta - \mathcal{D}_H H - \mathcal{D}_x H_x\\ &= \left(\frac{\partial\mathcal{D}}{\partial E^x} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial E^x}\right)\delta_\epsilon E^x + \left(\frac{\partial\mathcal{D}}{\partial K_\varphi} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial K_\varphi}\right)\delta_\epsilon K_\varphi + \left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\delta_\epsilon z - \mathcal{D}_H H - \mathcal{D}_x H_x = 0, \end{aligned}\tag{224}$$

where $z = (E^x)'/E^\varphi$ and $\beta = (E^\varphi)^2 q^{xx}/E^x$, and each partial derivative is taken by leaving the rest of the variables constant. (Thus, $\partial\mathcal{D}/\partial E^x$ does not act on the dependence of $\mathcal{D}$ on z and β.)

The condition $\mathcal{O} = 0$ can be analyzed by derivative conditions. For example, the derivative terms $\partial\mathcal{O}/\partial(E^\varphi)' = \partial\mathcal{O}/\partial(E^x)'' = 0$, which are both proportional to the overall factor in the Hamiltonian constraint, determine the coefficient $\mathcal{D}_H$ in terms of the observable $\mathcal{D}$,

$$\mathcal{D}_H = \frac{2\epsilon^x}{\sqrt{E^x}\lambda_0\cos^2(\lambda K_\varphi)}\left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right). \tag{225}$$

The derivative term $\partial\mathcal{O}/\partial(\epsilon^0)'$ does not have the necessary phase-space dependence to contribute to either H or H_x, so it must vanish independently and implies,

$$0 = \left(\frac{\partial\mathcal{D}}{\partial K_\varphi} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial K_\varphi}\right)\cos^2(\bar\lambda K_\varphi)z + \left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\left((4c_f + \bar\lambda^2 z^2)\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + 4q\cos(2\bar\lambda K_\varphi)\right). \tag{226}$$

Using this condition, we can obtain the coefficient $\mathcal{D}_x$ from the derivative term $\partial\mathcal{O}/\partial K_\varphi' = 0$,

$$\begin{aligned}\mathcal{D}_x &= \left(\frac{\partial\mathcal{D}}{\partial K_\varphi} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial K_\varphi}\right)\left(\frac{\epsilon^x}{E^\varphi} - \lambda_0\epsilon^0\frac{\sqrt{E^x}}{(E^\varphi)^2}\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}z\right)\\ &\quad + \left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\lambda_0\epsilon^0\frac{\sqrt{E^x}}{2(E^\varphi)^2}\left((4c_f + \bar\lambda^2 z^2)\cos(2\bar\lambda K_\varphi) - 16q\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}\right)\\ &= \frac{1}{z}\left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\left[\lambda_0\epsilon^0\frac{\sqrt{E^x}}{2(E^\varphi)^2}z\left((4c_f + \bar\lambda^2 z^2)\cos(2\bar\lambda K_\varphi) - 16q\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}\right)\right.\\ &\quad \left. - \sec^2(\bar\lambda K_\varphi)\left((4c_f + \bar\lambda^2 z^2)\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + 4q\cos(2\bar\lambda K_\varphi)\right)\left(\frac{\epsilon^x}{E^\varphi} - \lambda_0\epsilon^0\frac{\sqrt{E^x}}{(E^\varphi)^2}\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}z\right)\right]. \end{aligned}\tag{227}$$

With these results, the dependence of the condition $\mathcal{O} = 0$ on z (independently of the intrinsic dependence of $\mathcal{D}$, $\mathcal{D}_H$, $\mathcal{D}_x$, and $\sqrt{q^{xx}}$ on z) is polynomial up to order z^2. Therefore, we consider an expression for the observable of the form $\mathcal{D} = \mathcal{D}_0 + \mathcal{D}_1 z + \mathcal{D}_2 z^2$, with $\mathcal{D}_i = \mathcal{D}_i(E^x, K_\varphi)$ for $i = 0$, 1, 2, and then expand $\mathcal{O} = 0$ in z with highest order z^3. In addition, $\mathcal{O} = 0$ can be expanded in powers of $\sqrt{\beta}$ and K_x, which should vanish independently. The terms in $\mathcal{O} = 0$ proportional to K_x are

$$\begin{aligned}0 &= \left(\frac{\partial\mathcal{D}}{\partial K_\varphi} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial K_\varphi}\right)\lambda_0\epsilon^0\frac{\sqrt{E^x}}{E^\varphi}\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}z^2 - \left(\frac{\partial\mathcal{D}}{\partial z} + \frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\lambda_0\epsilon^0\frac{\sqrt{E^x}}{2E^\varphi}z\left((4c_f + \bar\lambda^2 z^2)\cos(2\bar\lambda K_\varphi) - 16q\bar\lambda^2\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}\right)\\ &\quad + \mathcal{D}_H\lambda_0\frac{\sqrt{E^x}}{2}\left((4c_f + \bar\lambda^2 z^2)\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + 4q\cos(2\bar\lambda K_\varphi)\right) + z\mathcal{D}_x E^\varphi, \end{aligned}\tag{228}$$

the vanishing of which is implied by (225)–(227).

We next expand $\mathcal{O}$ in powers of β, independently of the intrinsic dependence of $\mathcal{D}$ on β, giving

$$\mathcal{O} = \frac{\mathcal{D}^\beta}{\sqrt{\beta}} + \sqrt{\beta}\mathcal{D}_\beta + \mathcal{D}_0, \tag{229}$$

where

$$\mathcal{D}^{\beta} \propto \left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\left[\frac{\epsilon^0}{z}A_{-1}+\epsilon^x A_0+\epsilon^0 A_1 z+\epsilon^0 A_3 z^3+\epsilon^0 A_5 z^5\right], \tag{230}$$

$$\mathcal{D}_{\beta} \propto \left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\left[\frac{\epsilon^0}{z}B_{-1}+\epsilon^0 B_1 z\right], \tag{231}$$

and

$$\mathcal{D}_0 \propto \frac{\epsilon^0}{z}C_{-1}+\left(\frac{\partial\mathcal{D}}{\partial E^x}\epsilon^0 C_0^x+\left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\epsilon^x C_0^z\right)+\left(\frac{\partial\mathcal{D}}{\partial E^x}\epsilon^x C_1^x+\left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\epsilon^0 C_1^z\right)z$$
$$+\left(\frac{\partial\mathcal{D}}{\partial E^x}\epsilon^0 C_2^x+\left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\epsilon^x C_2^z\right)z^2+\left(\frac{\partial\mathcal{D}}{\partial z}+\frac{\partial\mathcal{D}}{\partial\beta}\frac{\partial\beta}{\partial z}\right)\epsilon^0 z^3. \tag{232}$$

The functions A_i are in general complicated expressions of the undetermined functions of the phase-space variables. We find that no β-dependence of $\mathcal{D}$ can properly mix the $\mathcal{D}^{\beta}$, $\mathcal{D}_{\beta}$, and $\mathcal{D}_0$ such that $\mathcal{D}^{\beta}$ and $\mathcal{D}_{\beta}$ are nontrivial. Therefore, and since the classical limit requires $\mathrm{d}\mathcal{D}/\mathrm{d}z\neq 0$, we must have $A_i=B_i=0$ and take $\partial\mathcal{D}/\partial\beta=0$. We start with the simplest of these expressions.

Since the phase-space variables are nonvanishing off shell, we are interested only in the dependence of A_i and B_i on the undetermined functions in the constraint, with the condition that the undetermined functions with nonvanishing classical limit cannot be trivial. We then have

$$A_0 \propto V_q = 0, \tag{233}$$

$$A_5 \propto \alpha_{2q} = 0. \tag{234}$$

Using this, the other terms simplify to

$$A_{-1} \propto A_1 \propto A_3 \propto \alpha_{0q} = 0 \tag{235}$$

which implies that the B_i terms automatically vanish.

With $V_q=\alpha_{0q}=\alpha_{2q}=0$, the Hamiltonian constraint takes the form of the expression previously obtained for vacuum in [5]. The solution to $\mathcal{O}=0$ is then straightforward, giving

$$\mathcal{D}=d_0+\frac{d_2}{2}\left(\exp\int\mathrm{d}E^x\frac{\alpha_2}{2E^x}\right)\left(c_f\frac{\sin^2(\bar\lambda K_\varphi)}{\bar\lambda^2}+2q\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}-\cos^2(\bar\lambda K_\varphi)\left(\frac{(E^x)'}{2E^\varphi}\right)^2\right)+\frac{d_2}{4}\int\mathrm{d}E^x\left(\left(\Lambda_0+\frac{\alpha_0}{E^x}\right)\exp\int\mathrm{d}E^x\frac{\alpha_2}{2E^x}\right), \tag{236}$$

where d_0 and d_2 are constants with classical limit $d_0\to 0$ and $d_2\to 1$.

In what follows, we impose the condition that this observable be preserved in the vacuum limit, thus restricting (222) to the case where

$$V_q, \bar f_0^q, \bar f_2^q \underset{\phi\to 0}{\longrightarrow} 0. \tag{237}$$

(This restriction eliminates the possibility of using V_q to introduce a cosmological constant coupled to the emergent space-time metric.)

11. Existence of a matter observable, and residual canonical transformation

The general Hamiltonian constraint takes the form,

$$H=-\frac{\sqrt{E^x}}{2}\lambda_0\bar{\mathscr{g}}\left[E^\varphi\bar f_0+K_x\bar f_1+P_\phi\bar h_0+\frac{{P_\phi}^2}{E^\varphi}\bar f_3+\frac{((E^x)')^2}{E^\varphi}\left(\bar f_2+\frac{K_x}{E^\varphi}\bar h+\frac{P_\phi}{E^\varphi}\bar h_1+\frac{{P_\phi}^2}{(E^\varphi)^2}\bar h_2\right)\right.$$
$$\left.+\frac{(\phi')^2}{E^\varphi}\bar f_4+\frac{(E^x)'\phi'}{E^\varphi}\left(\bar h_3+\frac{P_\phi}{E^\varphi}\bar h_4\right)+\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right]$$
$$-\frac{\sqrt{E^x}}{2}\lambda_0\sqrt{\beta}\left[E^\varphi\bar g\bar f_0^q+P_\phi\bar g\bar h_0^q+\frac{{P_\phi}^2}{E^\varphi}\bar g\bar f_3^q+\frac{((E^x)')^2}{E^\varphi}\left(\bar g\bar f_2^q+\frac{P_\phi}{E^\varphi}\bar g\bar h_1^q+\frac{{P_\phi}^2}{(E^\varphi)^2}\bar g\bar h_2^q\right)\right.$$
$$\left.+\frac{(\phi')^2}{E^\varphi}\bar g\bar f_4^q+\frac{(E^x)'\phi'}{E^\varphi}\bar g\bar h_3^q\right]+\frac{\lambda_0^2}{2}E^x\sqrt{q_{xx}}V_q, \tag{238}$$

if we write $\bar g=\lambda_0\bar{\mathscr{g}}$ and $q^{xx}=\beta\lambda_0^2E^x/E^\varphi$. We now consider a slight generalization of the symmetry generator (122)

$$G[\alpha] = \int \mathrm{d}x\,\alpha\left(P_\phi \frac{\partial f_\phi}{\partial \phi} + E^\varphi \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} f_\varphi\right), \tag{239}$$

for undetermined functions $f_\phi(\phi, E^x)$ and $f_\varphi(\phi, E^x)$, and a constant α. A canonical transformation of the form (213) such that $f_c^\phi = f_\phi$ simplifies the symmetry generator,

$$G[\alpha] = \int \mathrm{d}x\,\alpha\left(P_\phi + E^\varphi \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial \ln \lambda}{\partial \phi}\right), \tag{240}$$

where we have rewritten the transformed f_φ as $\partial \ln\lambda/\partial\phi$ for some undetermined function $\lambda(\phi, E^x)$. We may also redefine the functions in the constraint (238) such that they now depend on these new versions. This step completes factoring out the diffeomorphism-preserving canonical transformations.

We now require that the smeared phase-space function (240) Poisson-commutes with the Hamiltonian constraint (238) on shell when $V_q = 0$. Defining $\delta_{G[\alpha]} \cdot \equiv \{\cdot, G[\alpha]\}$, we find that the bracket $\delta_{G[\alpha]} H[\epsilon^0]$ contains an $(E^x)''$ term. The rest of the terms can then be rearranged to complement this term into reproducing the Hamiltonian constraint, which vanishes on shell and need not be considered for the existence of a global matter symmetry. In practice, it is easier to subtract such a term and require that the rest vanish. We do this together with the expansion,

$$\delta_{G[\alpha]} H[\epsilon^0] - H[\epsilon^0]\delta_{G[\alpha]} \ln\left(\frac{\bar{g}}{E^\varphi}\right) = H^{(-1)}/\sqrt{\beta} + H^{(0)} + H^{(1)}\sqrt{\beta}, \tag{241}$$

where each term must vanish independently. Further using the fact that all the undetermined functions are independent of the phase-space variables K_x, E^φ, and P_ϕ with density weight one and of derivatives, all the subterms obtained from the expansion (241) must vanish independently. Thus, the first term being zero implies the equations,

$$0 = B^{(-1)} \bar{f}_0^q, \tag{242}$$

$$0 = B^{(-1)} \bar{f}_2^q, \tag{243}$$

$$0 = B^{(-1)} \bar{f}_3^q, \tag{244}$$

$$0 = B^{(-1)} \bar{f}_4^q, \tag{245}$$

$$0 = B^{(-1)} \bar{h}_0^q, \tag{246}$$

$$0 = B^{(-1)} \bar{h}_1^q, \tag{247}$$

$$0 = B^{(-1)} \bar{h}_2^q, \tag{248}$$

$$0 = B^{(-1)} \bar{h}_3^q, \tag{249}$$

where

$$\begin{aligned} B^{(-1)} &= \frac{\partial \beta}{\partial \phi} + \frac{\partial \ln \lambda}{\partial \phi}\left(\frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial \beta}{\partial K_\varphi} - E^\varphi \sec^2(\bar{\lambda} K_\varphi) \frac{\partial \beta}{\partial E^\varphi}\right) \\ &= \left(\frac{\partial c_f}{\partial \phi}\cos^2(\bar{\lambda} K_\varphi) - 2\frac{\partial q}{\partial \phi}\bar{\lambda}^2 \frac{\sin(2\bar{\lambda} K_\varphi)}{2\bar{\lambda}}\right) - \frac{\partial \ln \lambda^2}{\partial \phi}\bar{\lambda}^2 \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}}\left(c_f \frac{\sin(2\bar{\lambda} K_\varphi)}{2\bar{\lambda}} + q\cos(2\bar{\lambda} K_\varphi)\right) \\ &\quad + \frac{\partial \ln \lambda^2}{\partial \phi}\left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2 \cos^2(\bar{\lambda} K_\varphi). \end{aligned} \tag{250}$$

The last term $H^{(1)} = 0$ being zero implies the equations,

$$\frac{\partial(\bar{g}\bar{f}_0^q)}{\partial \phi} = \left(2\bar{g}\bar{f}_0^q - \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial(\bar{g}\bar{f}_0^q)}{\partial K_\varphi}\right)\frac{\partial \ln \lambda}{\partial \phi} + \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \bar{g}\bar{h}_0^q \frac{\partial^2 \ln \lambda}{\partial \phi^2}, \tag{251}$$

$$\frac{\partial(\bar{g}\bar{f}_2^q)}{\partial \phi} = -\left(2\bar{\lambda}^2 \frac{\tan^2(\bar{\lambda} K_\varphi)}{\bar{\lambda}^2}\bar{g}\bar{f}_2^q + \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial(\bar{g}\bar{f}_2^q)}{\partial K_\varphi}\right)\frac{\partial \ln \lambda}{\partial \phi} + \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \bar{g}\bar{h}_1^q \frac{\partial^2 \ln \lambda}{\partial \phi^2}, \tag{252}$$

$$\frac{\partial(\bar{g}\bar{f}_3^q)}{\partial \phi} = -\left(2\bar{\lambda}^2 \frac{\tan^2(\bar{\lambda} K_\varphi)}{\bar{\lambda}^2}\bar{g}\bar{f}_3^q + \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial(\bar{g}\bar{f}_3^q)}{\partial K_\varphi}\right)\frac{\partial \ln \lambda}{\partial \phi}, \tag{253}$$

$$\frac{\partial(\bar{g}\bar{f}_4^q)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{g}\bar{f}_4^q + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{g}\bar{f}_4^q)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{254}$$

$$\frac{\partial(\bar{g}\bar{h}_0^q)}{\partial\phi} = \left(\frac{\cos(2\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{g}\bar{h}_0^q - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{g}\bar{h}_0^q)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + 2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{g}\bar{f}_3^q\frac{\partial^2\ln\lambda}{\partial\phi^2}, \tag{255}$$

$$\frac{\partial(\bar{g}\bar{h}_1^q)}{\partial\phi} = -\left(\frac{1+2\sin^2(\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{g}\bar{h}_1^q + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{g}\bar{h}_1^q)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + 2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{g}\bar{h}_2^q\frac{\partial^2\ln\lambda}{\partial\phi^2}, \tag{256}$$

$$\frac{\partial(\bar{g}\bar{h}_2^q)}{\partial\phi} = -\left(2\frac{1+\sin^2(\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{g}\bar{h}_2^q + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{g}\bar{h}_2^q)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{257}$$

$$\frac{\partial(\bar{g}\bar{h}_3^q)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{g}\bar{h}_3^q + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{g}\bar{h}_3^q)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}. \tag{258}$$

The last term $H^{(0)}=0$ being zero implies the equations,

$$\frac{\partial(\bar{\not{g}}\bar{f}_0)}{\partial\phi} = \left(2\bar{\not{g}}\bar{f}_0 - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{f}_0)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{h}_0\frac{\partial^2\ln\lambda}{\partial\phi^2} - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{f}_1\frac{\partial^2\ln\lambda}{\partial\phi\partial E^x}, \tag{259}$$

$$\frac{\partial(\bar{\not{g}}\bar{f}_1)}{\partial\phi} = \left(\frac{\cos(2\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{\not{g}}\bar{f}_1 - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{f}_1)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{260}$$

$$\frac{\partial(\bar{\not{g}}\bar{f}_2)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{\not{g}}\bar{f}_2 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{f}_2)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{h}_1\frac{\partial^2\ln\lambda}{\partial\phi^2} + \cos^2(\bar{\lambda}K_\varphi)\frac{\partial^2\ln\lambda}{\partial\phi\partial E^x}, \tag{261}$$

$$\frac{\partial(\bar{\not{g}}\bar{f}_3)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{\not{g}}\bar{f}_3 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{f}_3)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{262}$$

$$\frac{\partial(\bar{\not{g}}\bar{f}_4)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{\not{g}}\bar{f}_4 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{f}_4)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{263}$$

$$\frac{\partial(\bar{\not{g}}\bar{h}_0)}{\partial\phi} = \left(\frac{\cos(2\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{\not{g}}\bar{h}_0 - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{h}_0)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + 2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{f}_3\frac{\partial^2\ln\lambda}{\partial\phi^2}, \tag{264}$$

$$\frac{\partial(\bar{\not{g}}\bar{h}_1)}{\partial\phi} = -\left(\frac{1+2\sin^2(\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{\not{g}}\bar{h}_1 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{h}_1)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + 2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{h}_2\frac{\partial^2\ln\lambda}{\partial\phi^2}, \tag{265}$$

$$\frac{\partial(\bar{\not{g}}\bar{h}_2)}{\partial\phi} = -\left(2\frac{1+\sin^2(\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{\not{g}}\bar{h}_2 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{h}_2)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi}, \tag{266}$$

$$\frac{\partial(\bar{\not{g}}\bar{h}_3)}{\partial\phi} = -\left(2\bar{\lambda}^2\frac{\tan^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\bar{\not{g}}\bar{h}_3 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial(\bar{\not{g}}\bar{h}_3)}{\partial K_\varphi}\right)\frac{\partial\ln\lambda}{\partial\phi} + \left(1 + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\bar{\not{g}}\bar{h}_4\right)\frac{\partial^2\ln\lambda}{\partial\phi^2}, \tag{267}$$

$$\frac{\partial(\bar{\not{g}}\bar{h}_4)}{\partial\phi} = \left(-2\frac{1+2\sin^2(\bar{\lambda}K_\varphi)}{\cos^2(\bar{\lambda}K_\varphi)}\bar{\not{g}}\bar{h}_4 - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left(\frac{\partial(\bar{\not{g}}\bar{h}_4)}{\partial K_\varphi} + 2\bar{\lambda}^2\right)\right)\frac{\partial\ln\lambda}{\partial\phi}. \tag{268}$$

The condition for the existence of the matter observable is thus highly nontrivial, leading to the set of equations (242)–(249) and (251)–(268). These are, however, too complicated to be solved completely, and yet not sufficient to fully restrict the form of the Hamiltonian constraint. In order to make progress, we continue to impose additional conditions.

