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Hamiltonian analysis of curvature-squared gravity with or without conformal invariance

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We analyze gravitational theories with quadratic curvature terms, including the case of conformally invariant Weyl gravity, motivated by the intention to find a renormalizable theory of gravity in the ultraviolet region, yet yielding general relativity at long distances. In the Hamiltonian formulation of Weyl gravity, the number of local constraints is equal to the number of unstable directions in phase space, which in principle could be sufficient for eliminating the unstable degrees of freedom in the full nonlinear theory. All the other theories of quadratic type are unstable—a problem appearing as ghost modes in the linearized theory. We find that the full projection of the Weyl tensor onto a three-dimensional hypersurface contains an additional fully traceless component, given by a quadratic extrinsic curvature tensor. A certain inconsistency in the literature is found and resolved: when the conformal invariance of Weyl gravity is broken by a cosmological constant term, the theory becomes pathological, since a constraint required by the Hamiltonian analysis imposes the determinant of the metric of spacetime to be zero. In order to resolve this problem by restoring the conformal invariance, we introduce a new scalar field that couples to the curvature of spacetime, reminiscent of the introduction of vector fields for ensuring the gauge invariance.

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I. INTRODUCTION

One of the most interesting theories of gravity is the Weyl gravity [1], whose action is defined by the square of the Weyl tensor, $S=-\frac{1}{4}\int d^4x\sqrt{-g}C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma}$. The intriguing property of this theory is its invariance under the local conformal transformation of the metric, $g_{\mu\nu}\to\Omega^2(x)g_{\mu\nu}$, making it consequently insensitive to the angles. Furthermore, it is a power-counting renormalizable theory of gravity thanks to the presence of higher-order derivatives in the Lagrangian. Hence, it can be considered as an ultraviolet completion of gravity. For a review, see [2] and references therein. More generally, perturbative renormalization of general relativity requires us to add to the Einstein-Hilbert Lagrangian invariant counterterms that are quadratic in curvature [3–5]. Furthermore, Weyl gravity is also useful for the supergravity construction [6,7] and it also emerges from the twistor string theory [8].

Weyl gravity is a special case of higher-derivative theories of gravity which have been extensively studied, especially in the case of three dimensions. One such example is the new massive gravity in three dimensions [9], whose Lagrangian includes quadratic curvature terms that contain four-derivative contributions. There also exists a recent example of four-dimensional higher-derivative gravity, which is a combination of the Einstein gravity with cosmological constant, together with the contribution of the Weyl tensor squared term. An appropriate fine-tuning of the cosmological constant and the coefficient of the Weyl term produces the so-called critical gravity, where the additional massive spin-2 excitations around an anti–de Sitter background become massless [10]. The relation of such critical gravity to conformal gravity in four-dimensional spacetime has been studied in [11]. Recently it has been proposed that one can obtain solutions of four-dimensional Einstein gravity with cosmological constant by introducing a simple Neumann boundary condition into the conformally invariant Weyl gravity [12]. In a somewhat similar fashion, it has been argued that one can obtain ghost-free four-dimensional massive gravity by introducing Dirichlet boundary conditions into curvature-squared gravity on an asymptotically de Sitter spacetime [13]. Weyl action is also an important object in recent proposals, that relates the conformal symmetry group, gravity and particle physics [14,15]. It is possible that this idea is closely related to the earlier proposal by Sakharov on the generation of both Einstein-Hilbert action and higher-order curvature terms from the quantum fluctuations of vacuum when space is curved [16]. For further works on the generation of Einstein gravity as a quantum effect, see [17–19].

The inclusion of higher-order curvature terms is generally motivated by string theory, since such terms are known to appear in the low energy limit [20,21].

On the other hand, the price that we have to pay in order to achieve a renormalizable theory of gravity is the inclusion of extra gravitational degrees of freedom.

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They appear because of the higher-order time derivatives present in the Lagrangian. Moreover, those extra degrees of freedom often have negative kinetic terms, and are usually referred to as ghosts when the linearized theory is quantized. Typically, theories with ghosts are considered to be inconsistent, since they are either violently unstable or nonunitary, depending on whether the states associated with the higher-derivative degrees of freedom are considered to possess negative energy or positive energy but indefinite norm. However, there are attempts how to resolve this problem as for example in [22]; see also [23,24].

It is important to stress that there is an alternative way to construct a renormalizable theory of gravity, which is called Hořava-Lifshitz gravity [25,26]. It achieves renormalizability via reduction of the gauge symmetry. Since the theory is invariant under foliation preserving diffeomorphisms, one can exclude higher-order time derivatives from the action, avoiding the ghost problem. The lack of full diffeomorphism invariance has significant consequences for the structure of the theory. For reviews, see [27,28]. The Hamiltonian formulation of Hořava-Lifshitz gravity has been studied particularly in [29,30]. For a review, see [31]. Generalized Hořava-Lifshitz gravitational theories were proposed and analyzed in [32–35]. Proposals of covariant alternatives to Hořava-Lifshitz gravity were presented in [36,37] and their Hamiltonian structure was studied in [38,39].

Previous lines suggest that gravitational theories involving higher-order curvature terms are very interesting and deserve to be studied from different points of view. An important question is to understand their Hamiltonian dynamics. The strong coupling limit of conformal gravity was considered first in [40]. The Hamiltonian formulation of the higher-derivative theories of gravity (up to quadratic curvature terms) was performed in [41,42], and later also considered in [43,44]. The Hamiltonian analysis of more general $f(\text{Riemann})$ theories of gravity was considered in [45].

The main goal of the present paper is to perform the Hamiltonian analysis of the curvature-squared theories of gravity in greatest details. The previous analyses have not been complete in all respects, and due to the new interest in higher-derivative gravity they deserve a new detailed treatment. Specifically, we are interested in the structure of constraints which crucially depends on the values of the parameters that appear in the action, what will be introduced in the next section. It turns out that each case requires a separate treatment since the nature of various constraints and the number of physical degrees of freedom depend on the value of the parameters. The theory with most symmetries is the Weyl gravity. A surprising situation occurs when Weyl gravity is supplemented with a nonzero cosmological constant. It obviously breaks conformal invariance, but diffeomorphism invariance is retained. There is no evident reason why we could not include such a constant term into the action. However, the investigation of the structure of constraints reveals that the theory becomes inconsistent: the requirement of the preservation of a secondary constraint leads to the condition that the determinant of the metric of spacetime should be equal to zero, which is satisfied when either the lapse N or the determinant of the three-dimensional metric h is zero, $\sqrt{-g} = N\sqrt{h} = 0$. We analyze this situation further by introducing a scalar field ϕ into the action in order to regain the conformal invariance, following [46,47]. The scalar field has to couple to the scalar curvature and its kinetic term must have the wrong sign in order to obtain the Weyl invariant action. In the Hamiltonian analysis, we obtain a first-class constraint that is the generator of the Weyl symmetry. This symmetry can be gauge fixed by imposing the condition $\phi = \text{const}$. When we insert this condition into the action, we obtain the standard Einstein-Hilbert term with the condition that the original kinetic term for ϕ corresponds to the ghostlike degree of freedom.

II. GRAVITATIONAL ACTION WITH QUADRATIC CURVATURE TERMS

A. Action and its physical degrees of freedom

We consider the generally covariant theory of gravity in four-dimensional spacetime whose action consists of the Einstein-Hilbert part, the cosmological constant and the quadratic curvature terms. The gravitational action reads

$$S_C = \int d^4x\sqrt{-g}\left[\Lambda + \frac{R}{2\kappa} - \frac{\alpha}{4}C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma} + \frac{\beta}{8}R^2 + \gamma G\right], \tag{2.1}$$

where κ, α, β and γ are coupling constants. We consider all four-dimensional integrals to be taken over the whole spacetime $\mathcal{M}$. The Weyl tensor is defined as

$$C_{\mu\nu\rho\sigma} = R_{\mu\nu\rho\sigma} - \frac{2}{(d-2)}(g_{\mu[\rho}R_{\sigma]\nu} - g_{\nu[\rho}R_{\sigma]\mu}) + \frac{2}{(d-1)(d-2)}g_{\mu[\rho}g_{\sigma]\nu}R, \tag{2.2}$$

where d is the dimension of spacetime. The Weyl tensor is by definition the traceless part of the Riemann tensor. In the last term of the action (2.1), G is the Gauss-Bonnet-Chern curvature term,

$$G = R_{\alpha\beta\gamma\delta}R_{\mu\nu\rho\sigma}\epsilon^{\alpha\beta\mu\nu}\epsilon^{\gamma\delta\rho\sigma} = R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} - 4R_{\mu\nu}R^{\mu\nu} + R^2. \tag{2.3}$$

In four-dimensional spacetime, its integral $\int d^4x\sqrt{-g}G$ becomes a topological invariant which is proportional to the Euler characteristic of the spacetime manifold. Since we consider smooth variations of spacetime, which do not change its topology, the Gauss-Bonnet-Chern part of the action can be regarded as a constant. Hence we can drop it.

The Weyl tensor squared can be written as

$$C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma} = 2\left(R_{\mu\nu}R^{\mu\nu} - \frac{1}{3}R^2\right) + G. \tag{2.4}$$

Thus the action (2.1) becomes

$$S_R = \int d^4x\sqrt{-g}\left[\Lambda + \frac{R}{2\kappa} - \frac{\alpha}{2}R_{\mu\nu}R^{\mu\nu} + \left(\frac{\alpha}{6} + \frac{\beta}{8}\right)R^2 + \left(\gamma - \frac{\alpha}{4}\right)G\right]. \tag{2.5}$$

The actions (2.1) and (2.5) are of course identical. However, when we discard the Gauss-Bonnet-Chern topological invariant term in both actions, $\gamma \int d^4x\sqrt{-g}G$ and $(\gamma - \alpha/4)\int d^4x\sqrt{-g}G$, respectively, the resulting actions differ by a multiple of the said invariant, namely by $-(\alpha/4)\int d^4x\sqrt{-g}G$. Even though this topological invariant term has no impact on the physical dynamics of the theory, it affects the Hamiltonian formulation of the theory in a significant way. Namely, the structure of the constraints of the theory is considerably simpler for the action (2.1) than for the action (2.5), when both actions are considered without the explicit invariant term $\int d^4x\sqrt{-g}G$. In other words, the topological invariant part of the Weyl tensor squared (2.4) action simplifies the Hamiltonian analysis significantly.

The quadratic curvature terms are known to render the theory renormalizable when the cosmological constant is absent [48]. The theory is also known to possess the property of asymptotic freedom [49]. For nonvanishing couplings, the action (2.1) contains eight local degrees of freedom [48,50]. On the Minkowski background, two degrees of freedom are associated with the usual massless spin-2 graviton, five modes are associated with a massive spin-2 excitation, and one with a massive scalar. Moreover, the massive spin-2 component carries negative energy, which implies that the theory is unstable. Alternatively, the negative energy states can be regarded as positive energy states with indefinite norm, what leads to the violation of unitarity.

Although pure curvature-squared gravity without the Einstein-Hilbert part admits standard vacuum solutions, asymptotically flat solutions do not couple to a positive definite matter distribution [5,50], e.g., in the case of the Schwarzshild solution. For that reason the Einstein-Hilbert part of the action is necessary in the infrared region. As we already noted above, the Einstein-Hilbert action can be generated by quantum effects whenever the spacetime is allowed to be curved [16–19].

Some of the extra degrees of freedom can be removed by certain choices of the coupling constants. For $\Lambda = 0$, $\kappa^{-1} = \beta = \gamma = 0$ and $\alpha = 1$, the action (2.1) becomes the conformally invariant action of Weyl gravity,

$$S_{\mathrm{Weyl}} = -\frac{1}{4}\int d^4x\sqrt{-g}C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma}. \tag{2.6}$$

The additional local symmetry under conformal transformations removes one degree of freedom, but it is not sufficient for removing all the ghosts, namely the negative energy spin-2 excitations. On the Minkowski background, the six degrees of freedom are associated with ordinary massless spin-2 and spin-1 excitations, and with a massless spin-2 ghost [51].

On the cosmologically relevant anti–de Sitter backgrounds, the extra gravitational degrees of freedom can appear as a partially massless spin-2 field [12,52]. This is because the conventional connection between gauge invariance, masslessness and propagation on null cones holds generically only in flat four-dimensional spacetime [53]. On (anti–)de Sitter backgrounds, higher spin fields ($s > 1$) can become partially massless, carrying a number of degrees of freedom that is between the extremes of flat space, $2s + 1$ for massive and 2 for massless fields. This requires that the mass is appropriately tuned with respect to the cosmological constant [54].

On the other hand, setting $\alpha = 0$ in the action removes the negative energy spin-2 component, leaving only the extra scalar degree of freedom. The result would indeed be the simplest case of $f(R)$ gravity. But then renormalizability is lost. We consider the potentially renormalizable theories exclusively in this paper. Hence we assume $\alpha \neq 0$.

B. Equations of motion

The variation of the gravitational action with respect to the metric of spacetime $g^{\mu\nu}$ leads to the following equations of motion,

$$-g_{\mu\nu}\Lambda + \frac{1}{\kappa}\left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R\right) + \alpha(2\nabla^\rho\nabla^\sigma C_{\rho\mu\nu\sigma} + C_{\rho\mu\nu\sigma}R^{\rho\sigma}) + \frac{\beta}{2}\left[R\left(R_{\mu\nu} - \frac{1}{4}g_{\mu\nu}R\right) - \nabla_\mu\nabla_\nu R + g_{\mu\nu}\nabla^\rho\nabla_\rho R\right] = T_{\mu\nu}, \tag{2.7}$$

where the energy-momentum tensor of matter is defined as

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta S_{\mathrm{matter}}}{\delta g^{\mu\nu}}. \tag{2.8}$$

Matter is assumed to be coupled minimally to the metric of spacetime. The trace of the equations of motion is a linear inhomogeneous second-order differential equation for the scalar curvature,

$$-4\Lambda - \frac{1}{\kappa}R + \frac{3\beta}{2}\nabla^\mu\nabla_\mu R = T, \tag{2.9}$$

with no contribution from the Weyl gravity part of the action. The boundary terms which arise from the variation of the action are discussed next.

C. Boundary surface terms

We require that the solutions of Einstein field equations be extrema of the Einstein-Hilbert action when only the variation of the metric (and not its derivatives) is fixed to zero on the boundary of spacetime. In general relativity, we cannot fix derivatives of the variation of the metric on the boundary, because that would overconstrain the system. Therefore, we have to discuss the surface terms that arise in the variation of the action with respect to the metric of spacetime.

The variations of the metric are required to vanish on the boundary of spacetime, $\delta g_{\mu\nu} = 0$. In fact, it is sufficient to fix only the variation of the induced metric $\gamma_{\mu\nu}$ on the boundary of spacetime, $\delta\gamma_{\mu\nu} = 0$, while leaving the variation normal to the boundary free. This is because a variation of the action is invariant under diffeomorphism gauge transformations and there always exists a gauge transformation $\nabla_{(\mu}\xi_{\nu)}$ with $\xi_\nu = 0$ on the boundary, which transforms $\delta g_{\mu\nu}$ into $\delta\gamma_{\mu\nu}$.

Whenever the integrand of a surface term is proportional to $\delta g_{\mu\nu}$ or $\delta\gamma_{\mu\nu}$ on the boundary of spacetime, the surface term vanishes. Thus we only need to consider surface terms that involve derivatives of the variation of the metric.