12. Partial Abelianization

We apply the generalized techniques for partial Abelianization developed in [5] by simply including the new degree of freedom given by the scalar field. The procedure is identical to that of the earlier Sec. IV C up to the definition of the new structure function and using the modified constraint instead of the classical one.

We consider the following linear combination,

$$H^{(A)} = BH + AH_x \tag{269}$$

of the constraints, where A and $B \neq 0$ are so far undetermined phase-space functions, and H is the previous modified constraint. Reusing the definitions (97)–(102) for coefficients such as $\mathcal{A}^x$, now applied to the modified constraint, the structure function in the bracket of two $H^{(A)}$ is given by

$$q^{(A)} = B^2 q^{xx} + B\mathcal{A}^x. \tag{270}$$

Partial Abelianization is achieved by setting $q^{(A)} = 0$. Assuming the dependence $B = B(K_\varphi, E^x, \phi)$ and a constraint of the general form (238), we obtain

$$\begin{aligned} A &= \frac{\partial B}{\partial K_\varphi}\frac{\partial H}{\partial (E^\varphi)'} \\ &= -\frac{\sqrt{E^x}}{2}\lambda_0 \cos^2(\bar\lambda K_\varphi)\frac{\partial B}{\partial K_\varphi}\frac{(E^x)'}{(E^\varphi)^2} \end{aligned} \tag{271}$$

and

$$\begin{aligned} \mathcal{A}^x &= -\frac{\partial A}{\partial K_\varphi}\frac{\partial H}{\partial (E^\varphi)'} - \frac{\partial A}{\partial (E^x)'}\frac{\partial H}{\partial K_x} \\ &= -\lambda_0^2 \frac{E^x}{4}\frac{\cos^4(\bar\lambda K_\varphi)}{(E^\varphi)^2}\left[-\frac{\partial B}{\partial K_\varphi}\bar f_1 + \left(\frac{(E^x)'}{E^\varphi}\right)^2\left(\frac{\partial^2 B}{\partial K_\varphi^2} + \frac{3}{2}\frac{\partial B}{\partial K_\varphi}\frac{\partial \ln \bar g}{\partial K_\varphi}\right)\right] \\ &= -\lambda_0^2 E^x \frac{\cos^2(\bar\lambda K_\varphi)}{(E^\varphi)^2}\left[-\frac{\partial B}{\partial K_\varphi}\left(c_f \frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + q\cos(2\bar\lambda K_\varphi)\right) + \left(\frac{(E^x)'}{2E^\varphi}\right)^2\left(\frac{\partial^2 B}{\partial K_\varphi^2} - 3\bar\lambda^2 \frac{\partial B}{\partial K_\varphi}\frac{\tan(\bar\lambda K_\varphi)}{\bar\lambda}\right)\cos^2(\bar\lambda K_\varphi)\right]. \end{aligned} \tag{272}$$

Condition (270) for partial Abelianization, such that $q^{(A)} = 0$, then implies

$$\begin{aligned} 0 = &\left[B\left(c_f - 2q\bar\lambda^2 \frac{\tan(\bar\lambda K_\varphi)}{\bar\lambda}\right) - \frac{\partial B}{\partial K_\varphi}\left(c_f \frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + q\cos(2\bar\lambda K_\varphi)\right)\right]\cos^2(\bar\lambda K_\varphi) \\ &- \left(\frac{(E^x)'}{2E^\varphi}\right)^2\left(\frac{\partial^2 B}{\partial K_\varphi^2}\cos^2(\bar\lambda K_\varphi) + \bar\lambda^2 B - 3\bar\lambda^2 \frac{\partial B}{\partial K_\varphi}\frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda}\right)\cos^2(\bar\lambda K_\varphi). \end{aligned} \tag{273}$$

Since B is independent of $(E^x)'$, the two lines in this equation must vanish independently. The first line implies

$$B = \frac{\bar B}{\cos^2(\bar\lambda K_\varphi)}\left(c_f \frac{\sin(2\bar\lambda K_\varphi)}{2\bar\lambda} + q\cos(2\bar\lambda K_\varphi)\right), \tag{274}$$

where $\bar B$ is an undetermined function of E^x and ϕ. Substituting this result in the second line and demanding that it vanish, we obtain

$$\bar\lambda\, \bar B\, q \sec(\bar\lambda K_\varphi) = 0. \tag{275}$$

For a nontrivial Abelianization with nonzero $\bar\lambda$, this equation determines $q = 0$. The Abelianization coefficients are then

$$B^{(A)} = \bar B c_f \frac{\tan(\bar\lambda K_\varphi)}{\bar\lambda}, \qquad A^{(A)} = -\bar B \lambda_0 c_f \frac{\sqrt{E^x}}{2}\frac{(E^x)'}{(E^\varphi)^2}, \tag{276}$$

where we have included the superscript (A) in order to distinguish them from the previous coefficients in linear combinations. The coefficients (276) together with the condition that $q = 0$, implied by (275), Abelianize any constraint of the general form (238).

V. CLASSES OF CONSTRAINTS

There is a large number of free functions in the generic modified Hamiltonian constraint, subject to conditions that include coupled nonlinear differential equations. It is hard to solve these equations in complete generality, but several physically motivated conditions impose additional equations that can be used to simplify and solve the original restrictions on modification functions.

A. Constraints compatible with the classical-matter limit

A special class of modified constraints is given by those that recover classical matter behavior (on a modified background) in a certain limit. This requirement imposes additional conditions that can be used in order to solve for some of the free functions.

1. Anomaly freedom

In order to recover the Klein-Gordon Hamiltonian on a curved, emergent space-time, we must impose $\bar{f}_3^q \neq 0$ and $\bar{f}_4^q \neq 0$. Equations (244) and (245) then imply that the $B^{(-1)}$ factor (250) must vanish, which in turn implies that

$$\frac{\partial c_f}{\partial \phi} = \frac{\partial q}{\partial \phi} = \frac{\partial \lambda}{\partial \phi} = 0. \tag{277}$$

Hence, c_f, q, and λ can only depend on E^x. With these results, Eqs. (242)–(249) are trivially satisfied, while Eqs. (251)–(268) imply that $\bar{g}\bar{f}_0^q$ as well as $\bar{g}\bar{h}_j^q$, $\bar{f}_j$, and $\bar{h}_j$ for $j = 0, 1, 2, 3, 4$ must be independent of ϕ. Considering these conditions, the only undetermined function that is allowed to depend on ϕ is the global factor λ_0. Combined with the results for the existence of a gravitational vacuum observable, (237), we obtain

$$\bar{f}_{0q} = \bar{f}_0^q = \bar{f}_2^q = 0. \tag{278}$$

At this point, only the conditions for anomaly-freedom remain to be solved. The vanishing of the $((E^x)')^2 q^{xx}$ term in Eqs. (203) and (204) implies $\bar{h}_1^q = 0$ and $\bar{h}_2^q = 0$, respectively. The $((E^x)')^2\sqrt{q^{xx}}$ term in (204) then implies that $\bar{h}_2 = 0$. Five additional equations are derived from (200) and (204), implementing anomaly-freedom,

$$\frac{\partial(\bar{g}\bar{f}_3)}{\partial K_\varphi} = 2\bar{g}\bar{f}_3\bar{h}_4, \tag{279}$$

$$\frac{\partial(\bar{g}\bar{f}_3^q)}{\partial K_\varphi} = 2\bar{g}\bar{f}_3^q\bar{h}_4, \tag{280}$$

as well as

$$0 = P_\phi\left[-\bar{g}^2\frac{\partial \bar{f}_1}{\partial K_\varphi}(1 - \bar{g}\bar{f}_3^q\bar{g}\bar{f}_4^q) + 4\bar{g}\bar{f}_3\bar{g}\bar{f}_4 - \bar{g}\bar{f}_1\bar{g}\bar{h}_4\right], \tag{281}$$

$$0 = P_\phi[\bar{g}\bar{f}_3\bar{g}\bar{f}_4^q + \bar{g}\bar{f}_3^q\bar{g}\bar{f}_4], \tag{282}$$

$$P_\phi\left[\bar{g}\frac{\partial(\bar{g}\bar{h}_4)}{\partial K_\varphi}\right] = P_\phi\left[\bar{g}\bar{h}_4\left(\bar{g}\bar{h}_4 + \frac{1}{2}\frac{\partial \bar{g}}{\partial K_\varphi}\right) + \frac{1}{2}\bar{g}\frac{\partial^2 \ln \bar{g}}{\partial K_\varphi^2}(1 - \bar{f}_3^q\bar{g}\bar{f}_4^q)\right]. \tag{283}$$

One can solve (199) and (280) for $\bar{f}_4^q$ and $\bar{f}_3^q$ in terms of $\bar{h}_4$, substitute in (283), and solve for $\bar{h}_4$, which has the rather lengthy solution,

$$\bar{h}_4 = q\bar{\lambda}^2\left(c_f\cos^2(\bar{\lambda}K_\varphi)) - 2q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + c_{h4}q\bar{\lambda}^2|\cos(\lambda(K_\varphi + \mu_\varphi))| \times \sqrt{c_f\cos^2(\bar{\lambda}K_\varphi) - 2q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}}\right)^{-1}, \tag{284}$$

where c_{h4} is an undetermined function of E^x. Upon substitution in (282) and solving for $\bar{f}_3$ and $\bar{f}_4$ using (198) and (279), and substituting all the results in (281), consistency forces us to take the limit $c_{h4} \to \infty$, that is, the function involved must have the form,

$$\bar{h}_4 = \bar{f}_3 = \bar{f}_4 = 0, \tag{285}$$

$$\bar{g}\bar{f}_3^q = -\frac{\alpha_3}{E^x}, \tag{286}$$

$$\bar{g}\bar{f}_4^q = -\frac{E^x}{\alpha_3}, \tag{287}$$

where α_3 is an undetermined function of E^x with classical limit $\alpha_3 \to 1$.

The remaining equations for anomaly-freedom then simplify to

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_0)}{\partial K_\varphi} = \bar{g}\bar{h}_0\bar{g}\bar{h}_3 - 2\bar{g}\bar{f}_1\bar{g}\bar{f}_2 - \bar{g}\bar{f}_1\frac{\partial \bar{g}}{\partial E^x} + \bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x} + \frac{1}{4}\bar{g}^2\frac{\partial \bar{f}_1}{\partial K_\varphi}\bar{g}\bar{h}_0^q\bar{g}\bar{h}_3^q, \tag{288}$$

$$0 = \bar{h}_0^q\bar{h}_3 + \bar{h}_0\bar{h}_3^q, \tag{289}$$

$$\frac{\partial \bar{f}_2}{\partial K_\varphi} = -\frac{1}{2}\frac{\partial}{\partial K_\varphi}\frac{\partial \ln \bar{g}}{\partial E^x} + \bar{h}_1\bar{h}_3 - \frac{1}{8}\frac{\partial^2 \ln \bar{g}}{\partial K_\varphi^2}\bar{g}\bar{h}_0^q\bar{g}\bar{h}_3^q, \quad (290)$$

$$\bar{h}_1\bar{h}_3^q = 0, \quad (291)$$

as well as

$$P_\phi\left[\bar{g}\frac{\partial(\bar{g}\bar{h}_0)}{\partial K_\varphi}\right] = P_\phi\left[-2\bar{g}\bar{f}_1\bar{g}\bar{h}_1 + \frac{1}{2}\bar{g}^2\frac{\partial \bar{f}_1}{\partial K_\varphi}\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3^q\right], \quad (292)$$

$$P_\phi\left[\bar{g}\frac{\partial(\bar{g}\bar{h}_0^q)}{\partial K_\varphi}\right] = P_\phi[2\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3], \quad (293)$$

$$P_\phi\left[\frac{\partial \bar{h}_1}{\partial K_\varphi}\right] = P_\phi\left[-\frac{1}{4}\frac{\partial^2 \ln \bar{g}}{\partial K_\varphi^2}\bar{g}\bar{f}_3^q\bar{g}\bar{h}_3^q\right], \quad (294)$$

and

$$\bar{h}_3 = \frac{1}{2}\frac{\partial \ln \bar{f}_1}{\partial K_\varphi}\bar{g}\bar{h}_0^q\bar{g}\bar{f}_4^q, \quad (295)$$

$$2\bar{h}_0\bar{f}_4^q = \bar{f}_1\bar{h}_3^q, \quad (296)$$

$$\bar{g}\frac{\partial(\bar{g}\bar{h}_3)}{\partial K_\varphi} = \bar{g}\bar{h}_3\frac{1}{2}\frac{\partial \bar{g}}{\partial K_\varphi} - \frac{1}{4}\bar{g}^2\frac{\partial^2 \ln \bar{g}}{\partial K_\varphi^2}\bar{g}\bar{h}_0^q\bar{g}\bar{f}_4^q, \quad (297)$$

$$\frac{\partial(\bar{g}\bar{h}_3^q)}{\partial K_\varphi} = \bar{g}\bar{h}_3^q\frac{1}{2}\frac{\partial \ln \bar{g}}{\partial K_\varphi} + 2\bar{h}_1\bar{g}\bar{f}_4^q, \quad (298)$$

Combining Eqs. (291), (294), and (298), we conclude that

$$\bar{h}_1 = \bar{h}_3^q = 0, \quad (299)$$

such that these three equations are now satisfied. Using these results, Eqs. (289), (293), and (295)–(297) can all be solved, concluding that

$$\bar{h}_0^q = \bar{h}_0 = \bar{h}_3 = 0. \quad (300)$$

The remaining equations for anomaly-freedom now greatly simplify to

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_0)}{\partial K_\varphi} = -2\bar{g}\bar{f}_1\bar{g}\bar{f}_2 - \bar{g}\bar{f}_1\frac{\partial \bar{g}}{\partial E^x} + \bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x} \quad (301)$$

$$\frac{\partial \bar{f}_2}{\partial K_\varphi} = -\frac{1}{2}\frac{\partial}{\partial K_\varphi}\frac{\partial \ln \bar{g}}{\partial E^x}, \quad (302)$$

with the general solutions

$$\bar{g}\bar{f}_0 = \lambda_0\left(-\Lambda_0 + \frac{\alpha_0}{E^x} + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(c_f\frac{\alpha_2}{E^x} + 2\frac{\partial c_f}{\partial E^x}\right) + 2\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(q\frac{\alpha_2}{E^x} + 2\frac{\partial q}{\partial E^x}\right)\right),$$
$$\bar{g}\bar{f}_2 = -\frac{\alpha_2}{4E^x}\lambda_0\cos^2(\bar{\lambda}K_\varphi), \quad (303)$$

where Λ_0, α_i, and α_{iq} are undetermined functions of E^x. This exhausts all the anomaly-freedom equations. Here, Λ_0 and α_0, are not independent functions, but we keep them separate because of their physical significance in the classical limit, which will be explained below.

The general Hamiltonian constraint obtained from the assumed conditions is

$$H = -\lambda_0\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(-\Lambda_0 + \frac{\alpha_0}{E^x} + \left(c_f\frac{\alpha_2}{E^x} + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right) + 2E^\varphi\left(q\frac{\alpha_2}{E^x} + 2\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right.$$
$$+ 4K_x\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + q\cos(2\bar{\lambda}K_\varphi)\right) + \frac{((E^x)')^2}{E^\varphi}\left(-\frac{\alpha_2}{4E^x}\cos^2(\bar{\lambda}K_\varphi) + \bar{\lambda}^2\frac{K_x}{E^\varphi}\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)$$
$$\left. + \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right] + \frac{E^\varphi}{2}\sqrt{q^{xx}}\left[\frac{{P_\phi}^2}{E^\varphi}\frac{\alpha_3}{E^x} + \frac{(\phi')^2}{E^\varphi}\frac{E^x}{\alpha_3}\right] + \lambda_0^2\frac{E^x}{2}\sqrt{q_{xx}}V_q, \quad (304)$$

with structure function

$$q^{xx} = \left(\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi) - 2q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\lambda_0^2\frac{E^x}{(E^\varphi)^2}. \quad (305)$$

All free functions, except for the constant $\bar{\lambda}$, may depend on E^x, and only λ_0 may also depend on ϕ. We will discuss the different classical limits below.

2. Recovery of a nonconstant holonomy parameter

We have used canonical transformations in order to restrict the dependence of the Hamiltonian constraint and make it more manageable, in particular by setting $\bar{\lambda}$ equal to a constant. By undoing some of the canonical transformations, it is possible to replace $\bar{\lambda}$ with a function, at the expense of introducing additional terms in the constraint.

Our discussion of the symmetry generator implies that a nonconstant holonomy parameter λ replacing $\bar{\lambda}$ in (304) cannot depend on ϕ, but it may depend on E^x. In order to recover such nonconstant holonomy effects, we simply have to invert some of our canonical transformations and redefine the rest of the parameters accordingly. Redefining

$$\begin{aligned}&\lambda_0 \to \lambda_0 \frac{\bar{\lambda}}{\lambda}, \qquad q \to q \frac{\lambda}{\bar{\lambda}}, \qquad \Lambda_0 \to \Lambda_0 \frac{\lambda^2}{\bar{\lambda}^2}, \qquad \alpha_0 \to \alpha_0 \frac{\lambda^2}{\bar{\lambda}^2}, \\ &\alpha_2 \to \alpha_2 - 4E^x \frac{\partial \ln \lambda}{\partial E^x}, \qquad V_q \to V_q \frac{\lambda^2}{\bar{\lambda}^2},\end{aligned} \tag{306}$$

implies that the general constraint and structure function now resemble (119) and (120),

$$\begin{aligned}H = &-\frac{\bar{\lambda}}{\lambda}\lambda_0 \frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0 + \frac{\alpha_0}{E^x}\right) + \left(c_f\left(\frac{\alpha_2}{E^x} - 4\frac{\partial \ln \lambda}{\partial E^x}\right) + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\right. \\ &+ 2E^\varphi\left(q\left(\frac{\alpha_2}{E^x} - 2\frac{\partial \ln \lambda}{\partial E^x}\right) + 2\frac{\lambda}{\bar{\lambda}}\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + 4K_x\left(c_f \frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + \frac{\lambda}{\bar{\lambda}} q\cos(2\bar{\lambda}K_\varphi)\right) \\ &+ \frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\partial \ln \lambda}{\partial E^x} - \frac{\alpha_2}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi) + \bar{\lambda}^2 \frac{K_x}{E^\varphi}\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) + \left.\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right] \\ &+ \frac{E^\varphi}{2}\sqrt{q^{xx}}\left[\frac{{P_\phi}^2}{E^\varphi}\frac{\alpha_3}{E^x} + \frac{(\phi')^2}{E^\varphi}\frac{E^x}{\alpha_3}\right] + \lambda_0^2 \frac{E^x}{2}\sqrt{q_{xx}}V_q,\end{aligned} \tag{307}$$

with structure function

$$q^{xx} = \left(\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi) - 2q\frac{\lambda}{\bar{\lambda}}\bar{\lambda}^2 \frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2 \frac{E^x}{(E^\varphi)^2}. \tag{308}$$

A canonical transformation of the form (182) with $f_x^\varphi = \lambda/\bar{\lambda}$, $\tilde{\mu}_\varphi = 0$, $f_c^\phi = \phi$ then eliminates all traces of $\bar{\lambda}$,

$$\begin{aligned}H = &-\lambda_0 \frac{\sqrt{E^x}}{2}\left[E^\varphi\left(-\Lambda_0 + \frac{\alpha_0}{E^x} + \left(c_f\left(\frac{\alpha_2}{E^x} - 4\frac{\partial \ln \lambda}{\partial E^x}\right) + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\lambda K_\varphi)}{\lambda^2}\right)\right. \\ &+ 2E^\varphi\left(q\left(\frac{\alpha_2}{E^x} - 2\frac{\partial \ln \lambda}{\partial E^x}\right) + 2\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\lambda K_\varphi)}{2\lambda} + 4\left(K_x + E^\varphi K_\varphi \frac{\partial \ln \lambda}{\partial E^x}\right)\left(c_f \frac{\sin(2\lambda K_\varphi)}{2\lambda} + q\cos(2\lambda K_\varphi)\right) \\ &+ \frac{((E^x)')^2}{E^\varphi}\left(-\frac{\alpha_2}{4E^x}\cos^2(\lambda K_\varphi) + \lambda^2\left(\frac{K_x}{E^\varphi} + K_\varphi \frac{\partial \ln \lambda}{\partial E^x}\right)\frac{\sin(2\lambda K_\varphi)}{2\lambda}\right) + \left.\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\lambda K_\varphi)\right] \\ &+ \frac{E^\varphi}{2}\sqrt{q^{xx}}\left[\frac{{P_\phi}^2}{E^\varphi}\frac{\alpha_3}{E^x} + \frac{(\phi')^2}{E^\varphi}\frac{E^x}{\alpha_3}\right] + \lambda_0^2 \frac{E^x}{2}\sqrt{q_{xx}}V_q,\end{aligned} \tag{309}$$

and

$$q^{xx} = \left(\left(c_f + \left(\frac{\lambda(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\lambda K_\varphi) - 2q\lambda^2 \frac{\sin(2\lambda K_\varphi)}{2\lambda}\right)\lambda_0^2 \frac{E^x}{(E^\varphi)^2}. \tag{310}$$

now resemble (116) and (117). In these phase-space coordinates, the constraint is no longer periodic in K_φ (see the third and fourth lines of H), but the classical limit is now direct. This shows that we have properly taken into account all effects of a nonconstant λ.