The variation of the Einstein-Hilbert action with respect to the metric includes a nonvanishing surface term on the boundary of spacetime, which can be written as

$$\begin{aligned}&-\frac{1}{2\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}r_\mu(\nabla_\nu\delta g^{\mu\nu} - g_{\nu\rho}\nabla^\mu\delta g^{\nu\rho})\\ &\quad= -\frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}\delta K,\end{aligned} \tag{2.10}$$

where $\partial\mathcal{M}$ is the boundary of spacetime $\mathcal{M}$, natural integration measure on $\partial\mathcal{M}$ is assumed, r^μ is the outward-pointing unit normal to the boundary (with norm $\varepsilon = r_\mu r^\mu = \pm 1$), $\gamma_{\mu\nu} = g_{\mu\nu} - \varepsilon r_\mu r_\nu$ is the induced metric on the boundary, and δK is the variation of the trace of the extrinsic curvature of the boundary of spacetime, $K = \nabla_\mu r^\mu$. In order to obtain a variational principle consistent with Einstein equations when only the variation of the metric (and not its derivatives) is fixed to zero on the boundary $\partial\mathcal{M}$, we add the surface term $\frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}K$ into the Einstein-Hilbert action, so that the surface term in the variation of the original action gets canceled,

$$S_{\rm EH} = \frac{1}{2\kappa}\int d^4x\sqrt{-g}R + \frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}K. \tag{2.11}$$

This completion to Einstein-Hilbert action was originally found in [55] and later considered in [56]. It is regarded as the complete standard action of general relativity.

As long as the geometry of spacetime is spatially compact, the action (2.11) is well defined. But in spatially noncompact spacetimes, the action diverges. Then one must choose a reference background, including the metric of spacetime g_0 and matter fields ψ_0, and then define the physical action as the difference of the variable action compared to the action of the fixed background [57],

$$S_{\rm phys}[g,\psi] = S[g,\psi] - S[g_0,\psi_0]. \tag{2.12}$$

This physical action is finite if we require that the field variables and the reference fields induce the same field configuration on the boundary of spacetime (particularly at spatial infinity).

Does the variation of the curvature-squared part of the action (2.1) yield extra surface terms? The variation of the action indeed contains nonvanishing surface terms. The first one is obtained from the R^2 part of the action in a similar way as in the case of Einstein-Hilbert action,

$$\begin{aligned}&-\frac{\beta}{4}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}Rr_\mu(\nabla_\nu\delta g^{\mu\nu} - g_{\nu\rho}\nabla^\mu\delta g^{\nu\rho})\\ &\quad= -\frac{\beta}{2}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}R\delta K.\end{aligned} \tag{2.13}$$

The Weyl gravity part of the action implies the second surface term as

$$\begin{aligned}&\alpha\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}r_\mu\left[R_{\nu\rho}\nabla^\rho\delta g^{\mu\nu} - \frac{1}{2}\left(R_{\nu\rho} - \frac{2}{3}g_{\nu\rho}R\right)\nabla^\mu\delta g^{\nu\rho}\right.\\ &\quad\left. - \frac{1}{2}R^{\mu\nu}g_{\rho\sigma}\nabla_\nu\delta g^{\rho\sigma} - \frac{1}{3}R\nabla_\nu\delta g^{\mu\nu}\right].\end{aligned} \tag{2.14}$$

In general, it appears to be impossible to write either of these boundary contributions as a variation of a functional on the boundary of spacetime. Some cases of very high level of symmetry, e.g. maximally symmetric spacetime, might be an exception. Although in general relativity we cannot fix the covariant derivatives of the variation of the metric on the boundary, we are now considering a higher-derivative theory, where imposing boundary conditions on the derivatives of the variation might be both permitted and natural, because the metric carries extra degrees of freedom due to the higher-order time derivatives. We shall postpone the final discussion on surface terms until Sec. III D, where the theory is given in a first-order form using Arnowitt-Deser-Misner formulation generalized for higher-derivative theory. Surface terms arising in Hamiltonian formalism are discussed in Sec. IV.

The variation of the Gauss-Bonnet-Chern topological invariant vanishes identically when the spacetime has no boundary. When the spacetime has boundary, the variation contains a surface term that turns out to be a variation of a functional on the boundary of spacetime. That boundary term can then be added into the term $\int d^4\sqrt{-g}G$, thus obtaining a true topological invariant whose variations vanish identically. In the presence of boundaries, the topological invariant can be written as

$$\int d^4x\sqrt{-g}G + 4\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}\Big(RK - 2R_{\mu\nu}\gamma^{\mu\nu}K + 2R_{\mu\nu\rho\sigma}K^{\mu\rho}\gamma^{\nu\sigma} - \frac{4}{3}K_{\mu\nu}K^{\mu}_{\rho}K^{\nu\rho} + K_{\mu\nu}K^{\mu\nu}K - \frac{2}{3}K^3\Big) = -32\pi^2\chi(\mathcal{M}), \tag{2.15}$$

where $K_{\mu\nu}$ denotes the extrinsic curvature on the boundary of spacetime. The Euler characteristic of spacetime $\mathcal{M}$ is denoted by $\chi(\mathcal{M})$. For a brief review of Gauss-Bonnet-Chern theorem, see, e.g., [58].

III. FIRST-ORDER ARNOWITT-DESER-MISNER REPRESENTATION OF THE HIGHER-DERIVATIVE GRAVITATIONAL ACTIONS

We consider the ADM decomposition of the gravitational field [59]. In the first two subsections, however, we shall work in a more general formalism that does not assume any given basis. After that the more traditional formalism in ADM coordinate system is applied. For reviews and mathematical background, see [60].

A. Foliation of spacetime into spatial hypersurfaces

We consider a globally hyperbolic spacetime $\mathcal{M}$ that admits a foliation into a family of nonintersecting Cauchy surfaces Σ_t, which cover the spacetime. Each Cauchy surface Σ_t is a spacelike hypersurface, such that every causal curve intersects Σ_t exactly once. These spatial hypersurfaces are parametrized by a global time function t.

The metric tensor $g_{\mu\nu}$ of spacetime induces a metric $h_{\mu\nu}$ on the spatial hypersurface Σ_t,

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu, \tag{3.1}$$

where n_μ is the future-directed unit normal to Σ_t. The metric of spacetime has the signature $(-,+,+,+)$. Since n_μ is timelike, it has the norm $n_\mu n^\mu = -1$. Conversely, the metric of spacetime can be expressed in terms of the induced metric on Σ_t and the unit normal to Σ_t as $g_{\mu\nu} = h_{\mu\nu} - n_\mu n_\nu$. The induced metric $h_{\mu\nu}$ is sometimes referred to as the first fundamental form of the hypersurfaces Σ_t. With one spacetime index raised, $h^\mu{}_\nu = g^{\mu\rho}h_{\rho\nu} = h^{\mu\rho}h_{\rho\nu}$, it is the projection operator onto Σ_t:

$$h^\mu_\nu = \delta^\mu_\nu + n^\mu n_\nu. \tag{3.2}$$

The subscript $\perp$ in front of a tensor is used to denote that it has been projected onto Σ_t, thus orthogonal to the normal n^μ, e.g.,

$$_\perp T^\mu{}_\nu = h^\mu{}_\rho h^\sigma{}_\nu T^\rho{}_\sigma. \tag{3.3}$$

We denote the metric compatible covariant derivatives on $(\mathcal{M}, g_{\mu\nu})$ and $(\Sigma_t, h_{\mu\nu})$ by ∇ and D, respectively. The spatial covariant derivative D of a (k,l)-tensor field T on Σ_t is given in terms of the covariant derivative ∇ on spacetime as

$$D_\mu T^{\nu_1\cdots\nu_k}{}_{\rho_1\cdots\rho_l} = h^\sigma{}_\mu h^{\nu_1}{}_{\alpha_1}\cdots h^{\nu_k}{}_{\alpha_k} h^{\beta_1}{}_{\rho_1}\cdots h^{\beta_1}{}_{\rho_l} \times \nabla_\sigma T^{\alpha_1\cdots\alpha_k}{}_{\beta 1\cdots\beta l}, \tag{3.4}$$

where in the right-hand side one considers the extension of T on spacetime.

The extrinsic curvature tensor of the spatial hypersurface Σ_t is defined as the component of $\nabla_\mu n_\nu$ that is fully tangent to Σ_t,

$$K_{\mu\nu} = h^\rho{}_\mu \nabla_\rho n_\nu = \nabla_\mu n_\nu + n_\mu a_\nu, \tag{3.5}$$

where by a_μ we denote the acceleration of an observer with velocity n_μ,

$$a_\mu = \nabla_n n_\mu = n^\nu \nabla_\nu n_\mu. \tag{3.6}$$

The symmetry of $K_{\mu\nu}$ follows from the fact that the shape operator $u \mapsto \nabla_u n$ is self-adjoint, $K(u,v) = \nabla_u n\cdot v = u\cdot \nabla_v n = K(v,u)$, for any vectors u and v tangent to Σ_t. Incidentally, the extrinsic curvature (3.5) can be written as the Lie derivative of the induced metric $h_{\mu\nu}$ on Σ_t along the unit normal n to Σ_t,

$$K_{\mu\nu} = \frac{1}{2}\mathcal{L}_n h_{\mu\nu}. \tag{3.7}$$

The trace of the extrinsic curvature is denoted by $K = h^{\mu\nu}K_{\mu\nu}$. The extrinsic curvature is sometimes referred to as the second fundamental form of Σ_t.

B. Decomposition of curvature tensors with respect to spatial hypersurfaces

In order to write the gravitational actions (2.1) or (2.5) in terms of the fundamental forms of the spatial hypersurfaces Σ_t and the unit normal n_μ to these hypersurfaces, we have to decompose the curvature tensors into components tangent and normal to the hypersurfaces. A detailed account of these standard projection relations is presented, because one of our projection relations for the Weyl tensor differs from the ones found in the literature, namely in Ref. [41] and those following it.

The decomposition of the Riemann tensor of spacetime into components tangent and normal to the hypersurfaces Σ_t is given by the following projection relations:

(i) Gauss relation

$$ {}_{\perp}R_{\mu\nu\rho\sigma} \equiv h^{\alpha}{}_{\mu}h^{\beta}{}_{\nu}h^{\gamma}{}_{\rho}h^{\delta}{}_{\sigma}R_{\alpha\beta\gamma\delta} = {}^{(3)}R_{\mu\nu\rho\sigma} + K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho}; \quad (3.8) $$

(ii) Codazzi relation

$$ {}_{\perp}R_{\mu\nu\rho\boldsymbol{n}} \equiv h^{\alpha}{}_{\mu}h^{\beta}{}_{\nu}h^{\gamma}{}_{\rho}n^{\delta}R_{\alpha\beta\gamma\delta} = 2D_{[\mu}K_{\nu]\rho}; \quad (3.9) $$

(iii) Ricci relation

$$ {}_{\perp}R_{\mu\boldsymbol{n}\nu\boldsymbol{n}} \equiv h^{\alpha}{}_{\mu}n^{\beta}h^{\gamma}{}_{\nu}n^{\delta}R_{\alpha\beta\gamma\delta} = K_{\mu\rho}K_{\nu}{}^{\rho} - \mathcal{L}_n K_{\mu\nu} + D_{(\mu}a_{\nu)} + a_{\mu}a_{\nu}. \quad (3.10) $$

The remaining projections of the Riemann tensor are either zero or related to the given ones by the symmetries of the Riemann tensor. In the Gauss relation (3.8), ${}^{(3)}R^{\mu}{}_{\nu\rho\sigma}$ is the Riemann tensor of the three-dimensional hypersurface Σ_t. In the used notation, the tensor index $\boldsymbol{n}$ has a special meaning, since it refers to the contraction with the unit normal n^{μ}.

For the Ricci tensor $R_{\mu\nu} = R^{\rho}{}_{\mu\rho\nu}$ of spacetime we obtain the following projection relations

$$ {}_{\perp}R_{\mu\nu} = {}^{(3)}R_{\mu\nu} + K_{\mu\nu}K - 2K_{\mu\rho}K^{\rho}{}_{\nu} + \mathcal{L}_n K_{\mu\nu} - D_{(\mu}a_{\nu)} - a_{\mu}a_{\nu}, \quad (3.11) $$

$$ {}_{\perp}R_{\mu\boldsymbol{n}} = D_{\nu}K^{\nu}{}_{\mu} - D_{\mu}K, \quad (3.12) $$

$$ R_{\boldsymbol{nn}} = K_{\mu\nu}K^{\mu\nu} - h^{\mu\nu}\mathcal{L}_n K_{\mu\nu} + D_{\mu}a^{\mu} + a_{\mu}a^{\mu}, \quad (3.13) $$

which are obtained from the contractions of the Gauss, Codazzi and Ricci relations (3.8)–(3.10). Note that for any *covariant* tensor T which is tangent to Σ_t, its Lie derivative along n, $\mathcal{L}_n T$, is also tangent to Σ_t. This is because $\mathcal{L}_n h^{\mu}{}_{\nu} = n^{\mu}a_{\nu}$, and hence $\mathcal{L}_n T$ is equal to its projection on Σ_t, $\mathcal{L}_n T = \mathcal{L}_n {}_{\perp}T = {}_{\perp}\mathcal{L}_n T$.

The decomposition of the scalar curvature R of spacetime can be written as

$$ R = h^{\mu\nu}{}_{\perp}R_{\mu\nu} - R_{\boldsymbol{nn}} = {}^{(3)}R + K^2 - 3K_{\mu\nu}K^{\mu\nu} + 2h^{\mu\nu}\mathcal{L}_n K_{\mu\nu} - 2D_{\mu}a^{\mu} - 2a_{\mu}a^{\mu} = {}^{(3)}R + K_{\mu\nu}K^{\mu\nu} - K^2 + 2\nabla_{\mu}(n^{\mu}K - a^{\mu}), \quad (3.14) $$

where in the last equality we have written the Lie derivative as

$$ \mathcal{L}_n K_{\mu\nu} = \nabla_n K_{\mu\nu} + (K_{\mu}{}^{\rho} - n_{\mu}a^{\rho})K_{\rho\nu} + (K_{\nu}{}^{\rho} - n_{\nu}a^{\rho})K_{\mu\rho} \quad (3.15) $$

in order to write its trace as

$$ h^{\mu\nu}\mathcal{L}_n K_{\mu\nu} = \nabla_n K + 2K_{\mu\nu}K^{\mu\nu} = \nabla_{\mu}(n^{\mu}K) - K^2 + 2K_{\mu\nu}K^{\mu\nu}. \quad (3.16) $$

We also used the identity

$$ D_{\mu}a^{\mu} + a_{\mu}a^{\mu} = \nabla_{\mu}a^{\mu}, \quad (3.17) $$

which can be proven easily by applying (3.4) to $D_{\mu}a^{\mu}$ and obtaining the component of $\nabla_{\mu}a_{\nu}$ which is fully orthogonal to Σ_t, $n^{\mu}n^{\nu}\nabla_{\mu}a_{\nu} = -a_{\mu}a^{\mu}$. For such decompositions of covariant derivatives of tensors into components tangent and normal to Σ_t, see [39]. The last form in (3.14) is useful for the Einstein-Hilbert part of the action, since the last term in $\sqrt{-g}R$ is a covariant divergence that can be written as a surface term. The second form in (3.14) is useful for the curvature-squared part of the action, where the second-order time derivative terms cannot be written as a divergence.

The Ricci tensor squared is written as a sum of the squares of its projections (3.11)–(3.13):

$$ R_{\mu\nu}R^{\mu\nu} = {}_{\perp}R_{\mu\nu}{}_{\perp}R^{\mu\nu} - 2{}_{\perp}R_{\mu\boldsymbol{n}}{}_{\perp}R^{\mu}{}_{\boldsymbol{n}} + (R_{\boldsymbol{nn}})^2. \quad (3.18) $$

The combination of quadratic curvature invariants in the Weyl action (2.6) is obtained as

$$ R_{\mu\nu}R^{\mu\nu} - \frac{1}{3}R^2 = \left(h^{\mu\rho}h^{\nu\sigma} - \frac{1}{3}h^{\mu\nu}h^{\rho\sigma}\right){}_{\perp}R_{\mu\nu}{}_{\perp}R_{\rho\sigma} + \frac{2}{3}R_{\boldsymbol{nn}}(h^{\mu\nu}{}_{\perp}R_{\mu\nu} + R_{\boldsymbol{nn}}) - 2{}_{\perp}R_{\mu\boldsymbol{n}}{}_{\perp}R^{\mu}{}_{\boldsymbol{n}}. \quad (3.19) $$

Further, we decompose the Weyl tensor (2.2) of spacetime into components tangent and normal to the spatial hypersurfaces Σ_t. First we obtain the projections of Weyl tensor where one or two arguments are projected along the unit normal n while the rest are projected onto Σ_t:

$$ {}_{\perp}C_{\mu\nu\rho\boldsymbol{n}} = {}_{\perp}R_{\mu\nu\rho\boldsymbol{n}} + {}_{\perp}R_{\boldsymbol{n}[\mu}h_{\nu]\rho} = 2D_{[\mu}K_{\nu]\rho} + D_{\sigma}K^{\sigma}{}_{[\mu}h_{\nu]\rho} - D_{[\mu}Kh_{\nu]\rho} = 2(h^{\alpha}{}_{\mu}h^{\beta}{}_{\nu}h^{\gamma}{}_{\rho} - h^{\sigma}{}_{[\mu}h_{\nu]\rho}h^{\beta\gamma})D_{[\alpha}K_{\beta]\gamma} \quad (3.20) $$

and

$$
\begin{aligned}
{}_{\perp}C_{\mu n\nu n} &= {}_{\perp}R_{\mu n\nu n} + \frac{1}{2}{}_{\perp}R_{\mu\nu} - \frac{1}{2}h_{\mu\nu}R_{nn} - \frac{1}{6}h_{\mu\nu}R \\
&= \frac{1}{2}\left(h^{\rho}{}_{\mu}h^{\sigma}{}_{\nu} - \frac{1}{3}h_{\mu\nu}h^{\rho\sigma}\right)({}^{(3)}R_{\rho\sigma} + K_{\rho\sigma}K - \mathcal{L}_n K_{\rho\sigma} \\
&\quad + D_{(\rho}a_{\sigma)} + a_{\rho}a_{\sigma}). \qquad (3.21)
\end{aligned}
$$

Finally, we obtain the component of Weyl tensor which is fully tangent to Σ_t as

$$
\begin{aligned}
{}_{\perp}C_{\mu\nu\rho\sigma} &= {}_{\perp}R_{\mu\nu\rho\sigma} - h_{\mu[\rho}{}_{\perp}R_{\sigma]\nu} + h_{\nu[\rho}{}_{\perp}R_{\sigma]\mu} + \frac{1}{3}h_{\mu[\rho}h_{\sigma]\nu}R \\
&= \mathcal{K}_{\mu\nu\rho\sigma} + h_{\mu\rho}{}_{\perp}C_{\nu n\sigma n} - h_{\mu\sigma}{}_{\perp}C_{\nu n\rho n} \\
&\quad - h_{\nu\rho}{}_{\perp}C_{\mu n\sigma n} + h_{\nu\sigma}{}_{\perp}C_{\mu n\rho n}, \qquad (3.22)
\end{aligned}
$$

where we have defined a new tensor $\mathcal{K}_{\mu\nu\rho\sigma}$ as

$$
\begin{aligned}
\mathcal{K}_{\mu\nu\rho\sigma} &= K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho} - h_{\mu\rho}(K_{\nu\sigma}K - K_{\nu\tau}K^{\tau}{}_{\sigma}) \\
&\quad + h_{\mu\sigma}(K_{\nu\rho}K - K_{\nu\tau}K^{\tau}{}_{\rho}) + h_{\nu\rho}(K_{\mu\sigma}K - K_{\mu\tau}K^{\tau}{}_{\sigma}) \\
&\quad - h_{\nu\sigma}(K_{\mu\rho}K - K_{\mu\tau}K^{\tau}{}_{\rho}) \\
&\quad + \frac{1}{2}(h_{\mu\rho}h_{\nu\sigma} - h_{\mu\sigma}h_{\nu\rho})(K^2 - K_{\tau\upsilon}K^{\tau\upsilon}). \qquad (3.23)
\end{aligned}
$$

This tensor is the traceless part of the quadratic extrinsic curvature tensor $K_{\mu\rho}K_{\nu\sigma} - K_{\mu\sigma}K_{\nu\rho}$. Note that $\mathcal{K}_{\mu\nu\rho\sigma}$ inherits the common symmetries of Riemann and Weyl tensors. In (3.22), we used the fact that in any three-dimensional space, the Weyl tensor vanishes necessarily due to its symmetries,

$$
\begin{aligned}
{}^{(3)}C_{\mu\nu\rho\sigma} &= {}^{(3)}R_{\mu\nu\rho\sigma} - 2h_{\mu[\rho}{}^{(3)}R_{\sigma]\nu} + 2h_{\nu[\rho}{}^{(3)}R_{\sigma]\mu} \\
&\quad + h_{\mu[\rho}h_{\sigma]\nu}{}^{(3)}R = 0. \qquad (3.24)
\end{aligned}
$$

For this reason the traceless part of (3.22) consists only of the traceless quadratic extrinsic curvature tensor (3.23). Unlike the other projections of Weyl tensor, ${}_{\perp}C_{\mu\nu\rho\sigma}$ is not fully traceless, since it satisfies

$$
h^{\nu\sigma}{}_{\perp}C_{\mu\nu\rho\sigma} = {}_{\perp}C_{\mu n\rho n}. \qquad (3.25)
$$

Evidently ${}_{\perp}C_{\mu\nu\rho\sigma}$ has no trace-trace part, because ${}_{\perp}C_{\mu n\rho n}$ is traceless. The Weyl tensor squared is then obtained as [1]

$$
\begin{aligned}
C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma} &= \mathcal{K}_{\mu\nu\rho\sigma}\mathcal{K}^{\mu\nu\rho\sigma} + 8{}_{\perp}C_{\mu n\nu n}{}_{\perp}C^{\mu}{}_{n}{}^{\nu}{}_{n} \\
&\quad - 4{}_{\perp}C_{\mu\nu\rho n}{}_{\perp}C^{\mu\nu\rho}{}_{n}, \qquad (3.26)
\end{aligned}
$$

where as ever the indices of tensors tangent to Σ_t are raised (and lowered) by the induced metric (3.1) on the hypersurface.

We should emphasize that our result (3.22) for the component of Weyl tensor which is fully tangent to the spatial hypersurface differs from the one given in [41], which has been followed in the literature to date. In [41], the component ${}_{\perp}C_{\mu\nu\rho\sigma}$ is obtained in a form similar to (3.22) but without the first term $\mathcal{K}_{\mu\nu\rho\sigma}$. We obtain that ${}_{\perp}C_{\mu\nu\rho\sigma}$ actually has a nonvanishing traceless part $\mathcal{K}_{\mu\nu\rho\sigma}$, in addition to the vanishing three-dimensional Weyl tensor (3.24). In other words, the traceless quadratic extrinsic curvature tensor defined in (3.23), which is present in our result (3.22), is absent in [41].

C. ADM Variables

We introduce a timelike vector t^{μ} that satisfies $t^{\mu}\nabla_{\mu}t = 1$. This vector is decomposed into components normal and tangent to the spatial hypersurfaces Σ_t as $t^{\mu} = Nn^{\mu} + N^{\mu}$, where $N = -n_{\mu}t^{\mu}$ is the lapse function and $N^{\mu} = h^{\mu}{}_{\nu}t^{\nu}$ is the shift vector on the spatial hypersurface Σ_t. The ADM variables consist of the lapse function, the shift vector and the induced metric (3.1) on Σ_t. Together they describe the geometry of spacetime.

Then we introduce a coordinate system on spacetime. We regard the smooth function t as the time coordinate and introduce an arbitrary coordinate system $(x^i, i = 1, 2, 3)$ on the spatial hypersurfaces Σ_t. The unit normal to Σ_t can now be written in terms of the ADM variables as

$$
n_{\mu} = -N\nabla_{\mu}t = (-N, 0, 0, 0), \qquad n^{\mu} = \left(\frac{1}{N}, -\frac{N^i}{N}\right). \qquad (3.27)
$$

The invariant line element in spacetime is written as

$$
ds^2 = -N^2dt^2 + h_{ij}(dx^i + N^i dt)(dx^j + N^j dt). \qquad (3.28)
$$

The lapse function must be positive everywhere, $N > 0$, since Ndt measures the lapse of proper time between the hypersurfaces Σ_t and Σ_{t+dt}. In the given ADM coordinate basis, the components of the metric of spacetime read

$$
g_{00} = -N^2 + N_i N^i, \quad g_{0i} = g_{i0} = N_i, \quad g_{ij} = h_{ij}, \qquad (3.29)
$$

where $N_i = h_{ij}N^j$. The contravariant components of the metric of spacetime are

$$
g^{00} = -\frac{1}{N^2}, \qquad g^{0i} = g^{i0} = \frac{N^i}{N^2}, \qquad g^{ij} = h^{ij} - \frac{N^i N^j}{N^2}, \qquad (3.30)
$$

[1]Weyl tensor is expanded in terms of its projections as

$$
\begin{aligned}
C_{\mu\nu\rho\sigma} &= {}_{\perp}C_{\mu\nu\rho\sigma} - n_{\mu}{}_{\perp}C_{n\nu\rho\sigma} - n_{\nu}{}_{\perp}C_{\mu n\rho\sigma} - n_{\rho}{}_{\perp}C_{\mu\nu n\sigma} \\
&\quad - n_{\sigma}{}_{\perp}C_{\mu\nu\rho n} + n_{\mu}n_{\rho}{}_{\perp}C_{n\nu n\sigma} + n_{\mu}n_{\sigma}{}_{\perp}C_{n\nu\rho n} + n_{\nu}n_{\rho}{}_{\perp}C_{\mu n n\sigma} \\
&\quad + n_{\nu}n_{\sigma}{}_{\perp}C_{\mu n\rho n}.
\end{aligned}
$$

When squared, each component of this expansion gives a nonvanishing contribution only when contracted with itself.

where $h^{ij}h_{jk} = \delta^i_k$. The indices of tensors that are tangent to Σ_t can be lowered and raised using the induced metric h_{ij} on Σ_t and its inverse h^{ij}.

The extrinsic curvature tensor (3.5) is written as

$$K_{ij} = \frac{1}{2}\mathcal{L}_n h_{ij} = \frac{1}{2N}(\partial_t h_{ij} - 2D_{(i}N_{j)}), \tag{3.31}$$

where ∂_t denotes the partial derivative with respect to the time t. In the projection relations for the curvature tensors obtained in Sec. III B, the second-order time derivatives of the metric h_{ij} are contained in the Lie derivative of the extrinsic curvature,

$$\mathcal{L}_n K_{ij} = \frac{1}{N}(\partial_t K_{ij} - \mathcal{L}_{\vec{N}} K_{ij}), \tag{3.32}$$

where $\mathcal{L}_{\vec{N}}$ denotes the Lie derivative along the shift vector N^i on the spatial hypersurface.

The acceleration (3.6) is given by the spatial derivative of the logarithm of the lapse function as

$$a_\mu = D_\mu \ln N. \tag{3.33}$$

In the ADM coordinate basis, the time-components of tensors tangent to Σ_t are defined by the spatial components of the tensor and the shift vector. For example, $n^\nu A_\mu = n_\mu A^\mu = 0$, implies $A_0 = A_i N^i$ and $A^0 = 0$.

Then we can present the projection relations for the curvature tensors in terms of ADM variables. The projection relations (3.11)–(3.13) for the Ricci tensor are written as[2]

$$R_{ij} = \mathcal{L}_n K_{ij} + {}^{(3)}R_{ij} + K_{ij}K - 2K_{ik}K_j{}^k - \frac{1}{N}D_iD_jN, \tag{3.34}$$

$$R_{i\boldsymbol{n}} = D_jK^j{}_i - D_iK, \tag{3.35}$$

$$R_{\boldsymbol{nn}} = -h^{ij}\mathcal{L}_n K_{ij} + K_{ij}K^{ij} + \frac{1}{N}D^iD_iN, \tag{3.36}$$

where $K = h^{ij}K_{ij}$. The scalar curvature of spacetime (3.14) reads

$$R = 2h^{ij}\mathcal{L}_n K_{ij} + {}^{(3)}R + K^2 - 3K_{ij}K^{ij} - \frac{2}{N}D^iD_iN. \tag{3.37}$$

The projection relations (3.20)–(3.22) for the Weyl tensor are the following,

$$C_{i\boldsymbol{n}j\boldsymbol{n}} = -\frac{1}{2}\left(\delta^k_i\delta^l_j - \frac{1}{3}h_{ij}h^{kl}\right) \times \left(\mathcal{L}_n K_{kl} - {}^{(3)}R_{kl} - K_{kl}K - \frac{1}{N}D_kD_lN\right), \tag{3.38}$$

$$C_{ijk\boldsymbol{n}} = 2D_{[i}K_{j]k} + D_lK^l_{[i}h_{j]k} - D_{[i}Kh_{j]k}, \tag{3.39}$$

$$C_{ijkl} = \mathcal{K}_{ijkl} + h_{ik}C_{j\boldsymbol{n}l\boldsymbol{n}} - h_{il}C_{j\boldsymbol{n}k\boldsymbol{n}} - h_{jk}C_{i\boldsymbol{n}l\boldsymbol{n}} + h_{jl}C_{i\boldsymbol{n}k\boldsymbol{n}}, \tag{3.40}$$

where the traceless quadratic extrinsic curvature tensor is written as

$$\begin{aligned}\mathcal{K}_{ijkl} = {}& K_{ik}K_{jl} - K_{il}K_{jk} - h_{ik}(K_{jl}K - K_{jm}K^m{}_l) \\ &+ h_{il}(K_{jk}K - K_{jm}K^m{}_k) + h_{jk}(K_{il}K - K_{im}K^m{}_l) \\ &- h_{jl}(K_{ik}K - K_{im}K^m{}_k) + \frac{1}{2}(h_{ik}h_{jl} - h_{il}h_{jk}) \\ &\times (K^2 - K_{mn}K^{mn}).\end{aligned} \tag{3.41}$$

The Weyl tensor squared (3.26) is obtained in the form

$$C_{\mu\nu\rho\sigma}C^{\mu\nu\rho\sigma} = 8C_{i\boldsymbol{n}j\boldsymbol{n}}C^i{}_{\boldsymbol{n}}{}^j{}_{\boldsymbol{n}} - 4C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}, \tag{3.42}$$

since $\mathcal{K}_{ijkl}$ squared is zero due to the Cayley-Hamilton theorem. We indeed obtain

$$\mathcal{K}_{ikjl}K^{kl} = -3P(K)_{ij} = 0 \tag{3.43}$$

and consequently

$$\mathcal{K}_{ijkl}\mathcal{K}^{ijkl} = -6P(K)^i{}_jK^j{}_i = 0, \tag{3.44}$$

where $P(K)^i{}_j$ is the characteristic polynomial,[3] (B4), for the tensor $K^i{}_j = h^{ik}K_{kj}$ with the tensor itself as the argument, which is identically zero. This means that the correction to the projection relation (3.40)—namely the tensor (3.41)—has no impact on the Hamiltonian formulation of the given gravitational theories (2.1). If the Weyl tensor were coupled to a tensor (or tensors) other than itself, the contribution of $\mathcal{K}_{ijkl}$ would not vanish in general.

D. First-order ADM representation of the action

Let us consider the gravitational actions (2.1) and (2.5) without the Gauss-Bonnet-Chern topological invariant term proportional to $\int d^4x\sqrt{-g}G$, i.e. we set $\gamma = 0$ in (2.1), and $\gamma - \alpha/4 = 0$ in (2.5). We shall present the actions in terms of the foliation of spacetime into spatial hypersurfaces Σ_t, using the ADM variables and an associated coordinate system.