3. Polymerization of the scalar field

The quantization strategy of loop quantum gravity requires a "polymerization" of the scalar field, usually done by replacing ϕ with $\sin(\bar{\nu}\phi)/\bar{\nu}$ in the Hamiltonian constraint, where $\bar{\nu}$ is a constant and the classical limit is obtained for $\bar{\nu} \to 0$. Such a replacement might be performed in a version of the constraint that is to be turned into an operator, in which case the boundedness of $\sin(\bar{\nu}\phi)$ may be beneficial, or it could be used as an effective constraint that is supposed to mimic some of the effects of loop quantization in an analysis of classical type, revealing potential space-time effects.

However, this replacement is not compatible with the general constraint (309), where the classical $(\phi')^2$-term can only be multiplied by E^x-dependent functions while a loop quantization would require a version of the form $\sin(\bar{\nu}\phi)' = \bar{\nu}\cos(\bar{\nu}\phi)\phi'$ with a ϕ-dependent multiplier. This version of polymerization is therefore not a covariant modification that preserves the classical-matter limit.

In fact, there is no room for any modification involving the scalar matter field except for one undetermined function that can be used to this end: the overall factor λ_0. The remaining freedom in applying the polymerization procedure is nonunique, but it can be further restricted and completed by taking inspiration from how a polymerization of the gravitational variable K_φ emerges without the need of a canonical transformation.

Physically, polymerization of the scalar field should imply boundedness effects from the field dependence since the field ϕ itself appears, by definition of polymerization, as an argument of a trigonometric function. More generally, we may want to allow polymerization to have an E^x-dependent point-holonomy parameter $\nu(E^x)$, such that it is sensitive to distance and energy scales and automatically implies the classical limit $\nu \to 0$ for large spherical areas E^x if ν is a decreasing function. If possible, a substitution of the form $\phi \to \sin(\nu\phi)/\nu$ is preferable because it has been most commonly used, which is bounded by $|\sin(\nu\phi)/\nu| < 1/\nu$. Since the relationship between ϕ and $\sin(\nu\phi)/\nu$ is not one-to-one, we have to limit the range of ϕ after a canonical transformation to polymerized form such that $|\phi| \leq 1/\nu$ (in an E^x-dependent way) if the replacement $\phi \to \sin(\nu\phi)/\nu$ is to be implemented by a well-defined canonical transformation.

In order to have a dynamically stable range limited in this way, we compute the evolution equations of the scalar field and require that $\dot{\phi}|_{\phi\to 1/\nu} \to 0$. There is then no evolution transversal to the surface $\phi = 1/\nu$ in phase space, and it is consistent to assume that the value of the scalar field does not increase beyond this limit. Geometrically, this condition means that whenever there is a point or a region on where $\phi = 1/\nu$, we must have $\dot{\phi} = 0$ at this place. As a specific case, we assume that this condition is obtained in an extended spatial region that defines part of a hypersurface of a canonical foliation. Since we need to limit only the normal component of evolution on the hypersurface, we may assume $N^x = 0$. The condition then leads to the equations,

$$\begin{aligned}\dot{\phi}|_{\phi\to 1/\nu} &= \{\phi, H[N]\}\\ &= \frac{\bar{\lambda}}{\lambda}\lambda_0 N\sqrt{\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi) - 2q\frac{\lambda}{\bar{\lambda}}\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}}\frac{P_\phi}{E^\varphi}\frac{\alpha_3}{\sqrt{E^x}},\end{aligned} \tag{311}$$

$$\dot{P}_\phi|_{\phi\to 1/\nu} = \frac{\bar{\lambda}\lambda_0}{2\lambda}\frac{N\sqrt{E^x}E^\varphi\partial V_q/\partial\phi}{\sqrt{(c_f + (\bar{\lambda}(E^x)'/(2E^\varphi))^2)\cos^2(\bar{\lambda}K_\varphi) - 2q\lambda\bar{\lambda}\sin(2\bar{\lambda}K_\varphi)/(2\bar{\lambda})}}, \tag{312}$$

using (307), the second equation at spatial points where $\phi' = 0$ according to our assumption that the maximum ϕ is reached in a subset of a hypersurface where, if it is sufficiently small, E^x and therefore ν can be assumed to be nearly constant. In $\dot{P}_\phi$, we omitted the term implied by $\partial\lambda_0/\partial\phi$ because it vanishes on shell.

We need both expressions to vanish because λ_0 is always positive. The sign of P_ϕ must therefore change in order to start decreasing the value of ϕ past the hypersurface. The solution to this problem is nonunique because we are not restricting the rate at which P_ϕ approaches zero. Based on how boundedness comes about in the gravitational case where the limiting value of $\bar{\lambda}K_\varphi$ implies a similar transition hypersurface studied for instance in [7,8], we redefine the overall factor by

$$\lambda_0(E^x, \phi) \to \lambda_0(E^x, \phi)(1 - \nu^2\phi^2), \tag{313}$$

where the residual dependence of the redefined λ_0 on E^x and ϕ is required to be nonzero if $\phi = 1/\nu$ so as not to interfere with the bound.

After this preparation, we perform a canonical transformation of the form (213) with $f_c^\phi = \sin(\nu\phi)/\nu$. This transformation turns the right-hand side of the redefinition (313) into $\lambda_0^2\cos^2(\nu\phi)$, and the Hamiltonian constraint (307) into

$$
\begin{aligned}
H = & -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\nu\phi)\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0+\frac{\alpha_0}{E^x}\right)+\left(c_f\left(\frac{\alpha_2}{E^x}-4\frac{\partial\ln\lambda}{\partial E^x}\right)+2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\right. \\
& +2E^\varphi\left(q\left(\frac{\alpha_2}{E^x}-2\frac{\partial\ln\lambda}{\partial E^x}\right)+2\frac{\lambda}{\bar{\lambda}}\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+4\left(K_x+P_\phi\left(\phi-\frac{\tan(\nu\phi)}{\nu}\right)\frac{\partial\ln\nu}{\partial E^x}\right)\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+\frac{\lambda}{\bar{\lambda}}q\cos(2\bar{\lambda}K_\varphi)\right) \\
& +\frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\partial\ln\lambda}{\partial E^x}-\frac{\alpha_2}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi)+\bar{\lambda}^2\left(\frac{K_x}{E^\varphi}+\frac{P_\phi}{E^\varphi}\left(\phi-\frac{\tan(\nu\phi)}{\nu}\right)\frac{\partial\ln\nu}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) \\
& \left.+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right] \\
& +\frac{E^\varphi}{2}\sqrt{q^{xx}}\left[\frac{{P_\phi}^2}{E^\varphi\cos^2(\nu\phi)}\frac{\alpha_3}{E^x}+\frac{1}{E^\varphi}\frac{E^x}{\alpha_3}\left(\phi'\cos(\nu\phi)+\left(\phi\cos(\nu\phi)-\frac{\sin(\nu\phi)}{\nu}\right)\frac{\partial\ln\nu}{\partial E^x}(E^x)'\right)^2\right] \\
& +\lambda_0^2\cos^4(\nu\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q, \qquad (314)
\end{aligned}
$$

with structure function

$$
q^{xx}=\left(\left(c_f+\left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi)-2q\frac{\lambda}{\bar{\lambda}}\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\cos^4(\nu\phi)\frac{E^x}{(E^\varphi)^2}. \qquad (315)
$$

For nonconstant ν, this constraint is not periodic in ϕ. Performing a second canonical transformation of the form (213) with $f_c^\phi=(\bar{\nu}/\nu)\phi$ and a constant $\bar{\nu}$, the constraint is rendered periodic,

$$
\begin{aligned}
H = & -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0+\frac{\alpha_0}{E^x}\right)+\left(c_f\left(\frac{\alpha_2}{E^x}-4\frac{\partial\ln\lambda}{\partial E^x}\right)+2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\right. \\
& +2E^\varphi\left(q\left(\frac{\alpha_2}{E^x}-2\frac{\partial\ln\lambda}{\partial E^x}\right)+2\frac{\lambda}{\bar{\lambda}}\frac{\partial q}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+4\left(K_x-P_\phi\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+\frac{\lambda}{\bar{\lambda}}q\cos(2\bar{\lambda}K_\varphi)\right) \\
& \left.+\frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\partial\ln\lambda}{\partial E^x}-\frac{\alpha_2}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi)+\bar{\lambda}^2\left(\frac{K_x}{E^\varphi}-\frac{P_\phi}{E^\varphi}\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right] \\
& +\frac{\bar{\nu}^2}{\nu^2}\frac{\sqrt{q^{xx}}}{2}\left[\frac{{P_\phi}^2}{\cos^2(\bar{\nu}\phi)}\frac{\alpha_3}{E^x}+\frac{E^x}{\alpha_3}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}(E^x)'\right)^2\right]+\lambda_0^2\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q, \qquad (316)
\end{aligned}
$$

and the structure function becomes

$$
q^{xx}=\left(\left(c_f+\left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi)-2q\frac{\lambda}{\bar{\lambda}}\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{(E^\varphi)^2}. \qquad (317)
$$

We note that effects implied by boundedness of the scalar field in the polymerized constraint (314) are not due to the canonical transformations, which cannot change physical implications, but rather a consequence of the nonclassical overall factor λ_0 and its ϕ-dependence. The result has two general implications of importance for discussions of polymerization in models of loop quantum gravity. First, while the P_ϕ^2-term and the new $(\phi')^2$-term may look like something one may have chosen with standard polymerization, there are additional terms in the consistent Hamiltonian constraint depending on ϕ and P_ϕ. In particular, there is a coupling term between ϕ and the spatial derivative $(E^x)'$ in the last line, as well as a terms linear in P_ϕ in the third and fourth lines. Such terms are not part of standard polymerization procedures.

Secondly, the structure function necessarily depends on the scalar field even at the kinematical level, after redefining the overall factor in order to comply with a bounded ϕ-dependent function in the constraint. This result is physically meaningful only within our new viewpoint of emergent modified gravity, in which space-time geometry is not described directly by a fundamental field, but rather an emergent object composed of the truly fundamental fields, in this case both the gravitational degree of freedom and the scalar matter field.

The Hamiltonian constraint (316) is then periodic in both K_φ and ϕ as a modified constraint with holonomy or polymerization effects. It includes the option of polymerization functions with nonconstant parameters λ and ν upon using canonical transformations. The vacuum mass observable associated to (316) is given by

$$\mathcal{M} = d_0 + \frac{d_2}{2}\left(\exp\int \mathrm{d}E^x\left(\frac{\alpha_2}{2E^x} - \frac{\partial \ln\lambda^2}{\partial E^x}\right)\right)\left(c_f\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + 2\frac{\lambda}{\bar{\lambda}}q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} - \cos^2(\bar{\lambda}K_\varphi)\left(\frac{(E^x)'}{2E^\varphi}\right)^2\right)$$
$$+ \frac{d_2}{4}\int \mathrm{d}E^x\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(\Lambda_0 + \frac{\alpha_0}{E^x}\right)\exp\int \mathrm{d}E^x\left(\frac{\alpha_2}{2E^x} - \frac{\partial\ln\lambda^2}{\partial E^x}\right)\right), \tag{318}$$

and, when $V = V_q = V^q = 0$, its scalar-field observable by

$$G[\alpha] = \int \mathrm{d}^3x\,\alpha\frac{\nu}{\bar{\nu}}\frac{P_\phi}{\cos(\bar{\nu}\phi)}, \tag{319}$$

where α, d_0, and d_2 are constants. The associated conserved matter current J^μ has the components,

$$J^t = \frac{\nu}{\bar{\nu}}\frac{P_\phi}{\cos(\bar{\nu}\phi)}, \tag{320}$$

$$J^x = \frac{\partial G}{\partial P_\phi}\frac{\partial H}{\partial\phi'} = \frac{\bar{\nu}}{\nu}\sqrt{q^{xx}}\frac{E^x}{\alpha_3}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)' - (E^x)'\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right). \tag{321}$$

4. Partial Abelianization

The partial Abelianization of the constraint (316) is easily achieved by using the coefficients (276) under the redefinitions (306) and (313) and taking $q = 0$ according to the condition (275). The resulting Abelianized constraint is given by

$$\frac{H^{(A)}}{\bar{B}c_f} = -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0 + \frac{\alpha_0}{E^x}\right) + \left(c_f\left(\frac{\alpha_2}{E^x} - 4\frac{\partial\ln\lambda}{\partial E^x}\right) + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\right.$$
$$+ 4\left(K_x - P_\phi\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + \frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\partial\ln\lambda}{\partial E^x} - \frac{\alpha_2}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi)\right.$$
$$\left.\left. + \bar{\lambda}^2\left(\frac{K_x}{E^\varphi} - \frac{P_\phi}{E^\varphi}\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) + \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)\right]$$
$$- \frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{(E^x)'}{E^\varphi}\left(K_\varphi' - \frac{K_x}{E^\varphi}(E^x)' + \frac{P_\phi}{E^\varphi}\phi'\right)$$
$$+ \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\bar{\nu}^2}{\nu^2}\frac{\sqrt{q^{xx}}}{2}\left(\frac{{P_\phi}^2}{\cos^2(\bar{\nu}\phi)}\frac{\alpha_3}{E^x} + \frac{E^x}{\alpha_3}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)' - \frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}(E^x)'\right)^2\right)$$
$$+ \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q. \tag{322}$$

This Abelian constraint has kinematical divergences at $K_\varphi = \pm\pi/(2\bar{\lambda})$ in from the first line and last line. The latter can easily be resolved by simply restricting the constraint to the free scalar case, $V_q = 0$, while the divergence of the first line can be eliminated if the equation,

$$\lambda^2\left(-\Lambda_0 + \frac{\alpha_0}{E^x}\right) + 2\frac{\partial c_f}{\partial E^x} + \left(\frac{\alpha_2}{E^x} - 4\frac{\partial\ln\lambda}{\partial E^x}\right)c_f = 0, \tag{323}$$

holds. If this equation is interpreted as a condition on c_f, its general solution is not compatible with the classical limit. However, if we exclude the last term of this equation, it reduces to

$$\frac{\partial c_f}{\partial E^x} = \frac{\lambda^2}{2}\left(\Lambda_0 - \frac{\alpha_0}{E^x}\right) \tag{324}$$

which can be directly integrated to obtain a nonclassical c_f compatible with the classical limit. For instance, if we choose the classical values $\Lambda_0 = \Lambda$ and $\alpha_0 = 1$, and a constant $\lambda = \bar{\lambda}$, we obtain

$$c_f = 1 + \frac{\bar{\lambda}^2}{2}\left(\Lambda E^x - \ln\left(\frac{E^x}{c_0}\right)\right), \tag{325}$$

where c_0 is the constant of integration. If one instead chooses $\lambda^2 = \Delta/E^x$, motivated for instance by loop quantum gravity, one obtains

$$c_f = 1 + \frac{\Delta}{2}\left(\Lambda \ln\left(\frac{E^x}{c_0}\right) + \frac{1}{E^x}\right). \tag{326}$$

In [25] it was shown that a nonclassical function of the form (325) can be related to MOND via the logarithmic term. Similarly, the version (326) can be related to MOND effects, too, since it has a logarithmic term. With this procedure, only the term multiplying c_f in (322) retains its kinematical divergence.

5. Classical limits and conditions

We have different types of classical limits that can be demonstrated explicitly for the polymerized Hamiltonian constraint (314), on which the conditions for gravitational and matter observables have been imposed. The polymerization can always be undone by setting $\nu \to \bar{\nu}$ followed by $\bar{\nu} \to 0$. The following two canonical transformations will also be useful for the discussion of classical limits:

$$\begin{aligned} &\phi \to \phi, \qquad P_\phi \to P_\phi - E^\varphi \frac{\partial \ln \lambda}{\partial \phi} K_\varphi, \\ &K_\varphi \to \frac{\lambda}{\bar{\lambda}} K_\varphi, \qquad E^\varphi \to \frac{\bar{\lambda}}{\lambda} E^\varphi, \\ &K_x \to K_x + E^\varphi \frac{\partial \ln \lambda}{\partial E^x} K_\varphi, \qquad E^x \to E^x, \end{aligned} \tag{327}$$

where λ may depend on E^x and ϕ, and

$$\begin{aligned} &\phi \to \frac{\nu}{\bar{\nu}} \phi, \qquad P_\phi \to \frac{\bar{\nu}}{\nu} P_\phi, \\ &K_\varphi \to K_\varphi, \qquad E^\varphi \to E^\varphi, \\ &K_x \to K_x + P_\phi \frac{\partial \ln \nu}{\partial E^x}, \qquad E^x \to E^x, \end{aligned} \tag{328}$$

where ν may depend on E^x. We have the following limits:

(i) The classical-matter limit is given by first performing the canonical transformation (328), turning the constraint (316) into (314) where $\bar{\nu}$ no longer appears, followed by $\alpha_3 \to 1$, $\nu \to 0$, and V_q becoming the classical potential of the scalar field. The resulting Hamiltonian constraint implies the Klein-Gordon equation on a curved, emergent spacetime.

(ii) The classical-geometry limit is given by first performing the canonical transformations (328) and (327), eliminating $\bar{\nu}$ and $\bar{\lambda}$ respectively, followed by $\lambda_0, c_f \to 1$ and λ, $\nu \to 0$. In this limit, we recover residual canonical transformations linear in K_φ which can be used to eliminate q by absorbing it into Λ_0.

(iii) The classical-gravity limit is given by the classical-geometry limit together with $\Lambda_0 \to -\Lambda$, $\alpha_0, \alpha_2 \to 1$, α_3 becoming a constant, and V_q becoming a free function of ϕ only.

(iv) A comparison with the constraint (119), obtained from a linear combination of the classical constraints and subsequent canonical transformations, shows that the modified constraint under consideration cannot reproduce the limit of reaching the classical constraint surface unless we take the classical-geometry limit since q^{xx} appears explicitly in (316), but not in (119). However, the constraint (119) is incompatible with the classical-geometry limit. Thus, the limit of reaching the classical constraint surface for (316) is trivial, as it exists only in the full classical limit.