[2]Since we specialize to the ADM coordinates, from now on all tensors will be tangent to the hypersurface Σ_t, except the unit normal n. Hence we can omit the prefixed symbol $\perp$ from tensors that have been projected to the hypersurface, e.g., $R_{ij} \equiv {}_\perp R_{ij}$.

[3]See Appendix B for the Cayley-Hamilton theorem and the definition of the characteristic polynomial.

Since the invariant terms in the action which are quadratic in curvature contain second-order time derivatives (3.32), we are dealing with a higher-derivative theory. In the Lagrangian formalism this is not a problem at all, because the Euler-Lagrange equations can in principle contain any number of time derivatives, in the present case up to fourth order. In the Hamiltonian formalism, the equations of motion contain only a first-order time derivative, namely in the form $df/dt = \{f, H\}$. In order to achieve such a first-order description of the dynamics of the higher-derivative action, we shall introduce additional variables and constraints so that the action can be rewritten into a form which contains only first-order time derivatives. The additional variables describe the extra degrees of freedom implied by the higher-order time derivatives. In the present case, it is most convenient to regard the metric h_{ij} and the extrinsic curvature K_{ij} as independent variables. The fact that h_{ij} and K_{ij} are related is taken into account by imposing their relation (3.31) as a constraint, using Lagrange multipliers. Thus from now on we consider the higher-derivative gravitational Lagrangian as a functional of the independent variables N, N^i, h_{ij} and K_{ij}. It also depends on the first-order time derivative of K_{ij}, and we extend it with the constraint $\mathcal{L}_n h_{ij} - 2K_{ij} = 0$ multiplied by the Lagrange multiplier λ^{ij}. That is we understand the complete action (without matter) as a functional,

$$S[N, N^i, h_{ij}, \dot{h}_{ij}, K_{ij}, \dot{K}_{ij}, \lambda^{ij}], \tag{3.45}$$

where the dot denotes time derivative.[4] Now the extra degrees of freedom associated with the second-order time derivative of the metric are carried by the variables K_{ij}.

The first-order ADM representation of the action (2.1) can now be written as

$$\begin{aligned} S_C = \int dt \int_{\Sigma_t} d^3x N\sqrt{h}\Big[\Lambda + \frac{1}{2\kappa}({}^{(3)}R + K_{ij}K^{ij} - K^2) \\ - 2\alpha C_{\boldsymbol{i}n\boldsymbol{j}n}C^{i}{}_{\boldsymbol{n}}{}^{j}{}_{\boldsymbol{n}} + \alpha C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}} + \frac{\beta}{8}R^2 \\ + \lambda^{ij}(\mathcal{L}_n h_{ij} - 2K_{ij})\Big] + S_{\mathrm{surf}}, \end{aligned} \tag{3.46}$$

where the expressions (3.37)–(3.39) are assumed and S_{surf} contains the surface terms. Alternatively, we could use the action (2.5), whose first-order ADM representation is expressed as

$$\begin{aligned} S_R = \int dt \int_{\Sigma_t} d^3x N\sqrt{h}\Big[\Lambda + \frac{1}{2\kappa}({}^{(3)}R + K_{ij}K^{ij} - K^2) \\ - \frac{\alpha}{2}\left(h^{ik}h^{jl} - \frac{1}{3}h^{ij}h^{kl}\right)R_{ij}R_{kl} \\ - \frac{\alpha}{3}R_{\boldsymbol{nn}}({}^{(3)}R + K^2 - K_{ij}K^{ij}) + \alpha R_{i\boldsymbol{n}}R^{i}{}_{\boldsymbol{n}} \\ + \frac{\beta}{8}R^2 + \lambda^{ij}(\mathcal{L}_n h_{ij} - 2K_{ij})\Big] + S_{\mathrm{surf}}, \end{aligned} \tag{3.47}$$

and we assumed (3.34)–(3.37).

These two forms of the action (3.46) and (3.47) differ, as mentioned previously, only by a multiple of the Gauss-Bonnet-Chern topological invariant term, $-(\alpha/4)\int d^4x\sqrt{-g}G$, albeit this is no longer so evident because it too has been decomposed with respect to the spatial hypersurfaces as a part of the Weyl tensor squared term (2.4). First of all the kinetic part of the Lagrangian density of the action (3.46) is simpler than the one of (3.47). In particular, the Weyl gravity part of the Lagrangian density of (3.46) has no dependence on $h^{ij}\mathcal{L}_n K_{ij}$, whereas the Lagrangian density of (3.47) contains the linear term $\frac{\alpha}{3}h^{ij}\mathcal{L}_n K_{ij}({}^{(3)}R + K^2 - K_{kl}K^{kl})$. This difference has consequences for the structure of the constraints in the Hamiltonian formulations of these two forms of the gravitational action.

1. Surface terms

In the case of general relativity, the surface terms are obtained as

$$S_{\mathrm{surf}} = \frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}K + \frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}r_\mu(n^\mu K - a^\mu), \tag{3.48}$$

where $\gamma_{\mu\nu}$ and r_μ are the induced metric and the outward-pointing unit normal to the boundary $\partial\mathcal{M}$ of spacetime, respectively. We should emphasize that in the first surface term, K refers to the extrinsic curvature of the boundary $\partial\mathcal{M}$, while in the last term, K refers to the extrinsic curvature of the spatial hypersurfaces Σ_t. In our globally hyperbolic spacetime, the boundary $\partial\mathcal{M}$ consists of the initial and final Cauchy surfaces, say Σ_0 and Σ_1, respectively, and of the timelike hypersurface $\mathcal{B}$ that connects those spatial hypersurfaces. The timelike part of the boundary is the union $\mathcal{B} = \bigcup_{t\in\mathbb{R}}\mathcal{B}_t$ of the two-dimensional boundaries $\mathcal{B}_t$ of the Cauchy surfaces Σ_t (at spatial infinity). On the initial and final Cauchy surfaces Σ_0 and Σ_1, the surface integrals cancel each other entirely. Thus only the integral over $\mathcal{B}$ survives in the surface terms,

$$S_{\mathrm{surf}} = \frac{1}{\kappa}\int_{\mathcal{B}} d^3x\sqrt{-\gamma}(K_{\mathcal{B}} + r_\mu n^\mu K - r_\mu a^\mu). \tag{3.49}$$

Here the trace of the extrinsic curvature of $\mathcal{B}$ is denoted by $K_{\mathcal{B}} = \nabla_\mu r^\mu$, so that it is not confused with K which is to the

[4] There is some room for the choice of what is regarded as the time derivative in Hamiltonian formulation of the theory. This is discussed in Sec. IV.

trace of the extrinsic curvature of the surfaces Σ_t on its intersection with the boundary $\mathcal{B}$. If the surfaces $\mathcal{B}$ and Σ_t are assumed to be orthogonal, the normals to $\mathcal{B}$ and Σ_t are orthogonal as well, i.e., $r_\mu n^\mu = 0$, and hence we further obtain [57]

$$S_{\rm surf} = \frac{1}{\kappa}\int_{\mathcal{B}} d^3x\sqrt{-\gamma}h^{\mu\nu}\nabla_\mu r_\nu = \frac{1}{\kappa}\int dt \oint_{\mathcal{B}_t} d^2x\sqrt{\sigma}N^{(2)}K, \quad (3.50)$$

where σ_{ab} is the induced metric on $\mathcal{B}_t$ and ${}^{(2)}K$ is the extrinsic curvature of $\mathcal{B}_t$ embedded in Σ_t. In the case of nonorthogonal boundaries, one actually has to include extra two-dimensional surface terms regarding the intersection angle $\eta = r_\mu n^\mu$ of $\mathcal{B}$ and Σ_t as [61]

$$S_{\rm surf} = \frac{1}{\kappa}\int_{\mathcal{B}} d^3x\sqrt{-\gamma}(K_{\mathcal{B}} + \eta K - r_\mu a^\mu) + \frac{1}{\kappa}\int_{\mathcal{B}_0}^{\mathcal{B}_1} d^2x\sqrt{\sigma}\sinh^{-1}\eta, \quad (3.51)$$

where we denote the difference of the integrals over the two-dimensional final and initial surfaces $\mathcal{B}_1$ and $\mathcal{B}_0$ as $\int_{\mathcal{B}_0}^{\mathcal{B}_1} = \int_{\mathcal{B}_1} - \int_{\mathcal{B}_0}$.

As was noted in Sec. II C, if the spacetime is spatially noncompact, we must choose a reference background and define the physical action as the difference to the reference action. This also applies to all surface terms in the action

Let us then consider the variational principle for the higher-derivative gravitational action (3.45). Now the action depends on both the induced metric h_{ij} and extrinsic curvature K_{ij} on the hypersurface Σ_t, viewed as independent variables. Therefore, we should consider variations of the action for which both h_{ij} and K_{ij} are held fixed on the boundary of spacetime. Thus we require that the solutions to the equations of motion (2.7) lead to extrema of the action when the variations of all the variables are imposed to be zero on the boundary $\partial\mathcal{M}$. Now consider the surface terms obtained in Sec. II C. The surface terms (2.10) and (2.13) obtained from the Einstein-Hilbert and scalar curvature squared parts of the action clearly vanish under the variations with respect to the enlarged configuration space of the action (3.45), because now the variation δK of the trace of extrinsic curvature vanishes on the boundary $\partial\mathcal{M}$. The surface term (2.14) which is implied by the variation of the action of Weyl gravity is a more complicated matter. By decomposing the integrand of this surface term into components tangent and normal to the boundary surface, it can be shown that the integrand is linear in the variations of the ADM variables and the extrinsic curvature. (See [62] for the details of the calculation.) Thus the surface term (2.14) also is zero when the variations of the ADM variables and the extrinsic curvature are imposed to vanish on the boundary. Boundary terms in curvature-squared gravity have also been studied in [63] with the same result: boundary terms are no longer required when quadratic curvature invariants are added into the Einstein-Hilbert action. Recently, the same conclusion was reached in [64]. Therefore the only surface term at this point is the one that originates from the covariant total derivative in the decomposition of the scalar curvature (3.14) in the Einstein-Hilbert action, namely,

$$\frac{1}{\kappa}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}r_\mu(n^\mu K - a^\mu). \quad (3.52)$$

Note that this surface term could be easily avoided by using the second expression for the decomposition of the scalar curvature of spacetime (3.14) and keeping the time derivative of K_{ij}. We, however, prefer to use the last expression of (3.14), and hence obtain the surface term (3.52) whenever the Einstein-Hilbert action is present. The fact that no boundary terms are required in curvature-squared gravity does not mean that it is forbidden to include boundary terms into the gravitational action. Indeed, we can include any boundary term whose variation is linear in the variations of the ADM variables and the extrinsic curvature. Such boundary terms do not compromise the action principle due to the chosen boundary conditions on the variations. Whenever the Einstein-Hilbert action is present, we shall take advantage of this freedom by including the same boundary term that is required in general relativity, $\kappa^{-1}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}K$, so that combined with (3.52), the total surface term takes the same form as in general relativity (3.48): more specifically (3.50), when the hypersurfaces are orthogonal or (3.51), if the hypersurfaces are nonorthogonal. This choice is motivated by the fact that the surface term plays the role of total energy in the Hamiltonian formulation, and we prefer to obtain a similar total energy as in general relativity. (See [57] for the case of general relativity.) In pure curvature-squared gravity, when the Einstein-Hilbert action is absent, we shall not include any surface terms, $S_{\rm surf} = 0$.

IV. HAMILTONIAN ANALYSIS

The Hamiltonian formulation and canonical quantization of gravitational theories whose Lagrangians are quadratic in curvature were originally studied in [40–42]. These Hamiltonian formulations differ significantly. Kaku [40] formulated conformally invariant Weyl gravity in the strong-coupling approximation, both in Hamiltonian and Lagrangian forms, analogous to higher-derivative Yang-Mills theory. The differences of [41] and [42] are particularly interesting. Boulware [41] based his analysis on the action (2.1) without the topological invariant term $\gamma\int d^4x\sqrt{-g}G$, while Buchbinder and Lyahovich [42] considered an action of the form (2.5) without the topological invariant term. In Sec. III, we obtained first-order forms of both of these actions in terms of ADM variables.

They are given in (3.46) and (3.47), respectively. We shall choose the action (3.46) as the basis of our Hamiltonian formulation of curvature-squared gravity, because of its simpler kinetic part compared to the action (3.47). The Hamiltonian analysis based on the action (3.47) would indeed result into more complicated constraints, even if one uses a canonical transformation for its simplification [42]. Those complications in the structure of constraints will be remarked upon in the following analysis.

There are a few plausible choices for what is regarded as the time derivative in the Hamiltonian formulation of the given higher-derivative gravitational theory. The obvious and most common choice is to consider the partial derivative with respect to time as the concept of time differentiation for Hamiltonian formulation of gravity, following the original ADM formalism [59]. However, in principle, we could choose the derivative along any (nondynamical) timelike vector as a generalized time derivative for Hamiltonian formulation. Since the given gravitational Lagrangian of (3.46) or (3.47) is independent of the time derivatives of N and N^i, and we know from previous analyses that they behave as arbitrary Lagrange multipliers, the unit normal n^μ to the spacelike hypersurface is not a dynamical quantity. Furthermore, time derivatives in the actions appear only in the form of $\mathcal{L}_n h_{ij}$ and $\mathcal{L}_n K_{ij}$, thus making the Lie derivative $\mathcal{L}_n$ along the unit normal n^μ a tempting alternative for the concept of time differentiation for the Hamiltonian formulation.[5] This kind of approach was adopted in [41], and later followed in [43,44]. On the other hand, the nondynamical nature of N and N^i is a result of the Hamiltonian analysis, rather than its premise, because it is not evident from the beginning that N and N^i do not appear in any of the constraints of the theory in Hamiltonian formulation. We shall treat N and N^i as genuine variables in the Hamiltonian analysis, uncovering that they can be considered as Lagrange multipliers. We consider partial derivative with respect to time (∂_t) as the concept of time differentiation in the following Hamiltonian formulation of the theory.

The Lagrangian density in the action (3.46) is a function

$$\mathcal{L}_C(N, N^i, h_{ij}, \partial_t h_{ij}, K_{ij}, \partial_t K_{ij}, \lambda^{ij}). \tag{4.1}$$

The canonical momenta conjugated to N and N^i are primary constraints

$$p_N \approx 0, \qquad p_i \approx 0, \tag{4.2}$$

respectively, since the action is independent of the time derivatives of N and N^i. The weak equality ($\approx$) is understood in the sense introduced by Dirac [65]: a weak equality can be imposed only after all Poisson brackets have been evaluated, while a usual strong equality could be imposed anywhere. The tensor density defined by the Lagrange multiplier λ^{ij} is identified as the canonical momentum conjugated to h_{ij},

$$p^{ij} = \frac{\partial \mathcal{L}_C}{\partial(\partial_t h_{ij})} = \sqrt{h}\lambda^{ij}. \tag{4.3}$$

The canonical momentum conjugated to K_{ij} is defined as

$$\mathcal{P}^{ij} = \frac{\partial \mathcal{L}_C}{\partial(\partial_t K_{ij})} = \sqrt{h}\left(2\alpha C^i{}_{\boldsymbol{n}}{}^j{}_{\boldsymbol{n}} + \frac{\beta}{2} h^{ij} R\right). \tag{4.4}$$

Note that once we have identified $\sqrt{h}\lambda^{ij}$ as the canonical momentum p^{ij} conjugate to h_{ij} in (4.3), it is unnecessary to include the Lagrange multiplier λ^{ij} and its conjugated momentum p^λ_{ij} as extra canonical variables. If we include them, we obtain the extra primary constraints $p^{ij} - \sqrt{h}\lambda^{ij} \approx 0$ and $p^\lambda_{ij} \approx 0$. We can set these second-class constraints to zero strongly and eliminate the variables λ^{ij} and p^λ_{ij} by substituting $\sqrt{h}\lambda^{ij} = p^{ij}$ and $p^\lambda_{ij} = 0$. The Dirac bracket defined by these second-class constraints is equivalent to the Poisson bracket for all the remaining variables (see Appendix C for details). In general, this applies to any higher-derivative theory, where the relevant primary constraints are linear in the Lagrange multipliers.

The number and nature of constraints and physical degrees of freedom depends on the values of the coupling constants. Therefore we shall treat the different cases separately. We are particularly interested in the cases with $\alpha \neq 0$, which possess the potential to be renormalizable, that is consistent at high energies. The cases with $\alpha = 0$ include only general relativity and a special case of $f(R)$ gravity, $f(R) = R + bR^2$, with or without the cosmological constant term, which are well known and understood. First we shall consider the most interesting case, namely the conformally invariant Weyl gravity. Weyl gravity will serve as the reference theory to which all the other cases are compared.

A. Weyl gravity: $\Lambda = 0$, $\kappa^{-1} = \beta = \gamma = 0$, $\alpha \neq 0$

First we consider the case of conformally invariant Weyl gravity (2.6). The action is given in (3.46) with $\Lambda = 0$ and the couplings $\kappa^{-1} = \beta = 0$, $\alpha \neq 0$, and without any surface terms $S_{\text{surf}} = 0$. We could also set the coupling $\alpha = 1$, but we choose not to, because keeping it will help in comparing to the other cases. The topological invariant term in (2.1) has been discarded, $\gamma = 0$.

The momentum (4.4) consists only of the projection (3.38) of the Weyl tensor. It can be written as

[5]Another alternative for the concept of time differentiation would be the Lie derivative $\mathcal{L}_m$, where the vector $m^\mu = Nn^\mu = (1, -N^i)$ is the component of the time vector t^μ which is normal to the hypersurfaces Σ_t. Then we would have $\mathcal{L}_n h_{ij} = N^{-1}\mathcal{L}_m h_{ij}$ and $\mathcal{L}_n K_{ij} = N^{-1}\mathcal{L}_m K_{ij}$.

$$\mathcal{P}^{ij} = -\alpha\sqrt{h}\bar{\mathcal{G}}^{ijkl}\left(\mathcal{L}_n K_{kl} - {}^{(3)}R_{kl} - K_{kl}K - \frac{1}{N}D_k D_l N\right), \tag{4.5}$$

where we have defined a traceless generalized DeWitt metric as

$$\bar{\mathcal{G}}^{ijkl} = \frac{1}{2}(h^{ik}h^{jl} + h^{il}h^{jk}) - \frac{1}{3}h^{ij}h^{kl}. \tag{4.6}$$

Since the Weyl tensor is traceless, in other words the DeWitt metric has the metric as its null eigenvector, $g_{ij}\bar{\mathcal{G}}^{ijkl} = 0 = \bar{\mathcal{G}}^{ijkl}g_{kl}$, the trace of the momentum (4.5) is zero. Thus we have to define one more primary constraint,[6]

$$\mathcal{P} \approx 0. \tag{4.7}$$

We adopt the notation where the trace of a quantity is denoted without indices and the traceless part is denoted by the bar accent. For example, we denote

$$\mathcal{P} = h_{ij}\mathcal{P}^{ij}, \qquad \bar{\mathcal{P}}^{ij} = \mathcal{P}^{ij} - \frac{1}{3}h^{ij}\mathcal{P}. \tag{4.8}$$

The DeWitt metric (4.6) has the traceless inverse

$$\bar{\mathcal{G}}_{ijkl} = \frac{1}{2}(h_{ik}h_{jl} + h_{il}h_{jk}) - \frac{1}{3}h_{ij}h_{kl}, \tag{4.9}$$

which satisfies

$$\bar{\mathcal{G}}_{ijmn}\bar{\mathcal{G}}^{mnkl} = \delta_i^{(k}\delta_j^{l)} - \frac{1}{3}h_{ij}h^{kl}. \tag{4.10}$$

The definition of the momentum (4.5) can then be used to obtain

$$\begin{aligned}\mathcal{P}^{ij}\partial_t K_{ij} = {} & -N\frac{\bar{\mathcal{P}}_{ij}\bar{\mathcal{P}}^{ij}}{\alpha\sqrt{h}} + N\bar{\mathcal{P}}^{ij}({}^{(3)}R_{ij} + K_{ij}K) \\ & + \bar{\mathcal{P}}^{ij}D_i D_j N + \mathcal{P}^{ij}\mathcal{L}_{\vec{N}}K_{ij} \\ & + \frac{N}{3}\mathcal{P}h^{ij}\mathcal{L}_n K_{ij},\end{aligned} \tag{4.11}$$

where $\bar{\mathcal{P}}_{ij} = \bar{\mathcal{G}}_{ijkl}\mathcal{P}^{kl}$. The Lagrangian density of the action is written in terms of the canonical variables as

$$\begin{aligned}\mathcal{L}_C = {} & -N\left(\frac{\bar{\mathcal{P}}_{ij}\bar{\mathcal{P}}^{ij}}{2\alpha\sqrt{h}} + 2p^{ij}K_{ij} - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}\right) \\ & + p^{ij}\partial_t h_{ij} - 2p^{ij}D_{(i}N_{j)}.\end{aligned} \tag{4.12}$$

By definition, the total Hamiltonian is

$$\begin{aligned}H = {} & \int_{\Sigma_t} d^3x(p^{ij}\partial_t h_{ij} + \mathcal{P}^{ij}\partial_t K_{ij} - \mathcal{L}_C \\ & + u_N p_N + u^i p_i + u_{\mathcal{P}}\mathcal{P}) \\ = {} & \int_{\Sigma_t} d^3x(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda_N p_N + \lambda^i p_i + \lambda_{\mathcal{P}}\mathcal{P}) \\ & + H_{\text{surf}},\end{aligned} \tag{4.13}$$

where all the u and λ are arbitrary Lagrange multipliers accounting for the first two constraints in (4.2), as well as the constraint (4.7). In the Hamiltonian, we have defined the following quantities. The Hamiltonian constraint is given as

$$\begin{aligned}\mathcal{H}_0 = {} & 2p^{ij}K_{ij} - \frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{2\alpha\sqrt{h}} + \mathcal{P}^{ij\,(3)}R_{ij} + \mathcal{P}^{ij}K_{ij}K \\ & + D_i D_j\mathcal{P}^{ij} - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}},\end{aligned} \tag{4.14}$$

where $\mathcal{P}_{ij} = h_{ik}h_{jl}\mathcal{P}^{kl}$. We have written the Hamiltonian constraint in terms of all the components of the momentum $\mathcal{P}^{ij}$, absorbing terms depending on the trace component $\mathcal{P}$ into the Lagrange multiplier term $\lambda_{\mathcal{P}}\mathcal{P}$. The momentum constraint has the form

$$\mathcal{H}_i = -2h_{ij}D_k p^{jk} + \mathcal{P}^{jk}D_i K_{jk} - 2D_j(\mathcal{P}^{jk}K_{ik}), \tag{4.15}$$

or, in terms of partial derivatives,

$$\begin{aligned}\mathcal{H}_i = {} & -2h_{ij}\partial_k p^{jk} - (2\partial_j h_{ik} - \partial_i h_{jk})p^{jk} \\ & - 2K_{ij}\partial_k\mathcal{P}^{jk} - (2\partial_j K_{ik} - \partial_i K_{jk})\mathcal{P}^{jk}.\end{aligned} \tag{4.16}$$

The surface term in the Hamiltonian (4.13) is expressed as

$$\begin{aligned}H_{\text{surf}} = {} & \oint_{\mathcal{B}_t} d^2x s_i(D_j N\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_j p^{ij} \\ & + 2N^j\mathcal{P}^{ik}K_{jk}),\end{aligned} \tag{4.17}$$

where s_i is the unit normal to the spatial boundary $\mathcal{B}_t$ embedded in Σ_t. The surface terms appear for two reasons. The first two appear due to the integration by parts of the term

$$\int_{\Sigma_t} d^3x\mathcal{P}^{ij}D_i D_j N = \int_{\Sigma_t} d^3x ND_i D_j\mathcal{P}^{ij} + \oint_{\mathcal{B}_t} d^2x s_i(D_j N\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij}).$$

[6] If we based our Hamiltonian formulation on the action (3.47), instead of (3.46), this constraint would have the form

$$\mathcal{P} - \alpha\sqrt{h}({}^{(3)}R + K^2 - K_{ij}K^{ij}) \approx 0,$$

where the extra terms compared to (4.7) depend on both h_{ij} and K_{ij}. These extra terms would complicate the analysis significantly.

The last two surface terms come from the integration by parts of the momentum constraint. Indeed, we define a smeared momentum constraint as the functional

$$\Phi[\vec{X}] = \int_{\Sigma_t} d^3x X^i \mathcal{H}_i, \tag{4.18}$$

where $\vec{X}$ is an arbitrary test vector on Σ_t. The momentum constraint (4.18) can be written as

$$\Phi[\vec{X}] = \int_{\Sigma_t} d^3x (p^{ij}\mathcal{L}_{\vec{X}} h_{ij} + \mathcal{P}^{ij}\mathcal{L}_{\vec{X}} K_{ij}) - \oint_{\mathcal{B}_t} d^2x 2s_i (X_j p^{ij} + X^j \mathcal{P}^{ik} K_{ik}), \tag{4.19}$$

where $\mathcal{L}_{\vec{X}} h_{ij} = 2D_{(i}X_{j)}$, which shows the origin of the last two surface terms. Thus the momentum constraint evidently generates infinitesimal (time-dependent) spatial diffeomorphism for the dynamical variables (h_{ij}, p^{ij}, K_{ij}, $\mathcal{P}^{ij}$) on the hypersurface Σ_t. We can extend the momentum constraint to a generator of (time-dependent) spatial diffeomorphism for all variables by absorbing certain terms into the Lagrange multipliers of the primary constraints (4.2). It can be defined up to boundary terms as

$$\Phi[\vec{X}] = \int_{\Sigma_t} d^3x (p^{ij}\mathcal{L}_{\vec{X}} h_{ij} + \mathcal{P}^{ij}\mathcal{L}_{\vec{X}} K_{ij} + p_N \mathcal{L}_{\vec{X}} N + p_i \mathcal{L}_{\vec{X}} N^i). \tag{4.20}$$

In either case, the momentum constraint satisfies the Lie algebra

$$\{\Phi[\vec{X}], \Phi[\vec{Y}]\} = \Phi[[\vec{X}, \vec{Y}]], \tag{4.21}$$

due to the corresponding property of the Lie derivative,

$$\mathcal{L}_{\vec{X}}\mathcal{L}_{\vec{Y}} - \mathcal{L}_{\vec{Y}}\mathcal{L}_{\vec{X}} = \mathcal{L}_{[\vec{X},\vec{Y}]}, \qquad [\vec{X}, \vec{Y}]^i = X^j \partial_j Y^i - Y^j \partial_j X^i. \tag{4.22}$$

The variables N, N^i, h_{ij} and K_{ij} behave as regular scalar or tensor fields under the spatial diffeomorphisms, while their canonically conjugated momenta behave as scalar or tensor densities of unit weight. Thus we can see that all the constraints behave as scalar or tensor densities of unit weight under the spatial diffeomorphisms.

We also define a smeared version of the Hamiltonian constraint as

$$\mathcal{H}_0[\xi] = \int_{\Sigma_t} d^3x \xi \mathcal{H}_0, \tag{4.23}$$

where ξ is an arbitrary test function on Σ_t. It satisfies the following algebra with the momentum constraint

$$\{\Phi[\vec{X}], \mathcal{H}_0[\xi]\} = \mathcal{H}_0[\vec{X}(\xi)], \tag{4.24}$$

since $\mathcal{H}_0$ is a scalar density of unit weight and consequently it satisfies

$$\{\mathcal{H}_0, \Phi[\vec{X}]\} = \mathcal{L}_{\vec{X}}\mathcal{H}_0 = X^i \partial_i \mathcal{H}_0 + \partial_i X^i \mathcal{H}_0. \tag{4.25}$$

Note that in the Hamiltonian, we could alternatively replace $\mathcal{P}^{ij}$ with its traceless components $\bar{\mathcal{P}}^{ij}$, or vice versa, because any term depending on a positive power of the primary constraint $\mathcal{P}$ can be absorbed into the Lagrange multiplier term $\lambda_{\mathcal{P}}\mathcal{P}$. Thus we could equally well define $\mathcal{H}_0$ in (4.14) with every $\mathcal{P}^{ij}$ replaced by $\bar{\mathcal{P}}^{ij}$. We shall, however, write the Hamiltonian in terms of all the components of the momentum $\mathcal{P}^{ij}$, since it simplifies slightly the calculation of the Poisson brackets between the constraints. The same applies to the momentum constraint and the surface terms. Note that we have written the first two surface terms in (4.13) with the full momentum $\mathcal{P}^{ij}$, corresponding to the term $D_i D_j \mathcal{P}^{ij}$ in (4.14). The momentum constraint (4.15) too is written with all the momenta so that it generates diffeomorphisms also for the trace component $\mathcal{P}$. Hence the last surface term in the Hamiltonian involves all the components of $\mathcal{P}^{ij}$ as well.

1. Consistency of constraints in time and secondary constraints

Every constraint has to be preserved under time evolution. This means the algebra of constraints has to be closed under the Poisson bracket.

The consistency of the primary constraints p_N and p_i in time is ensured by imposing $\mathcal{H}_0$ and $\mathcal{H}_i$ as local constraints,

$$\mathcal{H}_0 \approx 0, \qquad \mathcal{H}_i \approx 0, \tag{4.26}$$

respectively. This is why they were above referred to as the Hamiltonian constraint and the momentum constraint, respectively. The momentum constraint means that the theory is invariant under diffeomorphisms on the spatial hypersurface, i.e., generally covariant. The Hamiltonian constraint contains the dynamics of the theory. These constraints (at every point of Σ_t) are independent restrictions on the canonical variables [66]. Because the time evolution of the lapse N and shift N^i variables is given by the arbitrary Lagrange multipliers λ_N and λ^i, the lapse and shift variables themselves behave indeed as arbitrary multipliers in the Hamiltonian.

The consistency condition for the primary constraint $\mathcal{P}$ implies a secondary constraint. We express this new constraint as[7]

[7]If we based our Hamiltonian formulation on the action (3.47), this constraint would contain an extra term of the form $\alpha\sqrt{h}(D^i D^j K_{ij} - D^i D_i K)$ (up to a numerical factor). This extra term would further complicate the analysis significantly.

$$\mathcal{Q} = 2p + \mathcal{P}^{ij}K_{ij} \approx 0. \quad (4.27)$$

Note that we have included the trace component $\mathcal{P} \approx 0$ in the constraint $\mathcal{Q}$, similarly as we did in the Hamiltonian and momentum constraints, and for the same reason. Thanks to the secondary constraint (4.27), $\mathcal{P}$ is preserved in time,

$$\{\mathcal{P}(x), H\} \approx \{\mathcal{P}(x), \mathcal{H}_0[N]\} = -N(\mathcal{Q} + \mathcal{P}K)(x) \approx 0. \quad (4.28)$$

The Poisson bracket between $\mathcal{P}$ and $\mathcal{Q}$ closes,

$$\{\mathcal{P}(x), \mathcal{Q}(y)\} = \mathcal{P}(y)\delta(x-y). \quad (4.29)$$

Then we have to ensure that the secondary constraint $\mathcal{Q}$ is preserved in time. We again have

$$\{\mathcal{Q}(x), H\} \approx \{\mathcal{Q}(x), \mathcal{H}_0[N]\},$$

and thus the consistency condition for $\mathcal{Q}$ requires that the Poisson bracket between $\mathcal{Q}$ and $\mathcal{H}_0[N]$ must be a constraint (or zero). No further constraints are required, since we obtain

$$\{\mathcal{Q}(x), \mathcal{H}_0[N]\} = N\mathcal{H}_0(x) + ND^iD_i\mathcal{P}(x) + 3D_iND^i\mathcal{P}(x) + 2D^iD_iN\mathcal{P}(x) \approx 0. \quad (4.30)$$

See (D.10) in Appendix D for the derivation of this result, including all the Poisson brackets between the Hamiltonian constraint and the canonical variables.