(v) The full classical limit is given by the classical-gravity limit together with the classical-matter limit.

(vi) The vacuum limit is given by $P_\phi, \phi, V_q \to 0$, recovering the vacuum constraint (222).

Moreover, the constraint (316) can easily be Abelianized by imposing the condition (275), which simply requires that we set $q = 0$.

As will be shown in Sec. VI, the constraint (119) implies a physical singularity at the maximum-curvature surface in spatially homogeneous dynamical solutions.

B. Constraints compatible with the classical constraint surface as a limit

A second class of tractable conditions is obtained by requiring that the modified constraint has a limit in which the classical constraint surface is recovered.

1. Anomaly freedom

We just found that the modified constraint compatible with the classical-matter limit is not compatible with the limit of reaching the classical constraint surface unless we take the full classical limit. Since the limit in which the classical constraint surface is reached is given by (119), the existence of this limit requires a modified constraint that can be reduced to this version.

By inspection of the constraint (119), we require that the functions $\bar{f}_0$, $\bar{f}_2$, $\bar{f}_3$, $\bar{f}_4$, $\bar{h}_0$, $\bar{h}_3$, $\bar{h}_4$ are nonvanishing such that it can match (122) in some limit. Direct substitution of the covariance solution (211) in the condition (260) for the existence of a matter observable implies the restriction,

$$\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial c_f}{\partial\phi}+q\frac{\partial\ln\lambda}{\partial\phi}=0. \tag{329}$$

For a nonzero $\bar{\lambda}$ to be possible, c_f must be independent of ϕ because the second term does not depend on K_φ, unlike the first one. The second term then leaves us with two mutually exclusive options, a ϕ-dependent λ or a nonvanishing q. It turns out that anomaly freedom restricts us to the first option, as we will show now.

First, if we assume $\bar{f}_4^q\neq 0$, Eq. (204) implies that $\bar{f}_4^q=\bar{h}_2=0$ from its $((E^x)')^2\sqrt{q^{xx}}$ and $((E^x)')^2 q^{xx}$ terms. This turns Eq. (204) into Eqs. (280)–(283) used in the previous section, which allowed us to conclude that $\bar{f}_3$, $\bar{f}_4$, and $\bar{h}_4$ must vanish for nonzero $\bar{f}_4^q$. This contradiction with our opening conditions shows that we must instead choose $\bar{f}_4^q=0$.

With $\bar{f}_4^q=0$, the $\sqrt{q^{xx}}$ and $((E^x)')^2\sqrt{q^{xx}}$ terms of (204) imply $\bar{f}_3^q=0$ and $\bar{h}_2^q=0$, respectively. One can then show that the consistency between the $((E^x)')^2 q^{xx}$ term of (201), the $((E^x)')^2$ term of (200), the $\sqrt{q^{xx}}$ and $((E^x)')^2\sqrt{q^{xx}}$ terms of (202) and (203), and the zeroth-order and $((E^x)')^2$ terms of (204) determine,

$$\bar{h}_0^q=\bar{h}_1^q=\bar{h}_3^q=0. \tag{330}$$

With this, the $\sqrt{q^{xx}}$, $((E^x)')^2\sqrt{q^{xx}}$ terms of (201) can be solved for

$$\bar{g}\bar{f}_2^q=-\frac{\alpha_{2q}}{4E^x}\cos^2(\bar{\lambda}K_\varphi), \tag{331}$$

$$\bar{g}\bar{f}_0^q=\frac{\alpha_{0q}}{E^x}+\frac{\alpha_{2q}}{E^x}\left(c_f\cos^2(\bar{\lambda}K_\varphi)+2q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right), \tag{332}$$

where α_{0q} and α_{2q} are undetermined functions of E^x and ϕ.

The nontrivial equations for anomaly freedom become,

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_0)}{\partial K_\varphi}=\bar{g}\bar{h}_0\bar{g}\bar{h}_3-2\bar{g}\bar{f}_1\bar{g}\bar{f}_2-\bar{g}\bar{f}_1\frac{\partial\bar{g}}{\partial E^x}+\bar{g}\frac{\partial(\bar{g}\bar{f}_1)}{\partial E^x}, \tag{333}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{f}_2)}{\partial K_\varphi}=\bar{g}\bar{f}_2\frac{\partial\bar{g}}{\partial K_\varphi}-\bar{g}^2\frac{1}{2}\frac{\partial}{\partial E^x}\frac{\partial\ln\bar{g}}{\partial K_\varphi}+\bar{g}\bar{h}_1\bar{g}\bar{h}_3, \tag{334}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{h}_0)}{\partial K_\varphi}=-2\bar{g}\bar{f}_1\bar{g}\bar{h}_1+\bar{g}\bar{h}_0\bar{g}\bar{h}_4+2\bar{g}\bar{f}_3\bar{g}\bar{h}_3, \tag{335}$$

$$\frac{\partial(\bar{g}\bar{h}_1)}{\partial K_\varphi}=2\bar{h}_2\bar{g}\bar{h}_3+\bar{g}\bar{h}_1\left(\bar{h}_4+\frac{\partial\ln\bar{g}}{\partial K_\varphi}\right), \tag{336}$$

$$\bar{g}\frac{\partial(\bar{g}\bar{h}_3)}{\partial K_\varphi}=\bar{g}\bar{h}_3\left(\bar{g}\bar{h}_4+\frac{1}{2}\frac{\partial\bar{g}}{\partial K_\varphi}\right)+2\bar{g}\bar{h}_1\bar{g}\bar{f}_4-\bar{g}^2\frac{1}{2}\frac{\partial^2\ln\bar{g}}{\partial\phi\partial K_\varphi}, \tag{337}$$

$$\bar{g}^2\frac{\partial\bar{f}_1}{\partial\phi}=\bar{g}\bar{f}_1\bar{g}\bar{h}_3-2\bar{g}\bar{h}_0\bar{g}\bar{f}_4, \tag{338}$$

and

$$\frac{\partial\ln(\bar{g}\bar{f}_4)}{\partial K_\varphi}=2\bar{h}_4, \tag{339}$$

$$\frac{\partial(\bar{g}\bar{f}_3)}{\partial K_\varphi}=2\bar{g}\bar{f}_3\bar{h}_4-2\bar{g}\bar{f}_1\bar{h}_2, \tag{340}$$

$$\frac{\partial\bar{h}_2}{\partial K_\varphi}=2\bar{h}_2\bar{h}_4, \tag{341}$$

$$0=P_\phi\left[-\bar{g}^2\frac{\partial\bar{f}_1}{\partial K_\varphi}+4\bar{g}\bar{f}_3\bar{g}\bar{f}_4-\bar{g}\bar{f}_1\bar{g}\bar{h}_4\right], \tag{342}$$

$$P_\phi\left[\bar{g}^2\frac{\partial\bar{h}_4}{\partial K_\varphi}\right]=P_\phi\left[\bar{g}^2\bar{h}_4\left(\bar{h}_4-\frac{1}{2}\frac{\partial\ln\bar{g}}{\partial K_\varphi}\right)+4\bar{g}\bar{h}_2\bar{g}\bar{f}_4+\frac{1}{2}\bar{g}^2\frac{\partial^2\ln\bar{g}}{\partial K_\varphi^2}\right]. \tag{343}$$

The last five equations form an overdetermined system of equations for $\bar{f}_3$, $\bar{f}_4$, $\bar{h}_2$, and $\bar{h}_4$, since we already know $\bar{g}$ and $\bar{f}_1$. This system is hard, if not impossible, to solve exactly, and we will split our analysis into two versions with additional assumptions. In the first version we assume $\bar{h}_2=0$, and in the second one $\bar{h}_4=0$. The former is compatible with the limit of reaching the classical constraint surface considered in this subsection, while the latter will be analyzed in the next subsection.

With $\bar{h}_2=0$, the general solution of Eq. (343) is

$$\bar{h}_4=-\bar{\lambda}^2\ \sec(\bar{\lambda}K_\varphi)\frac{\sin(\bar{\lambda}K_\varphi)/\bar{\lambda}+c_{h4}}{c_{h4}\bar{\lambda}\sin(\bar{\lambda}K_\varphi)+1} \tag{344}$$

with an integration function c_{h4} independent of K_φ. Equations (339) and (340) can now be directly integrated, yielding

$$\bar{g}\bar{f}_3=-\lambda_0\frac{\alpha_3}{E^x}\cos^2(\bar{\lambda}K_\varphi)\left(1+c_{h4}\bar{\lambda}^2\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)^{-2}, \tag{345}$$

$$\bar{g}\bar{f}_4=-\lambda_0\frac{E^x}{\alpha_4}\cos^2(\bar{\lambda}K_\varphi)\left(1+c_{h4}\bar{\lambda}^2\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)^{-2}, \tag{346}$$

where α_3 and α_4 are undetermined functions of E^x and ϕ that cannot identically vanish under the current assumptions. Inserting these results in (342), we obtain

$$0 = \cos(\bar{\lambda}K_\varphi)\left(-4c_f\cos(2\bar{\lambda}K_\varphi) + 16q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) + 4\frac{\alpha_3}{\alpha_4}\frac{\cos^3(\bar{\lambda}K_\varphi)}{(1+c_{h4}\bar{\lambda}\sin(\bar{\lambda}K_\varphi))^4}$$
$$+ 4\bar{\lambda}\frac{c_{h4}\bar{\lambda}\cos(2\bar{\lambda}K_\varphi) - \sin(\bar{\lambda}K_\varphi)}{1+c_{h4}\bar{\lambda}\sin(\bar{\lambda}K_\varphi)}\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + q\cos(\bar{\lambda}K_\varphi)\right), \quad (347)$$

which must hold for all K_φ. If $c_{h4} \neq 0$, the dependence of this equation on K_φ is such that it can be valid only if $\alpha_3 = 0$, which is not allowed by the classical limit. Therefore, we have $c_{h4} = 0$ and the equation simplifies to

$$0 = \left(c_f - \frac{\alpha_3}{\alpha_4}\right)4\cos^3(\bar{\lambda}K_\varphi) - 2q\bar{\lambda}(3\sin(\bar{\lambda}K_\varphi) + 3\cos^2(\bar{\lambda}K_\varphi)\sin(\bar{\lambda}K_\varphi) - \sin^3(\bar{\lambda}K_\varphi)) \quad (348)$$

again for all K_φ. This equation restricts the values of the following free functions:

$$c_{h4} = q = 0, \quad (349)$$

$$\alpha_3 = c_f\alpha_4. \quad (350)$$

We can now solve Eqs. (333)–(338) for anomaly-freedom, which again form an overdetermined system of equations. Equation (336), assuming $\bar{h}_2 = 0$ in the present case, has the general solution

$$\bar{g}\bar{h}_1 = \lambda_0 c_{h1}\frac{\cos^3(\bar{\lambda}K_\varphi)}{1+c_{h4}\bar{\lambda}\sin(\bar{\lambda}K_\varphi)} = \lambda_0 c_{h1}\cos^3(\bar{\lambda}K_\varphi), \quad (351)$$

where c_{h1} is an undetermined function of E^x and ϕ. Equation (337) can now be solved by

$$\bar{g}\bar{h}_3 = \lambda_0\cos^2(\bar{\lambda}K_\varphi)\left(c_{h3} - 2c_{h1}\frac{E^x}{\alpha_4}\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right), \quad (352)$$

where c_{h3} is an undetermined function of E^x and ϕ. Next, we solve Eq. (335) by

$$\bar{g}\bar{h}_0 = \lambda_0\left(c_{h0}\cos(\bar{\lambda}K_\varphi) - 2\left(c_{h3}\frac{\alpha_3}{E^x} + c_{h1}c_f\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right), \quad (353)$$

where c_{h0} is an undetermined function of E^x and ϕ. Inserting these results into (338), we obtain the condition

$$0 = \bar{\lambda}^2 c_{h0} - c_{h1}c_f(c_{h1}+2) + 3c_{h1}c_f\cos(2\bar{\lambda}K_\varphi) \quad (354)$$

for all K_φ, which determines

$$c_{h0} = c_{h1} = 0, \quad (355)$$

since the classical limit requires c_f and α_3 to be nonzero.

Using all the results obtained so far, we solve Eqs. (333) and (334),

$$\bar{g}\bar{f}_2 = -\lambda_0\frac{\alpha_2}{4E^x}\cos^2(\bar{\lambda}K_\varphi), \quad (356)$$

$$\bar{g}\bar{f}_0 = \lambda_0\left(-\Lambda_0 + \frac{\alpha_0}{E^x} - V + \left(\frac{\alpha_2}{E^x}c_f + 2\frac{\partial c_f}{\partial E^x} - c_{h3}{}^2\frac{\alpha_3}{E^x}\right)\times\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right), \quad (357)$$

where α_0, V, and α_2 are undetermined functions of E^x and ϕ. Here, as in a similar case before, V and Λ_0 are not independent of α_0, but we keep them separate so as to be able to define a scalar-field potential independent of the gravitational terms. This exhausts all the equations for anomaly freedom.

We now go back to the condition that there be a matter observable, since the choice $q = 0$ has been forced upon us by the conditions for anomaly freedom. For $\partial_\phi\lambda \neq 0$, conditions (242) and (249) for the existence of a matter observable imply that $\bar{f}_i^q$ and $\bar{h}_i^q$, for all i, must vanish, thus determining $\alpha_{0q} = \alpha_{2q} = 0$. With this, the conditions (251)–(258) for the existence of a matter observable and condition (237) for the existence of a gravitational observable are trivially satisfied. The last step is to substitute all our solutions into the conditions (259)–(268), which then become constraining equations for the undetermined functions. Equation (262) requires that $\partial\alpha_3/\partial\phi = 0$, and, similarly, Eq. (263) requires $\partial\alpha_4/\partial\phi = 0$. Using this, Eq. (264) implies,

$$\frac{\partial c_{h3}}{\partial\phi} = \frac{\partial^2\ln\lambda}{\partial\phi^2}, \quad (358)$$

and thus

$$c_{h3} = c_{h3}^x + \frac{\partial \ln \lambda}{\partial \phi}, \tag{359}$$

where c_{h3}^x is an undetermined function of E^x. Substitution in (267) shows $c_{h3}^x = 0$. Equation (261) implies

$$\frac{\partial \alpha_2}{\partial \phi} = -2E^x \frac{\partial^2 \ln \lambda^2}{\partial \phi \partial E^x}, \tag{360}$$

and thus

$$\alpha_2 = \alpha_2^x - 4E^x \frac{\partial \ln \lambda}{\partial E^x}, \tag{361}$$

where α_2^x is an undetermined function of E^x. Substituting all the above into (259) with $V = 0$ we obtain the equation

$$\frac{\partial \ln (\alpha_0 - E^x \Lambda_0)}{\partial \phi} = \frac{\partial \ln \lambda^2}{\partial \phi}, \tag{362}$$

and thus

$$\alpha_0 - E^x \Lambda_0 = \frac{\lambda^2}{\bar{\lambda}} (\alpha_0^x - E^x \Lambda_0^x), \tag{363}$$

where α_0^x and Λ_0^x are undetermined functions of E^x. Comparison with (119) suggests that we multiply V by the same factor, and we do so in what follows. This exhausts all the conditions for the existence of matter and gravitational observables.

2. General Hamiltonian constraint

In order to recover the full effects of nonconstant λ, it suffices to redefine

$$\lambda_0 \to \lambda_0 \frac{\bar{\lambda}}{\lambda}, \qquad V_q \to \frac{\lambda^2}{\bar{\lambda}^2} V_q, \tag{364}$$

such that the general constraint now resembles (119). The Hamiltonian constraint is then

$$\begin{aligned} H = &-\frac{\bar{\lambda}}{\lambda} \lambda_0 \frac{\sqrt{E^x}}{2} \Bigg[E^\varphi \left(\frac{\lambda^2}{\bar{\lambda}} \left(-\Lambda_0^x + \frac{\alpha_0^x}{E^x} - V \right) + \left(\frac{\alpha_2^x}{E^x} c_f + 2 \frac{\partial c_f}{\partial E^x} \right) \frac{\sin^2(\bar{\lambda} K_\varphi)}{\bar{\lambda}^2} + \left(\frac{K_x}{E^\varphi} - \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \frac{\partial \ln \lambda}{\partial E^x} \right) 4 c_f \frac{\sin(2\bar{\lambda} K_\varphi)}{2\bar{\lambda}} \right. \\ &\left. - \left(\frac{P_\phi}{E^\varphi} + \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \left(c_{h3}^x + \frac{\partial \ln \lambda}{\partial \phi} \right) \right)^2 \frac{\alpha_4}{E^x} c_f \cos^2(\bar{\lambda} K_\varphi) \right) + \frac{((E^x)')^2}{E^\varphi} \left(\left(\frac{\partial \ln \lambda}{\partial E^x} - \frac{\alpha_2^x}{4E^x} \right) \cos^2(\bar{\lambda} K_\varphi) + \bar{\lambda}^2 \frac{K_x}{E^\varphi} \frac{\sin(2\bar{\lambda} K_\varphi)}{2\bar{\lambda}} \right) \\ &+ \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi} \right) \cos^2(\bar{\lambda} K_\varphi) + \cos^2(\bar{\lambda} K_\varphi) \left(-\frac{(\phi')^2}{E^\varphi} \frac{E^x}{\alpha_4} + \frac{(E^x)' \phi'}{E^\varphi} \left(c_{h3}^x + \frac{\partial \ln \lambda}{\partial \phi} - \frac{P_\phi}{E^\varphi} \bar{\lambda}^2 \frac{\tan(\bar{\lambda} K_\varphi)}{\bar{\lambda}} \right) \right) \Bigg] \\ &+ \lambda_0^2 \frac{E^x}{2} \sqrt{q_{xx}} V_q \end{aligned} \tag{365}$$

with structure function

$$q^{xx} = \left(c_f + \left(\frac{\bar{\lambda} (E^x)'}{2E^\varphi} \right)^2 \right) \cos^2(\bar{\lambda} K_\varphi) \frac{\bar{\lambda}^2}{\lambda^2} \lambda_0^2 \frac{E^x}{(E^\varphi)^2}, \tag{366}$$

where all parameters are undetermined functions of E^x, except for λ_0, λ, V, and V_q which depend on both E^x and ϕ, and $\bar{\lambda}$ is a constant. For the constraint to be invariant under the transformation generated by (240), one must take $V = V_q = 0$. The classical limit can be obtained in different ways, as discussed below.

A canonical transformation of the form $K_\varphi \to (\lambda/\bar{\lambda}) K_\varphi$ eliminates all traces of $\bar{\lambda}$, but the constraint becomes nonperiodic in K_φ. This shows that we have properly taken into account all effects of the nonconstant λ.

3. Polymerization of the scalar field

Following the discussion of the previous section, we place an upper bound on the absolute value of the scalar matter field of the constraint (365) by using the redefinition (313). We can then take two consecutive canonical transformations of the form (213), the first one with $f_c^\phi = \sin(\nu \phi)/\nu$, and the second one with $f_c^\phi = (\bar{\nu}/\nu)\phi$. Applying these two transformations is equivalent to using the single canonical transformation,

$$\phi \to \frac{\sin(\bar{\nu}\phi)}{\nu}, \qquad P_\phi \to \frac{\nu}{\bar{\nu}} \frac{P_\phi}{\cos(\bar{\nu}\phi)},$$
$$K_x \to K_x - P_\phi \frac{\tan(\bar{\nu}\phi)}{\bar{\nu}} \frac{\partial \ln \nu}{\partial E^x}, \tag{367}$$

while all other phase-space variables remain unchanged.