Since $\mathcal{P}$ and $\mathcal{Q}$ are first-class constraints, they generate symmetry transformations. We again introduce smeared versions of the constraints

$$\mathcal{P}[\epsilon] = \int_{\Sigma_t} d^3x\epsilon\mathcal{P}, \qquad \mathcal{Q}[\epsilon] = \int_{\Sigma_t} d^3x\epsilon\mathcal{Q}, \quad (4.31)$$

which are the generators. The constraint $\mathcal{Q}$ generates a scale transformation for the following dynamical variables:

$$\{h_{ij}(x), \mathcal{Q}[\epsilon]\} = 2\epsilon h_{ij}(x),$$
$$\{p^{ij}(x), \mathcal{Q}[\epsilon]\} = -2\epsilon p^{ij}(x),$$
$$\{K_{ij}(x), \mathcal{Q}[\epsilon]\} = \epsilon K_{ij}(x),$$
$$\{\mathcal{P}^{ij}(x), \mathcal{Q}[\epsilon]\} = -\epsilon\mathcal{P}^{ij}(x). \quad (4.32)$$

Thus it is the generator of the conformal transformations. We could easily extend $\mathcal{Q}$ to a generator of scale transformations for all variables, just as we did above for the momentum constraint, by including the generators for the variables N, N^i and their conjugated momenta as $p_NN + p_iN^i$. Note that the conformal transformation leaves the scalars p and $\mathcal{P}^{ij}K_{ij}$ invariant, which implies $\mathcal{Q}$ itself is invariant, $\{\mathcal{Q}(x), \mathcal{Q}[\epsilon]\} = 0$. $\mathcal{P}$ is simply scaled under this transformation, $\{\mathcal{P}(x), \mathcal{Q}[\epsilon]\} = \epsilon\mathcal{P}(x)$. On the other hand, $\mathcal{P}$ generates a rather peculiar transformation:

$$\{h_{ij}(x), \mathcal{P}[\epsilon]\} = 0,$$
$$\{p^{ij}(x), \mathcal{P}[\epsilon]\} = -\epsilon\mathcal{P}^{ij}(x),$$
$$\{K_{ij}(x), \mathcal{P}[\epsilon]\} = \epsilon h_{ij}(x), \qquad \{\mathcal{P}^{ij}(x), \mathcal{P}[\epsilon]\} = 0. \quad (4.33)$$

It evidently transforms $\mathcal{Q}$ to $\mathcal{P}$, $\{\mathcal{Q}(x), \mathcal{P}[\epsilon]\} = -\epsilon\mathcal{P}(x)$.

The Hamiltonian constraint $\mathcal{H}_0$ is preserved under time evolution, since its Poisson bracket with itself is a sum of the momentum and $\mathcal{P}$ constraints (see Appendix D 1):

$$\{\mathcal{H}_0[\xi], \mathcal{H}_0[\eta]\} = \Phi[\xi\vec{D}\eta - \eta\vec{D}\xi] + 2\mathcal{P}[(\xi D_i\eta - \eta D_i\xi)h^{ij}(D^kK_{jk} - D_jK)]. \quad (4.34)$$

This ensures that the time evolution of the system is consistent with the structure of spacetime.

Since $\mathcal{Q}$ is a first-class constraint, we should include it into the total Hamiltonian with an arbitrary Lagrange multiplier:

$$H = \int_{\Sigma_t} d^3x(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda_Np_N + \lambda^ip_i + \lambda_{\mathcal{P}}\mathcal{P} + \lambda_{\mathcal{Q}}\mathcal{Q}) + H_{\text{surf}}. \quad (4.35)$$

2. Physical degrees of freedom and gauge fixing

The number of physical degrees of freedom in any constrained system can be counted according to Dirac's formula:

$$\text{Number of physical degrees of freedom} = \frac{1}{2}(\text{Number of canonical variables} - 2 \times \text{Number of first-class constraints} - \text{Number of second-class constraints}). \quad (4.36)$$

In the Hamiltonian formulation of Weyl gravity, there are 32 canonical variables, namely N, N^i, h_{ij}, $K_{ij}$and their canonically conjugated momenta p_N, p_i, p^{ij}, $\mathcal{P}^{ij}$. There exist ten first-class constraints, namely p_N, p_i, $\mathcal{H}_0$, $\mathcal{H}_i$, $\mathcal{P}$, $\mathcal{Q}$ and no second-class constraints. Thus the conformally invariant Weyl gravity has six physical degrees of freedom.

There exist many possible sets of gauge fixing conditions. The simplest way to fix the gauge freedom associated with the primary constraints $p_N = 0$ and $p_i = 0$, is to impose the lapse and shift variables to constant values everywhere. There do exist useful field-dependent choices for the conditions on N and N^i, but we do not consider them here. Hence we impose the conditions

$$\sigma_0 = N - 1 = 0, \qquad \sigma_i = N^i = 0. \tag{4.37}$$

The gauge freedom associated with the Hamiltonian and momentum constraints $\mathcal{H}_0 = 0$ and $\mathcal{H}_i = 0$ can be fixed by introducing four conditions among the components of the metric h_{ij}. The gauge freedom associated with the constraints $\mathcal{P} = 0$ and $\mathcal{Q} = 0$ can be fixed by imposing the traces of the metric and the extrinsic curvature to match those of the flat space. Thus we can choose the gauge conditions as

$$\chi_\mu(h_{ij}) = 0, \qquad \mu = 1, \ldots, 4, \tag{4.38}$$

$$K = 0, \qquad \chi_5 = \delta^{ij} h_{ij} - 3 = 0. \tag{4.39}$$

The four gauge conditions $\chi_\mu = 0$, $\mu = 1, \ldots, 4$, have to be such that they fix four components of the metric h_{ij}. These conditions are often referred to as coordinate conditions. This is because the conditions (4.37) and (4.38) essentially fix the coordinate system on spacetime and define how the spacetime is foliated.

An alternative choice of gauge fixing conditions, which is specific to Weyl gravity, is to replace the five conditions $\chi_\mu(h_{ij}) = 0$, $\mu = 1, \ldots, 5$, with conditions on the traceless component of the extrinsic curvature $\bar{K}_{ij}$, i.e., we replace (4.38) and (4.39) with

$$K = 0, \qquad \chi_\mu(\bar{K}_{ij}) = 0, \qquad \mu = 1, \ldots, 5. \tag{4.40}$$

The conditions $\chi_\mu(\bar{K}_{ij}) = 0$ have to be such that they fix each of the five independent components of $\bar{K}_{ij}$. This type of gauge is possible since the first-class constraints depend on all the components of the variables K_{ij}, $\mathcal{P}^{ij}$, as well as on all the components of the variables h_{ij}, p^{ij}. This enables a highly rich set of choices in the gauge fixing. When a gauge of the type (4.40) is chosen, we may regard that the 12 constraints define the variables K_{ij}, $\mathcal{P}^{ij}$ in terms of the independent variables h_{ij}, p^{ij}. For details on gauge fixing conditions, see [55,69] and the last reference in [60].

B. Weyl gravity with $\Lambda \neq 0$

In this subsection, we consider what happens to the Hamiltonian structure of Weyl gravity when the cosmological constant Λ is added into the Lagrangian. The cosmological constant term is added into the potential part of the Hamiltonian constraint as

$$\mathcal{H}_0 = 2p^{ij}K_{ij} - \frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{2\alpha\sqrt{h}} + \mathcal{P}^{ij\,(3)}R_{ij} + \mathcal{P}^{ij}K_{ij}K + D_iD_j\mathcal{P}^{ij} - \sqrt{h}\Lambda - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}. \tag{4.41}$$

All the primary constraints, the momentum constraint and the secondary constraint $\mathcal{Q}$ remain the same as in the conformally invariant Weyl gravity.

The consistency condition that ensures the secondary constraint $\mathcal{Q}$ to be preserved in time, now includes a cosmological constant term in addition to the terms involving the constraints $\mathcal{H}_0$ and $\mathcal{P}$:

$$\{\mathcal{Q}(x), H\} \approx \{\mathcal{Q}(x), \mathcal{H}_0[N]\} \approx 4\Lambda N\sqrt{h}(x). \tag{4.42}$$

Thus, whenever $\Lambda \neq 0$, we have to introduce another secondary constraint:

$$\mathcal{N} = N\sqrt{h} \approx 0. \tag{4.43}$$

In order to ensure the preservation of this constraint,

$$\{\mathcal{N}(x), H\} = NK\mathcal{N}(x) + \lambda_N\sqrt{h} \approx \lambda_N\sqrt{h}, \tag{4.44}$$

we set the Lagrange multiplier of the primary constraint p_N to zero,

$$\lambda_N = 0. \tag{4.45}$$

Thus we have a pair of second-class constraints $\mathcal{N}$ and p_N. The lapse does not evolve, $\partial_t N = 0$, i.e., it is frozen to its initial configuration. The Dirac bracket (4.71) is equivalent to the Poisson bracket for any quantities that are independent of N and p_N. $\mathcal{P}$ and $\mathcal{Q}$ are still first-class constraints:

$$\{\mathcal{N}(x), \mathcal{P}(y)\} = 0, \qquad \{\mathcal{N}(x), \mathcal{Q}(y)\} = 3\mathcal{N}(x)\delta(x - y). \tag{4.46}$$

The number of physical degrees of freedom is six, similar to the pure Weyl gravity. Unfortunately, the constraint (4.43) is physically unacceptable. The constraint (4.43) imposes the determinant of the metric of spacetime to be zero, $N\sqrt{h} = \sqrt{-g} = 0$. This destroys the geometry of spacetime.

For completeness, let us analyze the other possible secondary constraints in place of (4.43). If we impose the constraint $N \approx 0$, then N and p_N become a pair of second-class constraints. However, the time dimension collapses when $N = 0$. Recall that N must be positive since $N dt$ measures the lapse of proper time between the hypersurfaces at times t and $t + dt$.

Suppose we instead satisfy the condition (4.43) by imposing the constraint

$$\mathcal{Q}_{(2)} = \sqrt{h} \approx 0. \tag{4.47}$$

This constraint has a weakly vanishing Poisson bracket with the Hamiltonian constraint $\mathcal{H}_0[N]$ (D1),

$$\{\mathcal{Q}_{(2)}(x), \mathcal{H}_0[N]\} = N\sqrt{h}K(x) = NK\mathcal{Q}_{(2)}(x) \approx 0. \tag{4.48}$$

The Poisson brackets with $\mathcal{P}$ and $\mathcal{Q}$ are

$$\begin{aligned} &\{\mathcal{Q}_{(2)}(x), \mathcal{P}(y)\} = 0, \\ &\{\mathcal{Q}_{(2)}(x), \mathcal{Q}(y)\} = 2h_{ij}(y) \\ &\{\sqrt{h}(x), p^{ij}(y)\} = 3\mathcal{Q}_{(2)}(x)\delta(x-y). \end{aligned} \tag{4.49}$$

Thus the Poisson bracket between the secondary constraint $\mathcal{Q}_{(2)}$ and the Hamiltonian is proportional to $\mathcal{Q}_{(2)}$, and hence no further constraints are required. All the constraints appear to be first class, which is very strange, since we would expect to see some second-class constraint due to the violation of the conformal invariance. The extra first-class constraint $\mathcal{Q}_{(2)}$ implies the removal of one physical degree of freedom. Certainly the introduction of Λ into Weyl gravity should not remove any physical degrees of freedom! Compare this to Sec. 3.6 of [42], where four second-class constraints were found instead, denoted as $C^{(k)} \approx 0$, $k = 1, \ldots, 4$. It is however unclear why the constraint $C^{(4)}$ is required in [42], since $C^{(4)}$ is proportional to the constraint $C^{(3)}$ multiplied by K, and thus $C^{(4)}$ is redundant. With this redundant fourth second-class constraint $C^{(4)}$, the same number of physical degrees of freedom as in Weyl gravity were obtained in [42], that is six physical degrees of freedom. Our conclusion is the opposite: there exists one more first-class constraint compared to the Weyl gravity case, $\mathcal{Q}_{(2)}$, and thus the number of physical degrees of freedom is five.

The constraint (4.47) would generate a trivial (null) transformation. The transformations of most of the variables are zero strongly, while the only nontrivial transformation is that of the momentum p^{ij},

$$\begin{aligned} \{p^{ij}(x), \mathcal{Q}_{(2)}[\epsilon]\} &= -\epsilon(x)\frac{\Lambda}{2}\sqrt{h}h^{ij}(x) \\ &= -\frac{1}{2}h^{ij}\epsilon\mathcal{Q}_{(2)}(x) \approx 0, \end{aligned} \tag{4.50}$$

and even that vanishes weakly.

The constraint (4.47) would enable us to write the Hamiltonian as

$$\begin{aligned} H = \int_{\Sigma_t} d^3x(&N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda_N p_N + \lambda^i p_i + \lambda_{\mathcal{P}}\mathcal{P} \\ &+ \lambda_{\mathcal{Q}}\mathcal{Q} + \lambda^{(2)}_{\mathcal{Q}}\mathcal{Q}_{(2)}) + H_{\rm surf}, \end{aligned} \tag{4.51}$$

where the Hamiltonian constraint can now be written as

$$\begin{aligned} \mathcal{H}_0 = 2p^{ij}K_{ij} - \frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{2\alpha\sqrt{h}} + \mathcal{P}^{ij(3)}R_{ij} + \mathcal{P}^{ij}K_{ij}K \\ + D_iD_j\mathcal{P}^{ij}. \end{aligned} \tag{4.52}$$

As long as $\Lambda \neq 0$, the terms that are proportional to $\sqrt{h}$ can be absorbed into the Lagrange multiplier term $\lambda^{(2)}_{\mathcal{Q}}\mathcal{Q}_{(2)}$. The term $-\frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{2\alpha\sqrt{h}}$, however, appears to be divergent, since $h^{-1/2} \to \infty$. It is not surprising that the constraint (4.47) leads to such inconsistencies, since the metric of the spatial hypersurfaces Σ_t must be positive definite, $h = \det(h_{ij}) > 0$.

Thus every one of the possible secondary constraints (4.43), $N \approx 0$ or (4.47) implies a physically inconsistent Hamiltonian structure.

C. Including Λ into Weyl gravity with a scalar field

In order to resolve the previous problem with $\Lambda \neq 0$, following [46,47] we introduce a scalar field ϕ which is coupled to the metric of spacetime in a way that makes the theory invariant under conformal transformations, when the field ϕ transforms in an appropriate way. This is in a sense reminiscent of the introduction of gauge fields in order to ensure the invariance under local phase transformations. Since the theory is required to possess both the conformal and diffeomorphism invariances, the action for the scalar field must have the form [46,47]

$$S_\phi = \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + \frac{1}{12}R\phi^2 + \bar{\Lambda}\phi^4\right]. \tag{4.53}$$

We require that the scalar field transforms under conformal transformations as $\phi \to \Omega^{-1}\phi$, while the metric transforms in the usual way, $g_{\mu\nu} \to \Omega^2 g_{\mu\nu}$. The scalar curvature R transforms as

$$R \to \Omega^{-2}\left(R - 6g^{\mu\nu}\frac{\nabla_\mu\nabla_\nu\Omega}{\Omega}\right). \tag{4.54}$$

The value of $\bar{\Lambda}$ can be chosen freely, since it is not fixed by conformal invariance. Hence the action (4.53) is found to be conformally invariant. Consequently, the whole action of the theory, $S_{\rm Weyl,\Lambda} = S_{\rm Weyl} + S_\phi$, is conformally invariant as well.

In the action (4.53), notice that $\bar{\Lambda}$ is dimensionless, while the cosmological constant Λ has the dimension M^4, mass to the fourth power. The conformal invariance is broken spontaneously [67,68], when the scalar field ϕ has a nonzero vacuum expectation value. Naively, that would produce an effective cosmological constant as $\Lambda = \bar{\Lambda}\bar{\phi}^4$, where $\bar{\phi}$ is the vacuum expectation value of ϕ. However, it has been shown that the cosmological constant can be made to vanish at every order in perturbation theory [46,47], even though $\bar{\phi} \neq 0$ is required for the existence of a perturbation expansion.

For the Hamiltonian formulation we rewrite the action (4.53) in the $3+1$ form,

$$S_\phi = \int dt \int_{\Sigma_t} d^3x N\sqrt{h}\Big[-\frac{1}{2}(\nabla_n\phi)^2 + \frac{1}{2}h^{ij}\partial_i\phi\partial_j\phi - \frac{1}{3}K\phi\nabla_n\phi - \frac{1}{6\sqrt{h}}\partial_i(\sqrt{h}h^{ij}\partial_j\phi^2) + \frac{1}{12}(K_{ij}K^{ij} - K^2 + {}^{(3)}R)\phi^2 + \bar{\Lambda}\phi^4\Big] + S_{\rm surf}, \quad (4.55)$$

where $\nabla_n\phi = \frac{1}{N}(\partial_t\phi - N^i\partial_i\phi)$ and $S_{\rm surf}$ contains the boundary terms that appear due to integrations by parts. Then the momentum conjugate to ϕ has the form

$$p_\phi = -\sqrt{h}\nabla_n\phi - \frac{1}{3}\sqrt{h}K\phi. \quad (4.56)$$

The contribution of the scalar field to the Hamiltonian is

$$H_\phi = \int_{\Sigma_t} d^3x(p_\phi\partial_t\phi - \mathcal{L}_\phi) = \int_{\Sigma_t} d^3x(N\mathcal{H}_0^\phi + N^i\mathcal{H}_i^\phi) + H_{\rm surf}^\phi, \quad (4.57)$$

where

$$\mathcal{H}_0^\phi = -\frac{1}{2\sqrt{h}}\left(p_\phi + \frac{1}{3}\sqrt{h}K\phi\right)^2 - \frac{1}{2}\sqrt{h}h^{ij}\partial_i\phi\partial_j\phi + \frac{1}{6}\partial_i(\sqrt{h}h^{ij}\partial_j\phi^2) - \frac{1}{12}\sqrt{h}(K_{ij}K^{ij} - K^2 + {}^{(3)}R)\phi^2 - \bar{\Lambda}\sqrt{h}\,\phi^4, \quad (4.58)$$

$$\mathcal{H}_i^\phi = p_\phi\partial_i\phi, \quad (4.59)$$

and $H_{\rm surf}^\phi$ contains the boundary terms. Since we wish to obtain a boundary contribution only on the spatial boundary $\mathcal{B}_t$, we complement the action (4.53) with a boundary term $\frac{1}{6}\oint_{\partial\mathcal{M}} d^3x\sqrt{|\gamma|}K\phi^2$. The variations of this boundary term are proportional to the variations of the variables and hence vanish due to the boundary conditions. The boundary term in the Hamiltonian is obtained as

$$H_{\rm surf}^\phi = -\frac{1}{6}\oint_{\mathcal{B}_t} d^2xN\sqrt{\sigma}({}^{(2)}K\phi^2 + s_ih^{ij}\partial_j\phi^2). \quad (4.60)$$

The first term is similar to the boundary term of general relativity, but weighted by the scalar field factor $\frac{\kappa}{6}\phi^2$. The second term involves the gradient of the scalar factor ϕ^2 along the unit normal to the spatial boundary.

Preservation of the primary constraint $\mathcal{P} \approx 0$ leads to the following form of the secondary constraint $\mathcal{Q} \approx 0$:

$$\mathcal{Q} = 2p + \mathcal{P}^{ij}K_{ij} - p_\phi\phi. \quad (4.61)$$

The constraint $\mathcal{Q}$ is found to be the first-class constraint associated with the conformal symmetry. Indeed, we obtain

$$\{\mathcal{Q}(x), \mathcal{H}_0^\phi(y)\} = \mathcal{H}_0^\phi(x)\delta(x-y). \quad (4.62)$$

Now we can fix the constraint $\mathcal{Q} \approx 0$ by introducing the gauge fixing condition. Instead of the gauge condition χ_5 in (4.39), we may impose

$$\chi_\phi = \phi(x) - \phi_0 = 0, \qquad \phi_0 = \text{const}. \quad (4.63)$$

Then $\mathcal{Q}$ and χ_ϕ become the second-class constraints that vanish strongly and can be explicitly solved as

$$p_\phi = \frac{1}{\phi_0}(2p + \mathcal{P}^{ij}K_{ij}). \quad (4.64)$$

Note that the Dirac brackets between remaining phase space variables are the same as the Poisson brackets, since they have vanishing Poisson brackets with χ_ϕ.

The number of physical degrees of freedom is seven—one more than in the pure Weyl gravity. When the conformal gauge is fixed as in (4.63), the extra scalar degree of freedom is transferred to the metric variables. Alternatively, we can fix the gauge as in (4.39), keeping the scalar variables ϕ, p_ϕ.

We emphasize that the kinetic term of ϕ in the action (4.53) has the opposite sign compared to a regular scalar field. As a result, in the Hamiltonian (4.58), the kinetic term of ϕ is nonpositive.

D. General relativity plus Weyl gravity: $\kappa^{-1} \neq 0, \alpha \neq 0, \beta = \gamma = 0$

Here we consider the sum of Einstein-Hilbert and Weyl actions. This model is most relevant at long distances, where the Einstein-Hilbert action linear in curvature is expected to dominate the behaviour of the theory, while contribution of the Weyl action is suppressed by the higher-order derivatives. The cosmological constant can be either included or excluded, since its presence has no impact on the fundamental Hamiltonian structure of the theory when the Einstein-Hilbert action is included.

The Hamiltonian constraint is given as

$$\mathcal{H}_0 = 2p^{ij}K_{ij} - \frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{2\alpha\sqrt{h}} + \mathcal{P}^{ij(3)}R_{ij} + \mathcal{P}^{ij}K_{ij}K + D_iD_j\mathcal{P}^{ij} - \sqrt{h}\Lambda - \frac{\sqrt{h}}{2\kappa}({}^{(3)}R + K_{ij}K^{ij} - K^2) - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}. \tag{4.65}$$

The surface term $-\frac{1}{\kappa}\oint_{\mathcal{B}_t} d^2x\sqrt{\sigma}N^{(2)}K$ is now included in the total Hamiltonian (4.35) due to the presence of the Einstein-Hilbert action [see (3.50)]. In case the spacelike and timelike hypersurfaces Σ_t and $\mathcal{B}$ intersect nonorthogonally, we would include a surface term according to (3.51). Assuming the hypersurfaces are orthogonal, the surface term in the Hamiltonian is written as

$$H_{\text{surf}} = -\frac{1}{\kappa}\oint_{\mathcal{B}_t} d^2x\sqrt{\sigma}N^{(2)}K + \oint_{\mathcal{B}_t} d^2x s_i(D_jN\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_jp^{ij} + 2N^j\mathcal{P}^{ik}K_{jk}). \tag{4.66}$$

The secondary constraint $\mathcal{Q}$ now takes a different form

$$\mathcal{Q} = 2p + \mathcal{P}^{ij}K_{ij} + \frac{2}{\kappa}\sqrt{h}K \approx 0 \tag{4.67}$$

because of the presence of the Einstein-Hilbert part of the action. The Poisson bracket between $\mathcal{P}$ and $\mathcal{Q}$ no longer closes,

$$\{\mathcal{P}(x), \mathcal{Q}(y)\} = \left(\mathcal{P} - \frac{6}{\kappa}\sqrt{h}\right)(y)\delta(x-y). \tag{4.68}$$

Clearly the conformal symmetry of Weyl gravity has been broken. As a result, the consistency conditions that ensure the constraints $\mathcal{P}$ and $\mathcal{Q}$ to be preserved in time, determine the Lagrange multipliers of these constraints as

$$\lambda_{\mathcal{P}} = -N\left[\frac{2\kappa\Lambda}{3} + \frac{1}{2}({}^{(3)}R - K_{ij}K^{ij} + K^2)\right] \tag{4.69}$$

and

$$\lambda_{\mathcal{Q}} = 0. \tag{4.70}$$

Thus $\mathcal{P}$ and $\mathcal{Q}$ are now second-class constraints.

Recall that in the Hamiltonian formalism, second-class constraints become strong equalities if we replace the canonical Poisson bracket with the Dirac bracket. Given a set of second-class constraints ϕ_a, $a = 1, 2, \ldots, A$, the Dirac bracket is defined as

$$\{f_1(x), f_2(y)\}_{\text{D}} = \{f_1(x), f_2(y)\} - \iint_{\Sigma_t} d^3z d^3z' \sum_{a,b=1}^{A} \{f_1(x), \phi_a(z)\} \times M^{-1}_{ab}(z, z')\{\phi_b(z'), f_2(y)\}, \tag{4.71}$$

where $M^{-1}(x, y)$ is the inverse of the matrix $M(x, y)$ with the components

$$M_{ab}(x, y) = \{\phi_a(x), \phi_b(y)\}, \quad a, b = 1, 2, \ldots, A. \tag{4.72}$$

The constraints $\mathcal{P}$ and $\mathcal{Q}$ can be set to zero strongly, when we replace the Poisson bracket with the Dirac bracket.

The Dirac bracket between the canonical variables is defined as

$$\begin{aligned}
&\{h_{ij}(x), h_{kl}(y)\}_{\text{D}} = 0,\\
&\{h_{ij}(x), p^{kl}(y)\}_{\text{D}} = \left(\delta_i^{(k}\delta_j^{l)} + \frac{\kappa}{3}\frac{h_{ij}\mathcal{P}^{kl}}{\sqrt{h}}\right)(x)\delta(x-y),\\
&\{h_{ij}(x), K_{kl}(y)\}_{\text{D}} = -\frac{\kappa}{3}\frac{h_{ij}h_{kl}}{\sqrt{h}}(x)\delta(x-y),\\
&\{h_{ij}(x), \mathcal{P}^{kl}(y)\}_{\text{D}} = 0,\\
&\{p^{ij}(x), p^{kl}(y)\}_{\text{D}} = \left[\frac{\kappa}{3}\frac{\mathcal{P}^{ij}p^{kl} - p^{ij}\mathcal{P}^{kl}}{\sqrt{h}} + \frac{1}{6}K(\mathcal{P}^{ij}h^{kl} - h^{ij}\mathcal{P}^{kl})\right](x)\delta(x-y),\\
&\{p^{ij}(x), K_{kl}(y)\}_{\text{D}} = \left[\frac{\kappa}{3}\frac{p^{ij}h_{kl} - \frac{1}{2}\mathcal{P}^{ij}K_{kl}}{\sqrt{h}} + \frac{1}{6}h^{ij}h_{kl}K\right](x) \times \delta(x-y),\\
&\{p^{ij}(x), \mathcal{P}^{kl}(y)\}_{\text{D}} = \frac{\kappa}{6}\frac{\mathcal{P}^{ij}\mathcal{P}^{kl}}{\sqrt{h}}(x)\delta(x-y),\\
&\{K_{ij}(x), K_{kl}(y)\}_{\text{D}} = \frac{\kappa}{6}\frac{h_{ij}K_{kl} - K_{ij}h_{kl}}{\sqrt{h}}(x)\delta(x-y),\\
&\{K_{ij}(x), \mathcal{P}^{kl}(y)\}_{\text{D}} = \left(\delta_i^{(k}\delta_j^{l)} - \frac{1}{3}h_{ij}h^{kl} - \frac{\kappa}{6}\frac{h_{ij}\mathcal{P}^{kl}}{\sqrt{h}}\right)(x) \times \delta(x-y),\\
&\{\mathcal{P}^{ij}(x), \mathcal{P}^{kl}(y)\}_{\text{D}} = 0.
\end{aligned} \tag{4.73}$$

The total Hamiltonian is now written as

$$H = \int_{\Sigma_t} d^3x(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda_N p_N + \lambda^i p_i) + H_{\text{surf}}. \tag{4.74}$$

In the Hamiltonian formulation of the combination of Weyl and Einstein-Hilbert actions, there are 32 canonical variables (N, N^i, h_{ij}, K_{ij}) and their canonically conjugated momenta (p_N, p_i, p^{ij}, $\mathcal{P}^{ij}$). There exist eight first-class constraints (p_N, p_i, $\mathcal{H}_0$, $\mathcal{H}_i$) and two second-class constraints ($\mathcal{P}$, $\mathcal{Q}$). Thus the number of physical degrees of freedom is seven. Gauge fixing can be accomplished similarly as in Weyl gravity, but without the gauge conditions (4.39) which are associated with conformal invariance. For example, we can choose the gauge conditions as in (4.37) and (4.38).

We can now gain insight on the generality of the critical gravity proposal [10]. In the full nonlinear theory, the value of Λ has no impact on the structure of the constraints and the Hamiltonian. Since there exist eight first-class constraints (p_N, p_i, $\mathcal{H}_0$, $\mathcal{H}_i$) and two second-class constraints ($\mathcal{P}$, $\mathcal{Q}$), regardless of the presence or value of Λ, the number of local physical degrees of freedom is seven. This suggests that the possibility for the massive spin-2 excitations to become massless [10] is only an artefact of the linearized theory on the anti–de Sitter spacetime. This is likely related to the possibility of partial masslessness of higher spin fields on (anti–)de Sitter backgrounds [53,54]. In the linearized theory on Minkowski background, two modes are associated with the massless spin-2 graviton and five modes with a massive spin-2 field.

We have discovered a somewhat similar contrast between the linearized formulation of the so-called renormalizable covariant gravity on Minkowski spacetime and the Hamiltonian formulation of the full nonlinear theory in [39].

E. Curvature-squared gravity without conformal invariance

Here we consider the gravitational action (2.1), when the curvature-squared part of the action lacks conformal invariance. That is, we assume $\alpha \neq 0$ and $\beta \neq 0$ in the action (3.46). Cosmological constant and Einstein-Hilbert action can be either included or excluded, since the conformal invariance is already broken by the scalar curvature squared term.