The constraint (365) then becomes

$$H = -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}}\left(-\Lambda_0^x + \frac{\alpha_0^x}{E^x} - V\right) + \left(\frac{\alpha_2^x}{E^x}c_f + 2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right.\right.$$
$$+\left(\frac{K_x}{E^\varphi} - \frac{P_\phi}{E^\varphi}\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x} - \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial E^x}\right)4c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}$$
$$-\left(\frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)} + \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left(\frac{\bar{\nu}}{\nu}c^x_{h3} + \frac{\partial\ln\lambda}{\partial\phi}\right)\right)^2\frac{\alpha_4}{E^x}\frac{\nu^2}{\bar{\nu}^2}c_f\cos^2(\bar{\lambda}K_\varphi)\right) + \frac{((E^x)')^2}{E^\varphi}\left(\bar{\lambda}^2\frac{K_x}{E^\varphi}\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right.$$
$$\left.\left.+\cos^2(\bar{\lambda}K_\varphi)\left(\frac{\partial\ln\lambda}{\partial E^x} - \frac{\alpha_2^x}{4E^x} - \frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\left(\frac{\bar{\nu}}{\nu}c^x_{h3} + \frac{\partial\ln\lambda}{\partial\phi} + \frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\frac{E^x}{\alpha_4}\right)\right)\right)$$
$$+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi) + \cos^2(\bar{\lambda}K_\varphi)\left(-\frac{1}{E^\varphi}\left(\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\right)^2\frac{E^x}{\alpha_4} + \frac{(E^x)'}{E^\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\left(\frac{2E^x}{\alpha_4}\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right.\right.\right.$$
$$\left.\left.\left.\left.+\frac{\bar{\nu}}{\nu}c^x_{h3} + \frac{\partial\ln\lambda}{\partial\phi} - \frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}\bar{\lambda}^2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)\right)\right)\right] + \lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q, \tag{368}$$

with structure function

$$q^{xx} = \left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi)\frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{(E^\varphi)^2}. \tag{369}$$

The constraint (368) has been successfully polymerized; it is periodic in both K_φ and ϕ and allows for remnants of nonconstant holonomy parameters λ and ν.

The vacuum mass observable associated to (368) is given by

$$\mathcal{M} = d_0 + \frac{d_2}{2}\left(\exp\int dE^x\left(\frac{\alpha_2^x}{2E^x} - \frac{\partial\ln\lambda^2}{\partial E^x}\right)\right)\left(c_f\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} - \cos^2(\bar{\lambda}K_\varphi)\left(\frac{(E^x)'}{2E^\varphi}\right)^2\right)$$
$$+\frac{d_2}{4}\int dE^x\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(\Lambda_0^x + \frac{\alpha_0^x}{E^x}\right)\exp\int dE^x\left(\frac{\alpha_2^x}{2E^x} - \frac{\partial\ln\lambda^2}{\partial E^x}\right)\right), \tag{370}$$

and, when $V = V_q = V^q = 0$, its scalar-field observable by

$$G[\alpha] = \int d^3x\,\alpha\frac{\nu}{\bar{\nu}}\left(\frac{P_\phi}{\cos(\bar{\nu}\phi)} + E^\varphi\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial\phi}\right), \tag{371}$$

where α, d_0, and d_2 are constants. The associated conserved matter current J^μ has the components

$$J^t = \frac{\nu}{\bar{\nu}}\left(\frac{P_\phi}{\cos(\bar{\nu}\phi)} + E^\varphi\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial\phi}\right), \tag{372}$$

$$J^x = \frac{\partial G}{\partial P_\phi}\frac{\partial H}{\partial\phi'} = -\frac{\nu}{\bar{\nu}}\frac{\bar{\lambda}}{\lambda}\lambda_0\frac{\sqrt{E^x}}{2}\cos^2(\bar{\nu}\phi)\cos^2(\bar{\lambda}K_\varphi)\left(-\frac{2}{E^\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\frac{E^x}{\alpha_4}\right.$$
$$\left.+\frac{(E^x)'}{E^\varphi}\left(\frac{2E^x}{\alpha_4}\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x} + \frac{\bar{\nu}}{\nu}c^x_{h3} + \frac{\partial\ln\lambda}{\partial\phi} - \frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}\bar{\lambda}^2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)\right). \tag{373}$$

4. Partial Abelianization

The partial Abelianization of the constraint (365) is easily achieved by using the coefficients (276) under the redefinitions (364) and (313). The resulting Abelianized constraint is given by

$$\begin{aligned}
\frac{H^{(A)}}{\bar{B}c_f} = & -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\Bigg[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}}\left(-V-\Lambda_0^x+\frac{\alpha_0^x}{E^x}\right)+\left(\frac{\alpha_2^x}{E^x}c_f+2\frac{\partial c_f}{\partial E^x}\right)\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right. \\
& +\left(\frac{K_x}{E^\varphi}-\frac{P_\phi}{E^\varphi}\frac{\tan(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}-\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\frac{\partial\ln\lambda}{\partial E^x}\right)4c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} \\
& \left.-\left(\frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}+\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left(\frac{\bar{\nu}}{\nu}c_{h3}^x+\frac{\partial\ln\lambda}{\partial\phi}\right)\right)^2\frac{\alpha_4}{E^x}\frac{\nu^2}{\bar{\nu}^2}c_f\cos^2(\bar{\lambda}K_\varphi)\right) \\
& +\frac{((E^x)')^2}{E^\varphi}\left(\bar{\lambda}^2\frac{K_x}{E^\varphi}\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+\cos^2(\bar{\lambda}K_\varphi)\left(\frac{\partial\ln\lambda}{\partial E^x}-\frac{\alpha_2^x}{4E^x}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\left(\frac{\bar{\nu}}{\nu}c_{h3}^x+\frac{\partial\ln\lambda}{\partial\phi}+\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\frac{E^x}{\alpha_4}\right)\right)\right) \\
& +\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)+\cos^2(\bar{\lambda}K_\varphi)\left(-\frac{1}{E^\varphi}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\right)^2\frac{E^x}{\alpha_4}\right. \\
& \left.\left.+\frac{(E^x)'}{E^\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\left(\frac{2E^x}{\alpha_4}\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}+\frac{\bar{\nu}}{\nu}c_{h3}^x+\frac{\partial\ln\lambda}{\partial\phi}-\frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}\bar{\lambda}^2\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\right)\right)\right] \\
& -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{(E^x)'}{E^\varphi}\left(K_\varphi'-\frac{K_x}{E^\varphi}(E^x)'+\frac{P_\phi}{E^\varphi}\phi'\right)+\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q. \qquad (374)
\end{aligned}$$

This Abelian constraint has kinematical divergences at $K_\varphi = \pm\pi/(2\bar{\lambda})$ in the first line and last line. The latter can be easily resolved by simply restricting the constraint to the case $V_q = 0$. While the divergence of the first line can be treated as in the past section, such that it can be partially resolved if the equation

$$\frac{\partial c_f}{\partial E^x} = \frac{\lambda^2}{2}\left(V+\Lambda_0^x-\frac{\alpha_0^x}{E^x}\right) \qquad (375)$$

is solved for c_f. However, the difference between this equation and the one of the past section (324) is that the former involves the potential V. Recalling that c_f cannot depend on ϕ, we must either exclude the V-term from the equation (leaving it as a divergent term) or restrict the constraint to the free scalar case $V = 0$. Doing this, we recover Eq. (324).

5. Classical limits and conditions

The constraint (368) cannot reproduce the classical-matter limit because it does not have the necessary structure-function terms. It has the following limits:

(i) The classical-geometry limit is given by first performing the canonical transformations (328) and (327), which eliminate $\bar{\nu}$ and $\bar{\lambda}$, respectively, followed by $\lambda_0, c_f \to 1$ and $\lambda, \nu \to 0$. In this limit, we can absorb q into Λ_0 via a canonical transformation.

(ii) The classical-gravity limit is given by the classical-geometry limit together with $\Lambda_0^x \to -\Lambda$, $\alpha_0^x, \alpha_2^x \to 1$, α_4 becoming a constant, and $V(E^x, \phi) \to V(\phi)$ becoming a free function of ϕ only.

(iii) Unlike the constraint of the previous section, (368) has a nontrivial limit of reaching the classical constraint surface. This is given by taking the classical values for all the undetermined functions except λ_0 and $\bar{\lambda}$. The limit correspond precisely to (119).

(iv) The vacuum limit is given by $P_\phi, \phi, V_q \to 0$. However, the constraint (368) does not match the vacuum constraint (222) because it lacks the q-function.

The constraint (368) can easily be Abelianized by imposing the condition (275), which simply requires that we set $q = 0$.

As will be shown in Sec. VI, the constraint (368) develops a singularity at a maximum-curvature surface of spatially homogeneous dynamical solution.

C. Singularity-free constraints

Our final class of examples is given by constraints that have nonsingular space-time solutions at least for homogeneous spatial slices. While this statement does not guarantee complete removal of singularities, it sets this set of modified theories apart from the previous two classes.

We start with assumptions on some of the free functions that are apparently unrelated to the existence of nonsingular solutions. The next section will demonstrate the existence of solutions free of space-time singularities.

1. Anomaly freedom

We use the initial steps of the preceding subsection, but instead of using zero $\bar{h}_2$, we now assume $\bar{h}_2$ to be nonzero and $\bar{h}_4 = 0$. Equations (339) and (341) then imply that $\bar{h}_2$ and $\bar{g}\bar{f}_4$ are independent of K_φ. Equation (343) then has the solution,

$$\bar{g}\bar{f}_4 = -\lambda_0 \frac{E^x}{\alpha_3}, \tag{376}$$

$$\bar{h}_2 = -\bar{\lambda}^2 \frac{\alpha_3}{4E^x}, \tag{377}$$

where α_3 is an undetermined nonvanishing function of E^x and ϕ. We can now solve (340) by

$$\bar{g}\bar{f}_3 = \lambda_0 \left(c_{f3} - \frac{\alpha_3}{E^x} \left(c_f \cos^2(\bar{\lambda}K_\varphi) - 2q\bar{\lambda}^2 \frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} \right) \right), \tag{378}$$

where c_{f3} is an undetermined function of E^x and ϕ. Equation (342) then requires

$$c_{f3} = 0. \tag{379}$$

We next solve the system of equations (333)–(338), solving (336) for $\bar{h}_3$ in terms of $\bar{h}_1$ according to $\bar{g}\bar{h}_3 = (\bar{g}/2\bar{h}_2)\partial\bar{h}_1/\partial K_\varphi$. This solution together with (337) implies,

$$\frac{\bar{g}}{2\bar{h}_2} \frac{\partial^2 \bar{h}_1}{\partial K_\varphi^2} = -\frac{1}{2\bar{h}_2} \frac{\partial \bar{h}_1}{\partial K_\varphi} \frac{1}{2} \frac{\partial \bar{g}}{\partial K_\varphi} + 2\bar{h}_1 \bar{g}\bar{f}_4 - \bar{g}\frac{1}{2} \frac{\partial^2 \ln \bar{g}}{\partial \phi \partial K_\varphi}, \tag{380}$$

with general solution

$$\bar{h}_1 = c_{h1} \sec(\bar{\lambda}K_\varphi) + \bar{\lambda}^2 c_{h3} \frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}, \tag{381}$$

where c_{h1} and c_{h3} are undetermined functions of E^x and ϕ. Inserting this solution back into the previous expression, we obtain

$$\bar{g}\bar{h}_3 = -\lambda_0 \frac{2E^x}{\alpha_3} \left(c_{h3} + c_{h1} \frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} \right). \tag{382}$$

We now solve (335) by

$$\bar{g}\bar{h}_0 = \lambda_0 \left(c_{h0} + 4c_f \cos(\bar{\lambda}K_\varphi) \left(\frac{c_{h1}}{\bar{\lambda}^2} + c_{h3} \frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} \right) + 8q \left(-c_{h1} \frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} + c_{h3} \cos^2(\bar{\lambda}K_\varphi) \right) \right). \tag{383}$$

Using all these results in (338), we find the condition,

$$\begin{aligned} 0 = {} & \bar{\lambda}^2 c_{h0} + 2q\bar{\lambda}^2 \left(2c_{h3} - 3c_{h1} \left(\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} + \frac{\sin(3\bar{\lambda}K_\varphi)}{3\bar{\lambda}} \right) \right) + 4c_{h1} c_f \cos^3(\bar{\lambda}K_\varphi) \\ & - \frac{\alpha_3}{E^x} \cos^2(\bar{\lambda}K_\varphi) \left(\sin(2\bar{\lambda}K_\varphi) \frac{\partial c_f}{\partial \phi} + 2\bar{\lambda} \cos(2\bar{\lambda}K_\varphi) \frac{\partial q}{\partial \phi} \right), \end{aligned} \tag{384}$$

that must be valid for all K_φ, and therefore determines

$$\frac{\partial c_f}{\partial \phi} = \frac{\partial q}{\partial \phi} = c_{h1} = 0, \tag{385}$$

$$c_{h0} = -4qc_{h3}. \tag{386}$$

Finally, we solve the last two remaining equations for anomaly freedom, (333) and (334) by

$$\begin{aligned} \bar{g}\bar{f}_0 &= \lambda_0 \left(-\Lambda_0 + \frac{\alpha_0}{E^x} + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} \left(\frac{\alpha_2}{E^x} c_f + 2\frac{\partial c_f}{\partial E^x} \right) + 2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} \left(\frac{\alpha_2}{E^x} q + 2\frac{\partial q}{\partial E^x} \right) \right), \\ \bar{g}\bar{f}_2 &= \lambda_0 \left(-V - \frac{\alpha_2}{4E^x} \cos^2(\bar{\lambda}K_\varphi) - {c_{h3}}^2 \frac{E^x}{\alpha_3} \right), \end{aligned} \tag{387}$$

where α_0, α_2, Λ_0, and V are undetermined functions of E^x and ϕ.

We now use these results in the case of $V = V_q = 0$ in order to address Eqs. (242)–(249) and (251)–(268) for the existence of a matter observable. Equation (266) is turned into the condition

$$-\cos^2(\bar{\lambda}K_\varphi) \frac{\partial \ln \alpha_3}{\partial \phi} = \frac{\partial \ln \lambda^2}{\partial \phi}, \tag{388}$$

which implies that both α_3 and λ must be independent of ϕ.

The independence of λ on ϕ (as well as that of c_f and q) implies that Eqs. (242)–(249) are trivially satisfied because the B^{-1} factor (250) vanishes. Equation (252) requires that $\bar{g}\bar{f}_2^q$ is independent of ϕ which, together with condition (237) for the existence of a gravitational observable, implies that $\bar{f}_2^q = 0$. Similarly, Eq. (242) requires that $\bar{g}\bar{f}_2^q$ is independent of ϕ and must thus vanish.

In this case, we can introduce a new potential term $\bar{g}\bar{f}_2^q = V^q$, such that we recover the matter symmetry when $V^q = V_q = V = 0$. Finally, the right-hand sides of Eqs. (259)–(268) vanish, implying that all the remaining undetermined functions, except for λ_0, must be independent of ϕ.

2. General Hamiltonian constraint

As in the previous sections, we redefine

$$\begin{aligned}&\lambda_0 \to \lambda_0 \frac{\bar{\lambda}}{\lambda}, \qquad q \to q\frac{\lambda}{\bar{\lambda}}, \qquad \Lambda_0 \to \Lambda_0 \frac{\lambda^2}{\bar{\lambda}^2}, \qquad \alpha_0 \to \alpha_0 \frac{\lambda^2}{\bar{\lambda}^2}, \qquad \alpha_2 \to \alpha_2 - 4E^x \frac{\partial \ln \lambda}{\partial E^x},\\ &V \to V\frac{\lambda^2}{\bar{\lambda}^2}, \qquad V_q \to V_q \frac{\lambda^2}{\bar{\lambda}^2}, \qquad V^q \to V_q \frac{\lambda^2}{\bar{\lambda}^2},\end{aligned} \tag{389}$$

in order to recover all allowed effects of a nonconstant holonomy parameter λ. The Hamiltonian constraint is then

$$\begin{aligned}H = &-\frac{\bar{\lambda}}{\lambda}\lambda_0 \frac{\sqrt{E^x}}{2}\Bigg[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0 + \frac{\alpha_0}{E^x}\right) + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(\left(\frac{\alpha_2}{E^x} - 4\frac{\partial \ln\lambda}{\partial E^x}\right)c_f + 2\frac{\partial c_f}{\partial E^x}\right)\right)\\
&+ 2E^\varphi \frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(\left(\frac{\alpha_2}{E^x} - 2\frac{\partial\ln\lambda}{\partial E^x}\right)\frac{\lambda}{\bar{\lambda}}q + 2\frac{\lambda}{\bar{\lambda}}\frac{\partial q}{\partial E^x}\right) + 4(K_x + P_\phi c_{h3})\left(c_f \frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} + \frac{\lambda}{\bar{\lambda}} q\cos(2\bar{\lambda}K_\varphi)\right)\\
&- \frac{{P_\phi}^2}{E^\varphi}\frac{\alpha_3}{E^x}\left(c_f\cos^2(\bar{\lambda}K_\varphi) - 2\frac{\lambda}{\bar{\lambda}}q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right) - \frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\alpha_2}{4E^x} - \frac{\partial\ln\lambda}{\partial E^x}\right)\cos^2(\bar{\lambda}K_\varphi) - \left(\frac{K_x}{E^\varphi} + \frac{P_\phi}{E^\varphi}c_{h3}\right)\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right.\\
&\left. + \frac{{P_\phi}^2}{(E^\varphi)^2}\bar{\lambda}^2\frac{\alpha_3}{4E^x}\cos^2(\bar{\lambda}K_\varphi)\right) + \left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2} - \frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi) - \frac{(\phi' + c_{h3}(E^x)')^2}{E^\varphi}\frac{E^x}{\alpha_3} - \frac{\lambda^2}{\bar{\lambda}^2}E^\varphi V\Bigg]\\
&+ \lambda_0^2 \frac{E^x}{2}\sqrt{q_{xx}}V_q + \frac{\lambda^2}{\bar{\lambda}^2}\frac{(E^\varphi)^2}{2}\sqrt{q^{xx}}V^q,\end{aligned} \tag{390}$$

with structure function

$$q^{xx} = \frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\left(\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi) - 2\bar{\lambda}^2\frac{\lambda}{\bar{\lambda}}q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\frac{E^x}{(E^\varphi)^2}, \tag{391}$$

where all parameters are free functions of E^x, except for λ_0, V, and V_q, and V^q which may depend on both E^x and ϕ, while $\bar{\lambda}$ is a constant. The classical limit can be obtained in different ways, as discussed below. The matter symmetry is recovered for $V = V_q = V^q = 0$.

3. Partial Abelianization

The partial Abelianization of the constraint (393) is easily achieved by using the coefficients (276) under the redefinitions (313) and (389) and taking $q = 0$ according to the condition (275). The resulting Abelianized constraint is given by

$$\frac{H^{(A)}}{\bar{B}c_f} = -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-V-\Lambda_0+\frac{\alpha_0}{E^x}\right)+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(\left(\frac{\alpha_2}{E^x}-4\frac{\partial\ln\lambda}{\partial E^x}\right)c_f+2\frac{\partial c_f}{\partial E^x}\right)\right)\right.$$
$$+4\left(K_x+\frac{P_\phi}{\cos(\bar{\nu}\phi)}\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}-\frac{\nu^2}{\bar{\nu}^2}\frac{{P_\phi}^2}{E^\varphi\cos^2(\bar{\nu}\phi)}\frac{\alpha_3}{E^x}c_f\cos^2(\bar{\lambda}K_\varphi)$$
$$+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)-\frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\alpha_2}{4E^x}-\frac{\partial\ln\lambda}{\partial E^x}+\frac{\nu^2}{\bar{\nu}^2}\frac{{P_\phi}^2}{(E^\varphi)^2\cos^2(\bar{\nu}\phi)}\bar{\lambda}^2\frac{\alpha_3}{4E^x}\right)\cos^2(\bar{\lambda}K_\varphi)\right.$$
$$\left.-\left(\frac{K_x}{E^\varphi}+\frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)-\frac{1}{E^\varphi}\frac{\bar{\nu}^2}{\nu^2}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'\right.$$
$$\left.\left.+(E^x)'\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)^2\frac{E^x}{\alpha_3}\right]-\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\frac{(E^x)'}{E^\varphi}\left(K_\varphi'-\frac{K_x}{E^\varphi}(E^x)'+\frac{P_\phi}{E^\varphi}\phi'\right)$$
$$+\frac{\tan(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left(\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q+\frac{\lambda^2}{\bar{\lambda}^2}\frac{(E^\varphi)^2}{2}\sqrt{q^{xx}}V^q\right). \tag{392}$$

This Abelian constraint has some kinematical divergences at $K_\varphi = \pm\pi/(2\bar{\lambda})$ coming from the first line and the first term of the last line. The latter can be easily resolved by simply restricting the constraint to the case $V_q = 0$. While the divergence of the first line can be treated as in the past section, such that it can be partially resolved if Eq. (324) is solved for c_f in the free scalar case $V = 0$.

4. Polymerization of the scalar field

As discussed before, we place an upper bound on the absolute value of the scalar field in the constraint (365) by using the redefinition (313). We can then apply the canonical transformation (367), resulting in

$$H = -\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{\sqrt{E^x}}{2}\left[E^\varphi\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(-\Lambda_0+\frac{\alpha_0}{E^x}\right)+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(\left(\frac{\alpha_2}{E^x}-4\frac{\partial\ln\lambda}{\partial E^x}\right)c_f+2\frac{\partial c_f}{\partial E^x}\right)\right)\right.$$
$$+2E^\varphi\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(\left(\frac{\alpha_2}{E^x}-2\frac{\partial\ln\lambda}{\partial E^x}\right)\frac{\lambda}{\bar{\lambda}}q+2\frac{\lambda}{\bar{\lambda}}\frac{\partial q}{\partial E^x}\right)$$
$$+4\left(K_x+\frac{P_\phi}{\cos(\bar{\nu}\phi)}\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)\left(c_f\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}+\frac{\lambda}{\bar{\lambda}}q\cos(2\bar{\lambda}K_\varphi)\right)$$
$$-\frac{\nu^2}{\bar{\nu}^2}\frac{{P_\phi}^2}{E^\varphi\cos^2(\bar{\nu}\phi)}\frac{\alpha_3}{E^x}\left(c_f\cos^2(\bar{\lambda}K_\varphi)-2\frac{\lambda}{\bar{\lambda}}q\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)+\left(\frac{(E^x)'(E^\varphi)'}{(E^\varphi)^2}-\frac{(E^x)''}{E^\varphi}\right)\cos^2(\bar{\lambda}K_\varphi)$$
$$-\frac{((E^x)')^2}{E^\varphi}\left(\left(\frac{\alpha_2}{4E^x}-\frac{\partial\ln\lambda}{\partial E^x}\right)\cos^2(\bar{\lambda}K_\varphi)-\left(\frac{K_x}{E^\varphi}+\frac{P_\phi}{E^\varphi\cos(\bar{\nu}\phi)}\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)\bar{\lambda}^2\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right.$$
$$\left.\left.+\frac{\nu^2}{\bar{\nu}^2}\frac{{P_\phi}^2}{(E^\varphi)^2\cos^2(\bar{\nu}\phi)}\bar{\lambda}^2\frac{\alpha_3}{4E^x}\cos^2(\bar{\lambda}K_\varphi)\right)-\frac{1}{E^\varphi}\frac{\bar{\nu}^2}{\nu^2}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)'+(E^x)'\left(\frac{\nu}{\bar{\nu}}c_{h3}-\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right)^2\frac{E^x}{\alpha_3}-\frac{\lambda^2}{\bar{\lambda}^2}E^\varphi V\right]$$
$$+\lambda_0^2\cos^4(\bar{\nu}\phi)\frac{E^x}{2}\sqrt{q_{xx}}V_q+\frac{\lambda^2}{\bar{\lambda}^2}\frac{(E^\varphi)^2}{2}\sqrt{q^{xx}}V^q, \tag{393}$$

with structure function

$$q^{xx} = \frac{\bar{\lambda}^2}{\lambda^2}\lambda_0^2\left(\left(c_f+\left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi}\right)^2\right)\cos^2(\bar{\lambda}K_\varphi)-2\bar{\lambda}^2\frac{\lambda}{\bar{\lambda}}q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\right)\cos^4(\bar{\nu}\phi)\frac{E^x}{(E^\varphi)^2}. \tag{394}$$

The constraint (393) has been successfully polymerized. It is periodic in both K_φ and ϕ and allows for nonconstant holonomy parameters λ and ν.

The mass observable in vacuum associated with (393) is given by

$$\mathcal{M} = d_0 + \frac{d_2}{2}\left(\exp\int \mathrm{d}E^x\left(\frac{\alpha_2}{2E^x} - \frac{\partial \ln\lambda^2}{\partial E^x}\right)\right)\left(c_f\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + 2\frac{\lambda}{\bar{\lambda}}q\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}} - \cos^2(\bar{\lambda}K_\varphi)\left(\frac{(E^x)'}{2E^\varphi}\right)^2\right)$$
$$+\frac{d_2}{4}\int \mathrm{d}E^x\left(\frac{\lambda^2}{\bar{\lambda}^2}\left(\Lambda_0 + \frac{\alpha_0}{E^x}\right)\exp\int \mathrm{d}E^x\left(\frac{\alpha_2}{2E^x} - \frac{\partial\ln\lambda^2}{\partial E^x}\right)\right), \tag{395}$$

and, when $V = V_q = V^q = 0$, the scalar-field observable is

$$G[\alpha] = \int \mathrm{d}^3x\,\alpha\frac{\nu}{\bar{\nu}}\frac{P_\phi}{\cos(\bar{\nu}\phi)}, \tag{396}$$

where α, d_0, and d_2 are constants. The associated conserved matter current J^μ has the components

$$J^t = \frac{\nu}{\bar{\nu}}\frac{P_\phi}{\cos(\bar{\nu}\phi)}, \tag{397}$$

$$J^x = \frac{\partial G}{\partial P_\phi}\frac{\partial H}{\partial \phi'}$$
$$= \frac{\bar{\nu}}{\nu}\frac{\bar{\lambda}}{\lambda}\lambda_0\cos^2(\bar{\nu}\phi)\frac{(E^x)^{3/2}}{\alpha_3 E^\varphi}\left(\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right)' + (E^x)'\left(\frac{\nu}{\bar{\nu}}c_{h3} - \frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\frac{\partial\ln\nu}{\partial E^x}\right)\right). \tag{398}$$

5. *Classical limits and conditions*

The constraint (393) cannot reproduce the classical-matter limit because it does not have the necessary structure-function terms. It is not compatible with the limit of reaching the classical constraint surface because it does not have the $\bar{h}_4$-term.

The following limits can be realized:

(i) The classical-geometry limit is given by first performing the canonical transformations (328) and (327), which eliminate $\bar{\nu}$ and $\bar{\lambda}$, respectively, followed by the limit $\lambda_0, c_f \to 1$ and $\lambda, \nu \to 0$. In this limit, one can absorb q into Λ_0 via a canonical transformation.

(ii) The classical-gravity limit is given by the classical-geometry limit together with $\Lambda_0 \to -\Lambda$, α_0, $\alpha_2 \to 1$ and α_4 becoming a constant, while $V(E^x,\phi) \to V(\phi)$, $V_q(E^x,\phi) \to V_q(\phi)$, $V^q(E^x,\phi) \to V^q(\phi)$ are turned into free functions of ϕ only.

(iii) The vacuum limit is given by $P_\phi, \phi, V_q \to 0$, recovering the vacuum constraint (222).

The constraint (393) can be Abelianized by imposing the condition (275), which simply requires that we set $q = 0$.

As will be shown in Sec. VI, the constraint (368) is the only one of the three classes derived here that is nonsingular at a maximum-curvature surface of spatially homogeneous dynamical solutions.

VI. DYNAMICAL SOLUTIONS WITH HOMOGENEOUS SPATIAL SLICES

It is always difficult to find sufficiently many analytical solutions for inhomogeneous scalar field theories on a curved background in order to display characteristic physical effects. In our case, the different versions of consistent Hamiltonian constraints contain several new terms that distinguish them from minimally coupled theories of scalar fields on a modified background and which remain in the constraints even for spatially constant fields and backgrounds. In this homogeneous setting, suitable for instance for large-scale cosmological evolution or models of nonrotating interiors of black holes in a specific slicing, the original partial differential equations are reduced to ordinary differential equations that can often be solved exactly. As we will show now, their implications help us to distinguish between different versions of modified constraints.

A. Hamiltonian constraint compatible with the classical-matter limit

Our first class of modified theories is given by Hamiltonian constraints that are compatible with the classical-matter limit. These theories are most closely related to minimally coupled classical matter on a modified background.

1. Equations of motion

To be specific, we use the Hamiltonian constraint (314) compatible with the existence of matter observables and a polymerized scalar field. We only consider the simple case $q = V_q = \Lambda_0 = 0$, $c_f = \alpha_i = 1$ and constant λ_0, $\lambda = \bar{\lambda}$ and $\nu = \bar{\nu}$, looking for homogeneous solutions where $(E^x)' = (E^\varphi)' = P'_\phi = K'_x = K'_\varphi = \phi' = 0$. We call the time coordinate $t_{\rm h}$ and the spatial coordinate $x_{\rm h}$. A dot refers to a derivative with respect to $t_{\rm h}$, and a prime to a derivative with respect to $x_{\rm h}$. It can be shown that the partial gauge fixing,

$$N^x = 0, \qquad N' = 0, \tag{399}$$

allows initial homogeneous data to remain homogeneous during evolution. The conserved scalar charge is $G = P_\phi/\cos(\bar{\nu}\phi)$, such that $\dot{G} = 0$ even locally thanks to spatial homogeneity.

We now restrict ourselves to on shell solutions. The diffeomorphism constraint is automatically satisfied by the homogeneity condition, and we solve the Hamiltonian constraint (304) for

$$K_x = -\frac{E^\varphi}{4E^x}\frac{2\bar{\lambda}}{\sin(2\bar{\lambda}K_\varphi)} \times \left(1 + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} - \frac{G^2}{(E^\varphi)^2}|\cos(\bar{\lambda}K_\varphi)|\right). \tag{400}$$

We write equations of motion with respect to K_φ, using $\dot{A}/\dot{K}_\varphi = {\rm d}A/{\rm d}K_\varphi$ for any phase-space function A. We have

$$\frac{{\rm d}\ln((E^\varphi)^2/\cos^2(\bar{\lambda}K_\varphi))}{{\rm d}(\sin(\bar{\lambda}K_\varphi)/\bar{\lambda})} = 2\frac{\bar{\lambda}}{\sin(\bar{\lambda}K_\varphi)}\left(\left(1-\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\cos^2(\bar{\lambda}K_\varphi)\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} - G^2\frac{\cos(2\bar{\lambda}K_\varphi)}{|\cos(\bar{\lambda}K_\varphi)|}\right) \times \left(\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\cos^2(\bar{\lambda}K_\varphi)\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} + G^2|\cos(\bar{\lambda}K_\varphi)|\right)^{-1} \tag{401}$$

for the combination $(E^\varphi)^2/\cos^2(\bar{\lambda}K_\varphi)$ that appears in the emergent space-time metric,

$$\frac{{\rm d}\ln E^x}{{\rm d}K_\varphi} = -4\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + \frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}G^2|\cos(\bar{\lambda}K_\varphi|)\right)^{-1} \tag{402}$$

for the second configuration variable, and

$$\frac{\rm d}{{\rm d}K_\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right) = -2G\frac{\cos^3(\bar{\lambda}K_\varphi)}{E^\varphi}\left(|\cos(\bar{\lambda}K_\varphi)|\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right) + G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}\right)^{-1} \tag{403}$$

for the scalar field. The dependence on $t_{\rm h}$ is then given by using the solution of

$$\dot{K}_\varphi = -\lambda_0 N\frac{\cos^2(\bar{\nu}\phi)}{2\sqrt{E^x}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + \frac{G^2}{(E^\varphi)^2}|\cos(\bar{\lambda}K_\varphi)|\right). \tag{404}$$

Multiplying Eqs. (403) and (404), we see that the time derivative of $\sin(\bar{\nu}\phi)/\bar{\nu}$ vanishes at the extrema of the sine function. Evolution therefore respects the bounds of this function.

Equation (401) can be solved for E^φ such that

$$\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} = \frac{c_\varphi^2}{4}\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)^{-2}\left(1+\sqrt{1+\frac{4}{c_\varphi^2}\frac{G^2}{|\cos(\bar{\lambda}K_\varphi)|}\left(1+\frac{\bar{\lambda}^2}{\sin^2(\bar{\lambda}K_\varphi)}\right)}\right)^2, \tag{405}$$

where c_φ is the integration constant. We chose the sign of the square root so as to obtain a nonvanishing vacuum limit at $G \to 0$. The classical limit sets $c_\varphi^2 = 2M$. The right-hand side of (405) diverges as $\sec(\bar{\lambda}K_\varphi)$ at $K_\varphi = -\pi/(2\bar{\lambda})$. Multiplying with $\cos^2(\bar{\lambda}K_\varphi)$ shows that E^φ approaches zero at $K_\varphi = -\pi/(2\bar{\lambda})$ and does not diverge, but the relevant combination of E^φ and K_φ in the spatially homogeneous emergent space-time metric is $(E^\varphi)^2/\cos^2(\bar{\lambda}K_\varphi)$, given by the left-hand side of (405) without multiplication by $\cos^2(\bar{\lambda}K_\varphi)$. This combination diverges at $K_\varphi = -\pi/(2\bar{\lambda})$.

We can then use this result in (402) and (403) and directly integrate to get E^x and ϕ. The exact integrations are too complicated. However, it suffices to note that the right-hand sides of (402) and (403) remain finite even at $K_\varphi = -\pi/(2\bar{\lambda})$. The right-hand side of the ϕ-equation vanishes at this value, such that ϕ remains finite, independently of the bounded range of the sine function, and reaches a local maximum at $K_\varphi = -\pi/(2\bar{\lambda})$ if it has initially been increasing. The K_φ-derivative of $\ln(E^x)$ reaches a negative value at $K_\varphi = -\pi/(2\bar{\lambda})$, such that E^x continues to decrease from its initial value in a collapse model, staying finite. The crucial factor in the radial component q_{xx} of the emergent space-time metric is therefore (405) which diverges at $K_\varphi = -\pi/(2\bar{\lambda})$.

2. Internal time gauge

Instead of integrating (404), we can complete the gauge by choosing a new homogeneous time coordinate $t_\varphi = -K_\varphi$. The resulting consistency equation $\dot{K}_\varphi = -1$ then determines the lapse function,

$$N = \frac{1}{\lambda_0}\frac{2\sqrt{E^x}}{\cos^2(\bar{\nu}\phi)}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{G^2}{(E^\varphi)^2}|\cos(\bar{\lambda}K_\varphi)|\right)^{-1}. \tag{406}$$

Since $(E^\varphi)^2 \propto \cos(\bar{\lambda}K_\varphi)$ as $K_\varphi = -\pi/(2\bar{\lambda})$, the lapse function remains finite at $K_\varphi = -\pi/(2\bar{\lambda})$ provided $\phi \neq \pi/(2\bar{\nu})$.

The Ricci scalar of a spatially homogeneous metric of the form $\mathrm{d}s^2 = -N^2\mathrm{d}t_\varphi^2 + q_{xx}\mathrm{d}x^2 + E^x\mathrm{d}\Omega^2$ is given by

$$\begin{aligned} R = -\frac{1}{2N^2}\Bigg((\partial_{t_\varphi}\ln E^x)^2 &+ \left(\partial_{t_\varphi}\ln\frac{N^2}{(E^x)^2}\right)(\partial_{t_\varphi}\ln q_{xx}) \\ &+ (\partial_{t_\varphi}\ln q_{xx})^2 - 2\frac{\ddot{q}_{xx}}{{q_{xx}}^2} \\ &- 4\left(\frac{N^2}{E^x} - (\partial_{t_\varphi}\ln N)(\partial_{t_\varphi}\ln E^x) + \frac{\ddot{E}^x}{(E^x)^2}\right)\Bigg). \end{aligned} \tag{407}$$

At the maximum-curvature surface, $K_\varphi = -\pi/(2\bar{\lambda})$, the Ricci scalar diverges as

$$\begin{aligned} R|_{K_\varphi\approx-\pi/(2\bar{\lambda})} \propto \left(\partial_{t_\varphi}\ln\frac{N^2}{(E^x)^2}\right)(\partial_{t_\varphi}\ln q_{xx}) + ((\partial_{t_\varphi}\ln q_{xx}))^2 \\ - 2\frac{\ddot{q}_{xx}}{{q_{xx}}^2} \sim \tan^2(\bar{\lambda}K_\varphi). \end{aligned} \tag{408}$$

Thus, there is a physical singularity even though K_φ remains finite.

B. Hamiltonian constraints compatible with the limit of reaching the classical constraint surface

Constraints compatible with the limit of reaching the classical constraint surface are closest to modifications obtained from linear combinations of the classical constraints with phase-space dependent coefficients. They may therefore be considered matter versions of the nonsingular black hole models analyzed in [7,8]. However, here we will find that matter implies the existence of a physical singularity.

1. Equations of motion

We use the minimally coupled, polymerized version of the Hamiltonian constraint (368) compatible with the existence of a gravitational observable, considering only the case of $V_q = \lambda_0 = 0$, $\alpha_i^x = 1$ and constant λ_0. As in the previous example, we look for a homogeneous solution where $(E^x)' = (E^\varphi)' = P_\phi' = K_x' = K_\varphi' = \phi' = 0$. The time coordinate is again $t_{\rm h}$, and the spatial coordinate $x_{\rm h}$, a dot referring to derivative with respect to $t_{\rm h}$, a prime to a derivative with respect to $x_{\rm h}$, and the partial gauge fixing $N^x = 0$ and $N' = 0$ allows initial homogeneous data to remain homogeneous during evolution. The conserved charge is $G = P_\phi/\cos(\bar{\nu}\phi)$, such that $\dot{G} = 0$.

We now turn to on shell solutions. The diffeomorphism constraint is automatically satisfied by the homogeneity condition, and we solve the Hamiltonian constraint (368) for

$$K_x = \frac{E^\varphi}{4E^x}\frac{2\bar{\lambda}}{\sin(2\bar{\lambda}K_\varphi)}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}-\frac{G^2}{(E^\varphi)^2}\right). \tag{409}$$

We write the equations of motion using K_φ as the evolution parameter using $\dot{A}/\dot{K}_\varphi = \mathrm{d}A/\mathrm{d}K_\varphi$ for any phase space function A,

$$\begin{aligned} \frac{\mathrm{d}\ln((E^\varphi)^2/\cos^2(\bar{\lambda}K_\varphi))}{\mathrm{d}K_\varphi} &= \left(2\left(1-\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\frac{\bar{\lambda}\cos^2(\bar{\lambda}K_\varphi)}{\tan(\bar{\lambda}K_\varphi)} - G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}\frac{2\bar{\lambda}(1-3\cos(2\bar{\lambda}K_\varphi))}{\sin(2\bar{\lambda}K_\varphi)}\right) \\ &\quad\times\left(\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\cos^2(\bar{\lambda}K_\varphi) + G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}\right)^{-1}, \end{aligned} \tag{410}$$

$$\frac{\mathrm{d}\ln E^x}{\mathrm{d}K_\varphi} = -4\frac{\sin(2\bar{\lambda}K_\varphi)}{2\bar{\lambda}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{G^2}{(E^\varphi)^2}\right)^{-1}, \tag{411}$$

$$\frac{\mathrm{d}}{\mathrm{d}K_\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right) = -2\frac{G}{E^\varphi}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{G^2}{(E^\varphi)^2}\right)^{-1}, \tag{412}$$

where K_φ depends on $t_{\rm h}$ according to the solution of

$$\dot{K}_\varphi = -\lambda_0 N \frac{\cos^2(\bar{\nu}\phi)}{2\sqrt{E^x}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{G^2}{(E^\varphi)^2}\right). \tag{413}$$

Equation (410) can be solved for

$$\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} = \frac{c_\varphi^2}{4}\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)^{-2}\left(1+\sqrt{1+G^2\frac{4}{c_\varphi^2}\left(\frac{2\bar{\lambda}}{\sin(2\bar{\lambda}K_\varphi)}\right)^2\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^2, \tag{414}$$

where c_φ is an integration constant, and we chose the sign of the square root to obtain a nonvanishing vacuum limit if $G\to 0$. The classical limit determines $c_\varphi^2 = 2M$. The expression (414) diverges as $\sec^2(\bar{\lambda}K_\varphi)$, such that E^φ now remains finite at $K_\varphi = -\pi/(2\bar{\lambda})$. There is a clear distinction between this behavior for $G\neq 0$ and the vacuum limit of $G=0$, where E^φ approaches zero at $K_\varphi = -\pi/(2\bar{\lambda})$. For $G=0$, this model is equivalent to the minimal-coupling extension from [6] of the models analyzed in [7,8]. Singularity freedom observed in the latter papers is therefore shown to be unstable under the inclusion of minimally coupled matter.

Equation (409) then shows that K_x diverges as $\sec(\bar{\lambda}K_\varphi)$. Equations (411) and (412) imply that E^x and ϕ remain finite with E^x achieving its minimum value (in a collapse model) at $K_\varphi = -\pi/(2\bar{\lambda})$, while the value of ϕ depends on initial conditions.

2. Internal-time gauge

We complete the gauge by choosing a new time coordinate as $t_\varphi = -K_\varphi$. The consistency equation $\dot{K}_\varphi = -1$ determines the lapse function,

$$N = \frac{1}{\lambda_0}\frac{2\sqrt{E^x}}{\cos^2(\bar{\nu}\phi)}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{G^2}{(E^\varphi)^2}\right)^{-1}, \tag{415}$$

which remains finite at $K_\varphi = -\pi/(2\bar{\lambda})$ provided $\phi\neq\pi/(2\bar{\nu})$.

Using (407) for the expression of the Ricci scalar of a spatially homogeneous metric, we find that at the maximum-curvature surface, $K_\varphi = -\pi/(2\bar{\lambda})$, the Ricci scalar diverges as

$$\begin{aligned} R|_{K_\varphi\approx -\pi/(2\bar{\lambda})} &\propto \left(\partial_{t_\varphi}\ln\frac{N^2}{(E^x)^2}\right)(\partial_{t_\varphi}\ln q_{xx}) + ((\partial_{t_\varphi}\ln q_{xx}))^2 \\ &\quad - 2\frac{\ddot{q}_{xx}}{{q_{xx}}^2} \\ &\sim \tan^2(\bar{\lambda}K_\varphi). \end{aligned} \tag{416}$$

Thus, this hypersurface is a physical singularity for $G\neq 0$, as in the previous example. We emphasize again that the behavior of phase-space functions at the maximum-curvature hypersurface depends significantly on whether G is zero or nonzero. The nonsingular example of $G=0$ is therefore unstable under perturbation by matter terms.

C. Singularity-free Hamiltonian

Our last example of a class of consistent Hamiltonians was not motivated by the existence of specific limits or observables, but we now show that it improves the singularity behavior of the previous two examples.

1. Equations of motion

We again consider a special case, given by $c_f = \alpha_i = 1$, and $\lambda_0 = V = V_q = V^q = q = 0$, and look for a homogeneous solution where $(E^x)' = (E^\varphi)' = P_\phi' = K_x' = K_\varphi' = \phi' = 0$ in terms of a time coordinate $t_{\rm h}$ and a spatial coordinate $x_{\rm h}$, where a dot refers to a derivative with respect to the former and a prime to a derivative with respect to the latter. The partial gauge fixing $N^x = 0$ and $N' = 0$ allows initial homogeneous data to remain homogeneous during evolution. The conserved charge is $G = P_\phi/\cos(\bar{\nu}\phi)$, such that $\dot{G} = 0$.

For on shell solutions, the diffeomorphism constraint is automatically satisfied by the homogeneous condition, and we solve the Hamiltonian constraint, (393), for

$$\begin{aligned} K_x = &-\frac{E^\varphi}{4}\frac{2\bar{\lambda}}{\sin(2\bar{\lambda}K_\varphi)}\left(\frac{1}{2E^x}+\frac{1}{E^x}\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right) \\ &+\frac{G^2}{E^\varphi}\frac{1}{4E^x}\frac{\bar{\lambda}}{\tan(\bar{\lambda}K_\varphi)}. \end{aligned} \tag{417}$$

We now obtain the equations of motion with respect to K_φ, as the evolution parameter using $\dot{A}/\dot{K}_\varphi = {\rm d}A/{\rm d}K_\varphi$ for any phase space function A. After some simplifications, the equations are

$$\frac{\mathrm{d}\ln((E^\varphi)^2)}{\mathrm{d}K_\varphi} = 2\frac{2\bar{\lambda}}{\sin(2\bar{\lambda}K_\varphi)}\frac{\cos(2\bar{\lambda}K_\varphi) - \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} - G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}}{1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}}, \tag{418}$$

$$\frac{\mathrm{d}\ln E^x}{\mathrm{d}(\sin(\bar{\lambda}K_\varphi)/\bar{\lambda})} = -4\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + \frac{G^2}{E_\varphi^2}(1-\sin^2(\bar{\lambda}K_\varphi))\right)^{-1}, \tag{419}$$

and

$$\frac{\mathrm{d}(\sin(\bar{\nu}\phi)/\bar{\nu})}{\mathrm{d}(\sin(\bar{\lambda}K_\varphi)/\bar{\lambda})} = -2\frac{G}{E^\varphi}\cos(\bar{\lambda}K_\varphi)\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}\right)^{-1}, \tag{420}$$

where dependence on t_h is given by the solution of

$$\dot{K}_\varphi = -\lambda_0 N\frac{\cos^2(\bar{\nu}\phi)}{2\sqrt{E^x}}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+G^2\frac{\cos^2(\bar{\lambda}K_\varphi)}{(E^\varphi)^2}\right). \tag{421}$$

Equation (418) can be solved for

$$\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} = \frac{c_\varphi{}^2}{4}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)^{-2}\left(\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}+\sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{4G^2}{c_\varphi^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^2, \tag{422}$$

where c_φ is the integration constant, and we chose the sign of the square root to obtain the correct vacuum limit at $G\to 0$. Unlike in the previous two examples, this function does not diverge at $\bar{\lambda}K_\varphi = \pi/2$.

We can then use this result in (419) to solve for E^x by the complicated function

$$\begin{aligned} E^x = \frac{-c_x c_\varphi{}^{2/\sigma}}{2c_\varphi{}^2\sigma^2}&\left(-\sigma\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}+\sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{4G^2}{c_\varphi{}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^{2+2/\sigma}\\ &\times\left(1+\sigma\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)-\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{4G^2}{c_\varphi{}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)\\ &\times\left(1-\sigma\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)+\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{4G^2}{c_\varphi{}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^{-1}\\ &\times\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)^{-1}\left(\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{2G^2}{c_\varphi{}^2}\left(1+2\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)\right.\\ &\left.-\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}}\sigma\sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}+\frac{4G^2}{c_\varphi{}^2}\left(1+\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^{-1}, \end{aligned} \tag{423}$$

where c_x is a constant of integration and we have introduced $\sigma = \sqrt{1+4G^2/c_\varphi^2}$. Equation (420) can be solved for ϕ by

$$\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}} = \frac{\sin(\bar{\nu}\phi_\mathrm{H})}{\bar{\nu}} + \frac{2G}{c_\varphi\sigma}\ln\left(\frac{\sqrt{4G^2/c_\varphi^2+\sigma^2\sin^2(\bar{\lambda}K_\varphi)/\bar{\lambda}^2}-\sigma|\sin(\bar{\lambda}K_\varphi)|/\bar{\lambda}}{2G/c_\varphi}\right), \tag{424}$$

where ϕ_H is the integration constant, representing the value of the scalar field at $K_\varphi = 0$. Because this expression is bounded by $|\phi| = \pi/(2\bar{\nu})$, it implies a bound on the conserved quantity G and the initial condition ϕ_H.

2. Vacuum limit and homogeneous Schwarzschild gauge

In order to understand the role of the constants of integration, we look at the vacuum limit $\phi, G\to 0$ where the expressions reduce to

$$E^{\varphi} \to c_{\varphi}\left(1+\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2}\right)^{-1}\frac{\sin(2\bar{\lambda}K_{\varphi})}{2\bar{\lambda}}, \tag{425a}$$

and

$$E^x = \frac{-c_x c_{\varphi}^{2+O(G^2)}}{2c_{\varphi}^2(1+O(G^2))}\left(\frac{2G^2}{c_{\varphi}^2}\frac{\bar{\lambda}}{\sin(\bar{\lambda}K_{\varphi})}+O(G^4)\right)^{4+O(G^2)}(2+O(G^4))\left(-\frac{2G^4}{c_{\varphi}^4}\frac{\bar{\lambda}^2}{\sin^2(\bar{\lambda}K_{\varphi})}\left(1+\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2}\right)+O(G^6)\right)^{-1}$$
$$\times\left(1+\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2}\right)^{-1}\left(\frac{2G^4}{c_{\varphi}^4}\frac{\bar{\lambda}^2}{\sin^2(\bar{\lambda}K_{\varphi})}+O(G^6)\right)^{-1} \to c_x\left(1+\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2}\right)^{-2}, \tag{425b}$$

where K_{φ} depends on $t_{\rm h}$ according to

$$\dot{K}_{\varphi} \to -\lambda_0\frac{N}{2\sqrt{c_x}}\left(1+\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2}\right)^2 \tag{425c}$$

for a given N.

Alternatively, we can complete the gauge by assuming the (homogeneous) Schwarzschild condition $E^x = t_{\rm h}^2$ suitable for a black hole interior. We then obtain K_{φ} as a function of $t_{\rm h}$ by imposing the consistency equation $\dot{E}^x = 2t_{\rm h}$, using (423), and then inverting for K_{φ}. We simplify the required inversion by working with the vacuum equations (425b). We obtain

$$\frac{\sin^2(\bar{\lambda}K_{\varphi})}{\bar{\lambda}^2} = \frac{\sqrt{c_x}}{t_{\rm h}} - 1. \tag{426}$$

Inverting this expression for $K_{\varphi}(t_{\rm h})$, we have

$$\frac{E^{\varphi}}{\sqrt{E^x}} = \left(1-\bar{\lambda}^2\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)\right)^{-1/2}\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)^{-1/2}\frac{c_{\varphi}}{\sqrt{c_x}}, \tag{427}$$

and

$$N = \lambda_0^{-1}\left(1-\bar{\lambda}^2\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)\right)^{-1/2}\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)^{-1/2}, \tag{428}$$

The structure function is

$$q^{xx} = \left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)\frac{\lambda_0^2}{c_{\varphi}^2}, \tag{429}$$

and the emergent space-time metric reads

$$\mathrm{d}s^2 = -\left(1-\bar{\lambda}^2\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)\right)^{-1}\left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)^{-1}\frac{\mathrm{d}t_{\rm h}^2}{\lambda_0^2} + \left(\frac{\sqrt{c_x}}{t_{\rm h}}-1\right)^{-1}\frac{{c_{\varphi}}^2\mathrm{d}x_{\rm h}^2}{c_x\lambda_0^2} + t_{\rm h}^2\mathrm{d}\Omega^2. \tag{430}$$

A comparison with the exterior metric (or an application of the mass observable) then sets $c_x = 4M^2$ and $c_{\varphi} = 2M\lambda_0/\mu$ with μ a constant that scales the metric.

3. Internal time gauge

We can instead complete the gauge by using K_{φ} as our time coordinate, $t_{\varphi} = -K_{\varphi}$. The lapse function can then be obtained from the consistency equation $\dot{K}_{\varphi} = -1$,

$$N = \frac{2\sqrt{E^x}\sec^2(\bar{\nu}\phi)/\lambda_0}{1+\sin^2(\bar{\lambda}t_{\varphi})/\bar{\lambda}^2 + (G^2/(E^{\varphi})^2)\cos^2(\bar{\lambda}t_{\varphi})}. \tag{431}$$

The emergent space-time metric is determined by using this lapse function in the time component and the structure function (212) in the radial component, replacing the solutions (422)–(424) with $K_{\varphi} = -t_{\varphi}$. The expression is quite lengthy, but we can obtain meaningful results as follows.

Since the internal time takes the same values as K_{φ}, up to a sign difference, it suffices to restrict ourselves to the range $t_{\varphi} \in (0, \pi/\bar{\lambda})$. Comparing with the classical situation, $t_{\varphi} = 0$ represents the hypersurface matching the horizon of the black hole, while the midpoint $t_{\varphi} = \pi/(2\bar{\lambda})$ is a new hypersurface with maximum-curvature effects (the would-be classical singularity). Continuing through the allowed range, $t_{\varphi} = \pi/\bar{\lambda}$ would be the hypersurface matching the horizon of the black (or white) hole on the other side of the classical singularity in the spirit of [7,8,22]. These characteristic hypersurfaces allow us to take specific limits in their proximity, resulting in tractable equations. For an infalling matter field, we assume $P_{\phi} < 0$ initially, such that ϕ starts growing as a function of K_{φ} but remains bounded.

The geometry of this process is described by the emergent space-time metric, in which the inverse radial component, given by the structure function,

$$q^{xx} = \lambda_0^2 \cos^4(\bar{\nu}\phi) E^x \cos^2(\bar{\lambda}K_\varphi) \frac{1}{(E^\varphi)^2}$$
$$= \lambda_0^2 \cos^4(\bar{\nu}\phi) \frac{4}{c_\varphi^2} E^x \left(1 + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)^2 \left(\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} + \sqrt{\frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2} + \frac{4P_\phi^2}{c_\varphi^2}\left(1 + \frac{\sin^2(\bar{\lambda}K_\varphi)}{\bar{\lambda}^2}\right)}\right)^{-2}$$
$$\to \frac{4\lambda_0^2}{c_\varphi^2} \cos^4(\bar{\nu}\phi_0)(1+\bar{\lambda}^2)^2 \frac{E_0^x}{\bar{\lambda}^2}\left(1 + \sqrt{1 + \frac{4P_\phi^2}{c_\varphi^2}(1+\bar{\lambda}^2)}\right)^{-2}, \tag{432}$$

remains regular, provided $\phi_0 \neq \pi/(2\bar{\nu})$. This conclusion is stable with respect to matter perturbations.

4. Near the maximum-curvature hypersurface

Using the equations of motion, the behavior near the maximum-curvature hypersurface is given by

$$\frac{(E^\varphi)^2}{\cos^2(\bar{\lambda}K_\varphi)} \approx \frac{{c_\varphi}^2}{4}\left(\frac{\bar{\lambda}}{1+\bar{\lambda}^2}\right)^2\left(1 + \sqrt{1 + \frac{4G^2}{c_\varphi^2}(1+\bar{\lambda}^2)}\right)^2, \tag{433}$$

and

$$E^x \approx -\frac{\bar{\lambda}^2 c_x}{4(1+\bar{\lambda}^2)c_\varphi^2(c_\varphi^2+4G^2)}\left(\frac{\sqrt{c_\varphi^2 + 4(1+\bar{\lambda}^2)G^2} - \sqrt{c_\varphi^2+4G^2}}{\bar{\lambda}}\right)^{2c_\varphi/\sqrt{c_\varphi^2+4G^2}}$$
$$\times \frac{\bar{\lambda}^2 c_\varphi\sqrt{c_\varphi^2+4G^2} + (1+\bar{\lambda}^2)(c_\varphi^2+4G^2) - \sqrt{c_\varphi^2+4G^2}\sqrt{c_\varphi^2+(1+\bar{\lambda}^2)4G^2}}{\bar{\lambda}^2 c_\varphi\sqrt{c_\varphi^2+4G^2} - (1+\bar{\lambda}^2)(c_\varphi^2+4G^2) + \sqrt{c_\varphi^2+4G^2}\sqrt{c_\varphi^2+(1+\bar{\lambda}^2)4G^2}} \tag{434}$$

for the gravitational fields, and

$$\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}} \approx \frac{\sin(\bar{\nu}\phi_{\rm H})}{\bar{\nu}} + \frac{2G/c_\varphi}{\sqrt{1+4G^2/c_\varphi^2}}\ln\left(\frac{\sqrt{1+(4G^2/c_\varphi^2)(1+\bar{\lambda}^2)} - \sqrt{1+4G^2/c_\varphi^2}}{2\bar{\lambda}|G|/c_\varphi}\right) \tag{435}$$

for the scalar field. The lapse function, appearing in the time component of the emergent space-time metric, has the limit

$$N \approx \frac{2}{\lambda_0}\frac{\bar{\lambda}^2}{1+\bar{\lambda}^2}\sqrt{E^x}\sec^2(\bar{\nu}\phi) \tag{436}$$

and we have the time derivatives

$$\frac{{\rm d}((E^\varphi)^2/\cos^2(\bar{\lambda}t_\varphi))}{{\rm d}t_\varphi} \approx 0, \tag{437a}$$

$$\frac{{\rm d}E^x}{{\rm d}t_\varphi} \approx 0, \tag{437b}$$

$$\frac{\rm d}{{\rm d}t_\varphi}\left(\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}}\right) \approx 0, \tag{437c}$$

at first order, as well as

$$
\begin{aligned}
&\frac{\mathrm{d}^2((E^\varphi)^2/\cos^2(\bar\lambda t_\varphi))}{\mathrm{d}t_\varphi{}^2} \qquad (437\mathrm{d})\\
&= -\frac{(E^\varphi)^2}{\cos^2(\bar\lambda t_\varphi)}\Bigg(2\bar\lambda^2\sec^2(\bar\lambda t_\varphi) - 8\bar\lambda^2\frac{\cos(2\bar\lambda t_\varphi)}{\sin^2(2\bar\lambda t_\varphi)}\frac{\cos(2\bar\lambda t_\varphi) - \sin^2(\bar\lambda t_\varphi)/\bar\lambda^2 - G^2\cos^2(\bar\lambda t_\varphi)/(E^\varphi)^2}{1+\sin^2(\bar\lambda t_\varphi)/\bar\lambda^2 + G^2\cos^2(\bar\lambda t_\varphi)/(E^\varphi)^2}\\
&\quad + 4\frac{2(1+\bar\lambda^2) - G^2\bar\lambda\cos^2(\bar\lambda t_\varphi)/(\sin(2\bar\lambda t_\varphi)(E^\varphi)^2)\mathrm{d}\ln((E^\varphi)^2/\cos^2(\bar\lambda t_\varphi))/\mathrm{d}t_\varphi}{1+\sin^2(\bar\lambda t_\varphi)/\bar\lambda^2 + G^2\cos^2(\bar\lambda t_\varphi)/(E^\varphi)^2}\\
&\quad + 2\frac{\cos(2\bar\lambda t_\varphi) - \sin^2(\bar\lambda t_\varphi)/\bar\lambda^2 - G^2\cos^2(\bar\lambda t_\varphi)/(E^\varphi)^2}{(1+\sin^2(\bar\lambda t_\varphi)/\bar\lambda^2 + G^2\cos^2(\bar\lambda t_\varphi)/(E^\varphi)^2)^2}\left(4 - \frac{2G^2\bar\lambda}{\sin(2\bar\lambda t_\varphi)}\frac{\mathrm{d}\ln((E^\varphi)^2/\cos^2(\bar\lambda t_\varphi))}{\mathrm{d}t_\varphi}\right)\Bigg)\\
&\approx -c_\varphi{}^2\frac{\bar\lambda^6}{(1+\bar\lambda^2)^3}\left(1+\sqrt{1+\frac{4G^2}{c_\varphi^2}(1+\bar\lambda^2)}\right)^4\left(\left(1+\sqrt{1+\frac{4G^2}{c_\varphi^2}(1+\bar\lambda^2)}\right)^2 + \frac{4}{c_\varphi{}^2}G^2(1+\bar\lambda^2)\right)^{-1}\\
&= -\bar\lambda^2\frac{(E^\varphi)^2}{\cos^2(\bar\lambda K_\varphi)}\frac{\mathrm{d}^2E^x}{\mathrm{d}t_\varphi{}^2}, \qquad (437\mathrm{e})
\end{aligned}
$$

$$
\frac{\mathrm{d}^2E^x}{\mathrm{d}t_\varphi{}^2} \approx 4E^x\frac{\bar\lambda^2}{1+\bar\lambda^2}\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)^2\left(\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)^2 + \frac{4G^2(1+\bar\lambda^2)}{c_\varphi{}^2}\right)^{-1}. \tag{437f}
$$

$$
\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}t_\varphi{}^2}\left(\frac{\sin(\bar\nu\phi)}{\bar\nu}\right) &\approx -4G\bar\lambda\sin(\bar\lambda t_\varphi)\frac{E^\varphi}{\cos(\bar\lambda t_\varphi)}\left(\left(1+\frac{\sin^2(\bar\lambda t_\varphi)}{\bar\lambda^2}\right)\frac{(E^\varphi)^2}{\cos^2(\bar\lambda t_\varphi)} + G^2\right)^{-1}\\
&\approx -4\bar\lambda^2\frac{2G}{c_\varphi}\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)\left(\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)^2 + \frac{4G^2(1+\bar\lambda^2)}{c_\varphi{}^2}\right)^{-1}\\
&= -\frac{1+\bar\lambda^2}{E^x}\frac{2G}{c_\varphi}\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)^{-1}\frac{\mathrm{d}^2E^x}{\mathrm{d}t_\varphi{}^2},
\end{aligned} \tag{437g}
$$

at second order. It will also be useful to compute

$$
\dot q^{xx} = q^{xx}\left(\frac{\dot E^x}{E^x} - \frac{\cos^2(\bar\lambda t_\varphi)}{(E^\varphi)^2}\frac{\mathrm{d}((E^\varphi)^2/\cos^2(\bar\lambda t_\varphi))}{\mathrm{d}t_\varphi} - 4\bar\nu^2\frac{\tan(\bar\nu\phi)}{\bar\nu\cos(\bar\nu\phi)}\frac{\mathrm{d}}{\mathrm{d}t_\varphi}\left(\frac{\sin(\bar\nu\phi)}{\bar\nu}\right)\right) \approx 0 \tag{438}
$$

and

$$
\begin{aligned}
\ddot q^{xx} &\approx q^{xx}\left(\frac{\ddot E^x}{E^x} - \frac{\cos^2(\bar\lambda t_\varphi)}{(E^\varphi)^2}\frac{\mathrm{d}^2((E^\varphi)^2/\cos^2(\bar\lambda t_\varphi))}{\mathrm{d}t_\varphi{}^2} - 4\bar\nu^2\frac{\tan(\bar\nu\phi)}{\bar\nu\cos(\bar\nu\phi)}\frac{\mathrm{d}^2}{\mathrm{d}t_\varphi{}^2}\left(\frac{\sin(\bar\nu\phi)}{\bar\nu}\right)\right)\\
&\approx (1+\bar\lambda^2)q^{xx}\frac{\ddot E^x}{E^x}\left[1 + 4\bar\nu^2\frac{\tan(\bar\nu\phi)}{\bar\nu\cos(\bar\nu\phi)}\frac{2G}{c_\varphi}\left(1+\sqrt{1+\frac{4G^2(1+\bar\lambda^2)}{c_\varphi^2}}\right)^{-1}\right],
\end{aligned} \tag{439}
$$

which is finite.

Using (407) for the expression of the Ricci scalar of a spatially homogeneous metric we find that it is finite at the maximum-curvature hypersurface,

$$
R \approx \left(\frac{2}{E^x} + 2N^{-2}\frac{\ddot E^x}{(E^x)^2} - N^{-2}\ddot q^{xx}\right). \tag{440}
$$

Thus, the Ricci scalar is finite even in the presence of matter and when $\phi = \pi/(2\bar\nu)$. In this limiting case, we obtain

$$R\big|_{t_\varphi=\pi/(2\bar{\lambda}),\phi=\pi/(2\bar{\nu})} = \frac{2}{E^x}\bigg|_{t_\varphi=\pi/(2\bar{\lambda})}. \tag{441}$$

We conclude that the coordinate singularity at $\phi = \pi/(2\bar{\nu})$ is due to the scalar field reaching its maximal value when or before K_φ reaches its own maximum. In this case, ϕ would be a better indicator of the transition if it were used as an internal time instead of K_φ. The equations of motion with ϕ as the internal time are more complicated, but the solution would be qualitatively similar, just replacing K_φ with ϕ as the time coordinate.

5. Bounded-curvature and bounded-scalar effects

The solution (424) can be inverted,

$$\begin{aligned}\frac{\sin(\bar{\lambda}K_\varphi)}{\bar{\lambda}} &= -\frac{\sinh\left((\sin(\bar{\nu}\phi)/\bar{\nu} - \sin(\bar{\nu}\phi_{\rm H})/\bar{\nu})\sqrt{1+c_\varphi^2/(4G^2)}\right)}{\sqrt{1+c_\varphi^2/4G^2}} \\ &= -\frac{\sinh\left((\sin(\bar{\nu}\phi)/\bar{\nu} - \sin(\bar{\nu}\phi_{\rm H})/\bar{\nu})\sqrt{1+M^2\lambda_0^2/(\mu^2G^2)}\right)}{\sqrt{1+M^2\lambda_0^2/(\mu^2G^2)}}. \end{aligned} \tag{442}$$

If the mass M is considered to be supplied primarily by the scalar field, then we must have $\mu|G| \sim M$. Furthermore, the left-hand side of this expression is bounded, implying the inequality

$$\frac{1}{\bar{\lambda}} \gtrsim \frac{1}{\sqrt{2}}\sinh\left(\frac{1}{\sqrt{2}}\frac{\sin(\bar{\nu}\phi)}{\bar{\nu}} - \frac{1}{\sqrt{2}}\frac{\sin(\bar{\nu}\phi_{\rm H})}{\bar{\nu}}\right). \tag{443}$$

(The right-hand side is also bounded as a function of ϕ, but the gravitational bound is more universal as it may apply to multiple matter fields, and it is more instructive regarding space-time singularities.) The maximum effect of the scalar field is achieved at $\phi = \phi/(2\bar{\nu}) \gg \phi_H$. In this extreme case we have

$$\frac{1}{\bar{\lambda}} \gtrsim \frac{1}{\sqrt{2}}\sinh\left(\frac{1}{\sqrt{2}\bar{\nu}} - \frac{1}{\sqrt{2}}\frac{\sin(\bar{\nu}\phi_{\rm H})}{\bar{\nu}}\right). \tag{444}$$

Since we expect $\bar{\lambda}, \bar{\nu} \ll 1$, we can approximate this expression by

$$\frac{1}{\bar{\lambda}} \gtrsim \frac{1}{2\sqrt{2}}\exp\left(\frac{1}{\sqrt{2}\bar{\nu}}\right). \tag{445}$$

This result imposes a theoretical limit on the value of $\bar{\nu}$ in terms of $\bar{\lambda}$, as given by the specific dynamical solution to this model. Since $\bar{\lambda}$ is then exponentially smaller than $\bar{\nu}$, we can expect its effects to be in general much weaker. Nonclassical matter properties are therefore more pronounced in the extreme case of ϕ reaching its maximal value, compared with gravitational effects, in parallel with standard quantum effects that are usually more relevant for matter than for gravity, as seen for instance in various applications of quantum matter fields on a curved background in early Universe cosmology. Scalar collapse into a black hole should therefore be a promising line of research in emergent modified gravity.

VII. A NEW OUTLOOK ON SCALAR-TENSOR THEORIES

We have demonstrated that there are many interesting and previously unrecognized theories of spherically symmetric emergent modified gravity coupled to a scalar field. This outcome suggests several new options for scalar-tensor theories that may be useful for phenomenological studies in astrophysics and cosmology. Our new theories do not go beyond the second-order nature of field equations and do not encounter the Ostrogradski problem [37]. In some cases, they have intriguing new features such as the absence of physical singularities and, as shown in [25], make it possible to implement intermediate-scale modifications of general relativity such as MOND.

A new challenge that so far has not been explored much, but could be the origin of new and useful physical effects, is a possible dependence of the emergent space-time metric on the scalar field. Such a dependence is not always necessary but may be implied indirectly by additional physical requirements, as demonstrated in our specific classes of modified theories. In some of these cases, the same conditions also imply deviations of consistent scalar-field couplings from minimal coupling to the emergent space-time metric.

We found that physical conditions on the combined gravity-matter theory sometimes rule out minimal coupling of a scalar field, as seen for instance in (304) for constraints compatible with the classical-matter limit, where the matter terms,

$$\sqrt{q^{xx}}(\alpha_3 P_\phi{}^2/E^x + \alpha_3^{-1}(\phi')^2 E^x) + \lambda_0^2 E^x \sqrt{q_{xx}} V_q, \tag{446}$$

must separate different dependencies on E^x and ϕ, such that α_3 may depend only on E^x and λ_0 on both E^x and ϕ. In terms of the spatial part q_{ab} of the emergent space-time metric, the factors of $\sqrt{q^{xx}}/E^x = 1/\sqrt{\det q}$ in the kinetic term, of $\sqrt{q^{xx}}E^x = q^{xx}\sqrt{\det q}$ in the spatial-derivative term and of $\sqrt{q_{xx}}E^x = \sqrt{\det q}$ are as expected for minimal coupling, even in cases in which the structure function q^{xx} depends on K_φ and ϕ. However, all terms considered, we do not have minimal coupling unless $\alpha_3 = 1$ and $\lambda_0 = 1$. Polymerization of the scalar field, (316), then generates completely new terms in the modified Hamiltonian constraint, such as those linear in P_ϕ.

In other classes of modified constraints, minimal coupling is completely ruled out, for instance in the constraints (365) which requires a term of the form $P_\phi \phi'$ for any modification with $\bar{\lambda} \neq 0$, or in the singularity-free constraints (390) which have a simple $1/\alpha_3$-modification of the $(\phi')^2$-term,

$$\frac{\bar{\lambda}\lambda_0}{\lambda} \frac{(E^x)^{3/2}}{E^\varphi} \frac{(\phi')^2}{\alpha_3}, \tag{447}$$

with the classical-type metric factor $q^{xx}_{\rm class}\sqrt{\det q_{\rm class}} = (E^x)^{3/2}/E^\varphi$ not using the emergent spatial metric, but a more complicated P_ϕ^2-term,

$$\begin{aligned} &\frac{\alpha_3 \bar{\lambda}\lambda_0}{\lambda} \frac{P_\phi^2}{E^\varphi \sqrt{E^x}} \left(\left(c_f + \left(\frac{\bar{\lambda}(E^x)'}{2E^\varphi} \right)^2 \right) \cos^2(\bar{\lambda} K_\varphi) \right. \\ &\quad \left. - 2 \frac{\lambda}{\bar{\lambda}} q \bar{\lambda}^2 \frac{\sin(2\bar{\lambda} K_\varphi)}{2\bar{\lambda}} \right) \\ &= \frac{\alpha_3 \lambda}{\bar{\lambda}\lambda_0} q^{xx} \frac{E^\varphi}{(E^x)^{3/2}} P_\phi^2 = \frac{\alpha_3 \lambda}{\bar{\lambda}\lambda_0} \frac{\sqrt{\det q_{\rm class}}}{\det q} \end{aligned} \tag{448}$$

that makes use of a combination of the emergent and the classical spatial metric. The classical-type potential term $(\lambda\lambda_0/\bar{\lambda})\sqrt{E^x}E^\varphi V$ in this case just uses the classical volume element $\sqrt{\det q_{\rm class}} = \sqrt{E^x}E^\varphi$ rather than the emergent spatial metric, as in the $(\phi')^2$-term, but it has an extra factor of $\lambda^2\bar{\lambda}^2$ compared with the latter, potentially changing its E^x-dependence through λ. Moreover, there is a possibility of two new scalar potentials in

$$\lambda_0^2 \frac{E^x}{2} \sqrt{q_{xx}} V_q + \frac{\lambda^2}{\bar{\lambda}^2} \frac{(E^\varphi)^2}{2} \sqrt{q^{xx}} V^q \tag{449}$$

that do make use of the emergent spatial metric q_{xx}, one with the expected emergent spatial volume element $E^x\sqrt{q_{xx}}$ and one with the combination $(E^\varphi)^2\sqrt{q^{xx}} = \det q_{\rm class}/\sqrt{\det q}$ of a geometric mean of the two determinants. Some of these equations resemble bimetric theories, but only for spatial metric tensors in nonstandard couplings in the constraints. These theories are not bimetric in the usual meaning because only the emergent metric q_{xx} has a consistent space-time extension in our theories, but not the classical metric $q_{xx}^{\rm class}$.

So far, it remains unclear how emergent modified gravity could be constructed explicitly without restrictions such as symmetry reduction. However, in cases in which the emergent space-time metric does not depend on the scalar field, it is possible to use a spherically symmetric modified solution as a background for a nonspherical scalar field provided backreaction can be ignored. For a scalar-independent emergent space-time line element, the scalar coupling can be minimal and derived from a standard action,

$$S[\phi] = \frac{1}{2}\int {\rm d}^4x \sqrt{-\det g}(g^{\mu\nu}(\nabla_\mu\phi)(\nabla_\nu\phi) + V(\phi)), \tag{450}$$

with a spherically symmetric emergent space-time metric $g_{\mu\nu}$ and a nonspherical scalar field ϕ. More generally, it is possible to use a scalar-dependent emergent space-time metric as a spherically symmetric background for additional minimally coupled scalar fields that do not backreact on the background and may be nonspherical. The background can then be considered a scalar-tensor description of space-time geometry, on which other matter scalar fields evolve. If the emergent metric depends on the first scalar field, minimal coupling of matter scalar fields then implies characteristic coupling terms between all the scalar fields. There are therefore many new possibilities for scalar-tensor theories and their phenomenology.

VIII. DISCUSSION

We have extended emergent modified gravity in spherically symmetric space-times by including a scalar matter field, suggesting several consistency conditions for physically meaningful modifications of general relativity coupled to a Klein-Gordon field. Most importantly, we derived the condition that the Hamiltonian constraint must satisfy for both gravity and the scalar field to be covariant, given by Eq. (12). We studied implications of the hypersurface-deformation brackets (83) and the specific covariance conditions (93)–(95) in the general second-order Hamiltonian constraint (125) for spherically symmetric models with a scalar field. These conditions, together with factoring out diffeomorphism-preserving canonical transformations (178), completely determine the general Hamiltonian constraint (238) and its structure function (212) up to several free functions of the radial configuration variable E^x and the scalar field ϕ. The structure function, together with a lapse function according to gauge conditions or solutions of the equations of motion, determines the emergent space-time metric (92).

The general setting of emergent modified gravity allows for several modification functions that are introduced in a technical way through the terms by which they appear in the Hamiltonian constraint. There are certain differences between different classes of modification functions. For instance the modification functions λ_0, c_f, q, and λ are characteristic of emergent modified gravity because they appear directly in the emergent metric and hence have no counterpart in general relativity. The functions α_0 and α_2, by contrast, survive even when the metric is rendered classical. These functions can be identified with the extensively studied dilaton potential of two-dimensional gravity models, or as inverse-triad corrections of loop quantum gravity. The functions ν and λ may also be related to effects expected from loop quantum gravity, in this case holonomy modifications. The fact that these terms do appear in the emergent metric highlights the additional subtlety of holonomy terms compared with inverse-triad corrections as well as their more challenging nature regarding compatibility with general covariance. Another source of specific modification function of the kind found here may be Hamiltonian renormalization, which in emergent modified gravity can lead to more general functions then expected in the traditional approach [25]. Further analysis of dynamical solutions as well as phenomenological studies may be used to provide additional characterizations of the modification functions and all the effects of emergent modified gravity.

As a new observation related to matter couplings, the emergent space-time metric in general depends not only on the gravitational phase-space degrees of freedom but also on the scalar field through some of the free functions of a modified theory. This unexpected feature is realized even at the kinematical level before any field equations are solved, using only covariance conditions for the space-time line element. While it is possible to assume that all free functions of a modified Hamiltonian constraint that also appear in the emergent space-time metric are independent of the matter field, this property is not generic and therefore not representative of an effective theory of gravity coupled to scalar matter. Moreover, we have shown in specific classes of modified theories that this choice violates physically desirable conditions, mainly the existence of certain limits and observables. Therefore, if we view emergent modified gravity as a collection of possible effective theories that can describe covariant implications of quantum gravity, our result implies that a quantum-gravity theory coupled to scalar matter cannot have a space-time geometry derived solely from the fundamental gravitational degrees of freedom, assumed to set up the canonical theory by a phase-space formulation. The off shell constraint system, rather than the kinematical phase space alone, determines the meaning of gravity, geometry, and matter. Possible extensions to multiple matter fields of different kinds, including fermions perhaps with supersymmetry, present an interesting but still open question.

This outcome presents a new viewpoint on possible implications of modified or quantum gravity. One of the most important features we have come to understand from general relativity is that gravity is the geometry of space-time, which may be dynamically affected by matter but does not directly depend on the matter fields. Implicitly, higher-curvature or other traditional effective actions use this observation as an assumption because they are built on the basic statement that there is a space-time metric that directly appears as a fundamental degree of freedom for a gravitational action, coupled in different ways to matter fields. Our result shows that this assumption is not necessary, so far at least in spherically symmetric models, and rules out a large class of emergent modified theories. The kinematical equivalence of gravity and space-time geometry need no longer hold in quantum gravity, depending on the quantization procedure: According to the examples of (315), (369), and (394) space-time geometry is gravity and matter in particular in covariant models with characteristic modifications suggested by loop quantum gravity.

For instance, if one computes the volume of a certain space-time region in emergent modified gravity, one must know the gravitational field and the scalar field in that region. In practice, we would have two independent measurements, one of the volume in terms of distances and one of the energy or density of matter. In general relativity, volume measurements allow us to draw conclusions about the metric in a given coordinate system, with a direct connection with the gravitational field in this case. The same field appears in energy or density expressions for matter, which allow us to compute the values of matter fields from volume and density measurements. In emergent modified gravity, however, the metric and density depend nontrivially on both the gravitational and matter fields. Extracting the field values from measurements is therefore a more involved procedure. The new property also implies that field equations for matter are more challenging even for a free field without self-interactions and if dynamical backreaction on the gravitational degrees of freedom is ignored. If metric coefficients in the field equations depend not only on a background gravitational fields but also on the matter field, even free-field equations on a background are nonlinear. As another example, geodesic motion of test masses or light rays is determined by the emergent metric because it provides the only valid space-time geometry in emergent modified gravity. In models in which the emergent metric depends on the gravitational and matter variables, matter distributions would nontrivially affect the dynamics of these objects.

Conceptually, the result is a step towards unification of gravity and matter, given by a relational theory in which space-time is an emergent concept derived from the fundamental fields on phase space. Space-time becomes identical with gravity only in the vacuum limit, but even in this case the emergent metric depends nontrivially on both the configuration and momentum degrees of freedom of gravity. The dependence simplifies to the well-known configuration dependence of general relativity only in the complete classical limit of gravity and matter.

In some cases, we were able to obtain complete solutions of the field equations, but given the complexity of gravity-matter coupling in this framework, this was possible only in the simple (yet instructive) case of a space-time slicing that allows spatially homogeneous fields. In this setting, we found that different classes of scalar couplings in emergent modified gravity imply different conclusions about the fate of classical singularities. In specific examples, we demonstrated instability of vacuum results about singularity avoidance under matter perturbations, while one new class was able to maintain a singularity-free homogeneous behavior even in the presence of unrestricted matter.

Given the vast set of new covariant theories in spherical symmetry, many physical implications can now be explored. It remains to be seen how covariant modified gravity, for instance with terms such as point holonomies or partial Abelianizations motivated by loop quantum gravity, describes cosmological inhomogeneity in an expanding universe, the collapse of matter into a black hole, a modified form of Hawking radiation in models of black hole evaporation, or critical properties of gravitational collapse studied numerically in [38] using a model now known to violate covariance [39]. We expect that the kinematical dependence of space-time on the scalar field will imply new and previously unforeseen challenges to these questions, such as a suitable treatment of Hawking radiation.

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