The momentum (4.4) canonically conjugate to K_{ij} can be written as

$$\begin{aligned}\mathcal{P}^{ij} &= -\alpha\sqrt{h}\mathcal{G}^{ijkl}\mathcal{L}_n K_{kl}\\ &\quad + \alpha\sqrt{h}\bar{\mathcal{G}}^{ijkl}\left({}^{(3)}R_{kl} + K_{kl}K - \frac{1}{N}D_k D_l N\right)\\ &\quad + \frac{\beta}{2}\sqrt{h}h^{ij}\left({}^{(3)}R - 3K_{kl}K^{kl} + K^2 - \frac{2}{N}D^k D_k N\right),\end{aligned} \tag{4.75}$$

where we have defined a generalized DeWitt metric as

$$\mathcal{G}^{ijkl} = \frac{1}{2}(h^{ik}h^{jl} + h^{il}h^{jk}) - \frac{\alpha + 3\beta}{3\alpha}h^{ij}h^{kl}. \tag{4.76}$$

Since $\alpha \neq 0$ and $\beta \neq 0$, unlike the traceless DeWitt metric (4.6), this generalized DeWitt metric (4.76) has full rank, and hence its inverse can be obtained as

$$\mathcal{G}_{ijkl} = \frac{1}{2}(h_{ik}h_{jl} + h_{il}h_{jk}) - \frac{\alpha + 3\beta}{9\beta}h_{ij}h_{kl}. \tag{4.77}$$

We can now solve the definition of the momentum (4.75) in terms of the velocities $\partial_t K_{ij}$ and obtain

$$\begin{aligned}\mathcal{P}^{ij}\partial_t K_{ij} &= -N\frac{\mathcal{P}^{ij}\mathcal{G}_{ijkl}\mathcal{P}^{kl}}{\alpha\sqrt{h}} + N\mathcal{P}^{ij}({}^{(3)}R_{ij} + K_{ij}K)\\ &\quad + \mathcal{P}^{ij}D_i D_j N - \frac{N}{2}\mathcal{P}({}^{(3)}R - K_{ij}K^{ij} + K^2)\\ &\quad + \mathcal{P}^{ij}\mathcal{L}_{\vec{N}}K_{ij}.\end{aligned} \tag{4.78}$$

The Lagrangian density of the action is written in terms of the canonical variables as

$$\mathcal{L}_C = -N\left(\frac{\mathcal{P}^{ij}\mathcal{G}_{ijkl}\mathcal{P}^{kl}}{2\alpha\sqrt{h}} + 2p^{ij}K_{ij} - \sqrt{h}\Lambda - \frac{\sqrt{h}}{2\kappa}({}^{(3)}R + K_{ij}K^{ij} - K^2) - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}\right) + p^{ij}\partial_t h_{ij} - 2p^{ij}D_{(i}N_{j)}. \tag{4.79}$$

The total Hamiltonian is obtained as

$$H = \int_{\Sigma_t} d^3x(N\mathcal{H}_0 + N^i\mathcal{H}_i + \lambda_N p_N + \lambda^i p_i) + H_{\text{surf}}, \tag{4.80}$$

with the following quantities. The Hamiltonian constraint is defined as

$$\begin{aligned}\mathcal{H}_0 &= 2p^{ij}K_{ij} - \frac{\mathcal{P}^{ij}\mathcal{G}_{ijkl}\mathcal{P}^{kl}}{2\alpha\sqrt{h}} + \mathcal{P}^{ij(3)}R_{ij} + \mathcal{P}^{ij}K_{ij}K + D_i D_j\mathcal{P}^{ij} - \frac{\mathcal{P}}{2}({}^{(3)}R - K_{ij}K^{ij} + K^2) - \sqrt{h}\Lambda\\ &\quad - \frac{\sqrt{h}}{2\kappa}({}^{(3)}R + K_{ij}K^{ij} - K^2) - \alpha\sqrt{h}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}.\end{aligned} \tag{4.81}$$

The surface term is defined as

$$H_{\text{surf}} = -\frac{1}{\kappa}\oint_{\mathcal{B}_t} d^2x\sqrt{\sigma}N^{(2)}K + \oint_{\mathcal{B}_t} d^2x s_i(D_j N\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_j p^{ij} + 2N^j\mathcal{P}^{ik}K_{jk}), \tag{4.82}$$

where the surface term of general relativity, i.e., the first term, is included whenever the Einstein-Hilbert action is included.

The algebra of constraints has the same form as in general relativity. The Poisson bracket between Hamiltonian constraints is given as a sum of momentum constraints with a h^{ij}-dependent multiplier,

$$\{\mathcal{H}_0[\xi],\mathcal{H}_0[\eta]\} = \int_{\Sigma_t} d^3x(\xi D_i\eta - \eta D_i\xi)h^{ij}\mathcal{H}_j = \Phi[\xi\vec{D}\eta - \eta\vec{D}\xi]. \tag{4.83}$$

In the Hamiltonian formulation of curvature-squared gravity without conformal symmetry, and possibly with the cosmological constant and the Einstein-Hilbert action included, there are 32 canonical variables, namely N, N^i, h_{ij}, K_{ij} and their canonically conjugated momenta p_N, p_i, p^{ij}, $\mathcal{P}^{ij}$. There exist eight first-class constraints, namely p_N, p_i, $\mathcal{H}_0$, $\mathcal{H}_i$, and no second-class constraints. Thus the number of physical degrees of freedom is eight.

Gauge fixing can be accomplished in the same way as in the previous case in Sec. IV D. For example, we can choose the gauge conditions (4.37) and (4.38). Alternatively, we could impose the four gauge conditions (4.38) on the variables K_{ij} (or $\mathcal{P}^{ij}$). But in these conformally noninvariant theories, only part of the variables K_{ij} can be constrained, unlike in Weyl gravity (4.40).

F. Physical Hamiltonian and total gravitational energy

For a system which is invariant under time reparameterization, the Hamiltonian is typically a first-class constraint. The same is true for generally covariant field theories with diffeomorphism invariance. In a generally covariant system, time evolution is just the unfolding of a gauge transformation. The bulk part of the gravitational Hamiltonian is a sum of first-class constraints, like in (4.13) or in any other Hamiltonian considered in this paper. However, the surface contribution $H_{\rm surf}$ on the boundary of spatial hypersurface does not vanish on the constraint surface. This indeed provides us the concept of total energy.

First, in order to obtain the physical Hamiltonian, we need to subtract the reference background. Consider a given background solution and an arbitrary (variable) configuration. The variable configuration and the reference background should induce the same configuration on the spatial boundary $\mathcal{B}_t$, at least asymptotically. Hence the volume element on the boundary is identical for them. Since the background is a solution to the field equations, the constraints associated with the solution vanish. Thus the Hamiltonian for the background consists solely of the boundary terms $H_{\rm b} = H_{\rm b,\,surf}$. The physical Hamiltonian is the difference:

$$H_{\rm phys} = H - H_{\rm b}. \tag{4.84}$$

Furthermore, for a stationary background solution, the canonical momenta $p_{\rm b}^{ij}$ and $\mathcal{P}_{\rm b}^{ij}$ vanish, since the time derivatives of the variables $\partial_t h_{{\rm b},ij}$ and $\partial_t K_{{\rm b},ij}$ are zero. The spatial slices of the stationary background can be labeled so that its lapse matches the lapse of the variable configuration, $N_{\rm b} = N$. Then the Hamiltonian of the background is obtained as follows:

(i) for pure Weyl or curvature-squared gravity,

$$H_{\rm b} = 0, \tag{4.85}$$

(ii) for Weyl gravity with Λ included via a scalar field,

$$H_{\rm b} = -\frac{1}{6}\oint_{\mathcal{B}_t} d^2x N\sqrt{\sigma}({}^{(2)}K_{\rm b}\phi_{\rm b}^2 + s_i h_{\rm b}^{ij}\partial_j\phi_{\rm b}^2), \tag{4.86}$$

(iii) for general relativity with (or without) curvature-squared terms,

$$H_{\rm b} = -\frac{1}{\kappa}\oint_{\mathcal{B}_t} N\sqrt{\sigma}{}^{(2)}K_{\rm b}. \tag{4.87}$$

We can now define the total energy associated with the time translation along $t^\mu = Nn^\mu + N^\mu$ for any given solution of the equations of motion as the value of the physical Hamiltonian on the constraint surface. Since the constraint part of the Hamiltonian is zero for any solution, the total energy is given by the difference of the surface terms:

$$E = H_{\rm surf} - H_{\rm b}. \tag{4.88}$$

We obtain

(i) for pure Weyl or curvature-squared gravity,

$$E = \oint_{\mathcal{B}_t} d^2x s_i(D_jN\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_jp^{ij} + 2N^j\mathcal{P}^{ik}K_{jk}), \tag{4.89}$$

(ii) for Weyl gravity with Λ included via a scalar field,

$$E = -\frac{1}{6}\oint_{\mathcal{B}_t} d^2xN\sqrt{\sigma}[{}^{(2)}K\phi^2 - {}^{(2)}K_{\rm b}\phi_{\rm b}^2 + s_i(h^{ij}\partial_j\phi^2 - h_{\rm b}^{ij}\partial_j\phi_{\rm b}^2)] + \oint_{\mathcal{B}_t} d^2xs_i(D_jN\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_jp^{ij} + 2N^j\mathcal{P}^{ik}K_{jk}), \tag{4.90}$$

(iii) for general relativity with curvature-squared terms,

$$E = -\frac{1}{\kappa}\oint_{\mathcal{B}_t} d^2xN\sqrt{\sigma}({}^{(2)}K - {}^{(2)}K_{\mathrm{b}}) + \oint_{\mathcal{B}_t} d^2xs_i(D_jN\mathcal{P}^{ij} - ND_j\mathcal{P}^{ij} + 2N_jp^{ij} + 2N^j\mathcal{P}^{ik}K_{jk}). \quad (4.91)$$

These generic expressions for the total energy can be used to obtain the total energy with respect to different kinds of backgrounds, as in general relativity [57]. The two most relevant cases being the asymptotically flat spacetimes [59] and the asymptotically anti–de Sitter spacetimes [70]. The energy formulae could also be generalized for nonorthogonally intersecting boundaries Σ_t and $\mathcal{B}$, as in [61].

The energy of pure curvature-squared gravity (4.89) is equivalent to the previous results in the literature. When the Einstein-Hilbert action is included, our expression for the total energy (4.91) includes the familiar contribution of general relativity. A physical interpretation is that the Einstein-Hilbert term is expected to dominate at great distances. In the case of Sec. IV C, the energy (4.90) contains the contribution of the scalar field ϕ thanks to its coupling to the scalar curvature of spacetime.

Recall that the total energy is always positive in general relativity [71,72], except for flat Minkowski spacetime, which has zero energy. Similarly, when the coupling constants of the curvature-squared terms satisfy $\alpha\beta \leq 0$, the total energy of curvature-squared gravity (4.89) has been shown to be zero for all exact solutions representing isolated systems [73] (see also [74]). This can be seen as the result of energy confinement. The inclusion of the Einstein-Hilbert term does not change this feature. In fact the Einstein-Hilbert contribution in (4.91) is the dominate one, since the curvature falls off quicker in the asymptotic region when the Einstein-Hilbert term is included. In the case of (4.90), the asymptotic boundary condition for the scalar field can be chosen so that the total energy resembles the case of (4.91): in an asymptotically flat spacetime, $\phi = C + O(r^{-b})$ where C is a constant and $b > 1$, so that the gradient term of ϕ is suppressed and $C^2/3$ takes the role of the gravitational constant κ^{-1}.

G. Alternative Hamiltonian formulations

We emphasize that the first-order ADM forms of the actions and the discussion of the boundary surface terms presented in Sec. III, as well as the following Hamiltonian analysis presented in Sec. IV, are specific to the chosen independent variables of the action (3.45). For any higher-derivative theory, there exists many possible choices for the independent variables. Since the higher-order derivatives imply the existence of extra degrees of freedom, one introduces extra independent variables which carry the extra degrees of freedom of the theory. The choice of independent variables defines the form of the first-order action, which in turn defines the Hamiltonian structure of the theory. The different Hamiltonian formulations of a given higher-derivative theory should be related by canonical transformations [42]. Hence they should be physically equivalent (at least classically). For an example of an alternative Hamiltonian formulation of higher-derivative gravity, see [45].

Furthermore, the choice of boundary conditions is not unique. For instance, if the curvature tensor of spacetime would be considered as an independent variable, it would be natural to impose boundary conditions on the curvature tensor. Since such variables and their boundary conditions involve second-order derivatives, the formulation would clearly differ from the present formulation, where the extrinsic curvature (3.31) is chosen to be an independent variable of the first-order action.

V. CONCLUSIONS

We have presented a Hamiltonian analysis of Weyl gravity and of other fully diffeomorphism-invariant curvature-squared gravitational models. We concentrated on the potentially renormalizable theories, whose linearized actions are known to include notorious ghost fields with negative energy. All the surface terms on the boundary of spacetime were accounted for in each theory, as well as the freedom to include surface terms that vanish due to the expanded configuration space of higher-derivative gravity, which includes both the fundamental forms of the hypersurfaces. The expression for the total energy was obtain in each case with respect to a generic stationary background.

Compared to the seminal work in [41], a correction to the component of Weyl tensor that is fully tangent to the spatial hypersurface was discovered in (3.40). A fully traceless component appears, namely the properly symmetrized, traceless, quadratic extrinsic curvature tensor $\mathcal{K}_{ijkl}$ defined in (3.41). The square of $\mathcal{K}_{ijkl}$ vanishes due to the Cayley-Hamilton theorem. Hence the correction makes a difference in theories where the Weyl tensor is coupled to something else than itself. But it does not appear in the action of curvature-square gravity (2.1). Therefore the Hamiltonian structures presented in Secs. IV A, IV D, and IV E are similar to those found in the literature (see [41–45]). The only relevant difference is the presence of the surface Hamiltonian of general relativity–the first term in (4.66)—when the Einstein-Hilbert action is included ($\kappa^{-1} \neq 0$). In that case, the expression for total energy (4.91) is complemented by the energy term of general relativity—the first term in (4.91)—which is the dominant contribution in asymptotically flat spacetimes.

We found in Sec. IV B that including a nonvanishing cosmological constant into Weyl gravity implies a severe problem. Since the determinant of the metric of spacetime is forced to zero by a secondary constraint (4.43), the Hamiltonian structure becomes physically inconsistent. Thus Weyl gravity with $\Lambda \neq 0$ is not a well-defined theory.

In Sec. IV C, we analyzed the possibility to include a scalar field which is coupled to the scalar curvature of spacetime in way that preserves conformal invariance [46,47]. Conformal invariance is broken spontaneously if the scalar field has a nonzero vacuum expectation value, producing an effective Einstein-Hilbert term and possibly a cosmological constant. The kinetic term of the scalar field is nonpositive, what may jeopardize the stability of the system.

In all the cases that include the Weyl action, i.e., when $\alpha \neq 0$ in the action (2.1), the Ostrogradskian form of the Hamiltonian is clearly visible in the first term $2p^{ij}K_{ij}$ of the Hamiltonian constraint, which is linear in the momentum p^{ij}. This implies the appearance of the Ostrogradskian instability. In the absence of conformal invariance, there exist five or six unstable degrees of freedom depending on whether $\beta = 0$ or $\beta \neq 0$, respectively, which are associated with the five or six independent time derivatives of the components of the extrinsic curvature on the spatial hypersurface. Since there exists only four first-class constraints—associated with the diffeomorphism invariance—the constraints cannot restrain the higher-derivative degrees of freedom. Only in the case of conformally invariant Weyl gravity, there exist as many constraints as there are unstable directions in phase space. This follows from the fact that the Weyl action contains the five independent traceless components of the time derivative of the extrinsic curvature, and it possesses five first-class constraints which are associated with the diffeomorphism and conformal invariance. Hence in principle, only the conformally invariant Weyl gravity has enough local constraints to be able to restrain the unstable degrees of freedom. In all the other potentially renormalizable cases, the number of independent second-order derivatives in the Lagrangian exceeds the number of local invariances. Thus Weyl gravity is the only potentially renormalizable theory of the type (2.1) that might avoid the problem with instability, which manifests itself as ghosts and lacks unitarity in the linearized theory.[8]

However, perturbative analyses suggest that even Weyl gravity cannot escape the ghost problem. On the flat background, linearized Weyl gravity includes a massless spin-2 ghost [51]. The inclusion of Einstein-Hilbert action implies the appearance of a massive spin-2 ghost, as well as a massive scalar ghost if $\beta \neq 0$ in (2.1). The dilemma of generally covariant higher-derivative gravity is that the spin-2 ghost is required for renormalizability [48]. In the full nonlinear theory, further study of the problem is still required.

The recent claim of obtaining a critical case of curvature-squared gravity [10], where the spin-2 ghost becomes massless, was concluded in our Sec. IV D to be a specific feature of the linearized theory on the anti–de Sitter background. In the full nonlinear theory, however, it was shown in Sec. IV D that the number and nature of local physical degrees of freedom are independent of the value of the cosmological constant, when both the Einstein-Hilbert and Weyl actions are included.

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APPENDIX A: NOTATION

The metric tensor $g_{\mu\nu}$ of spacetime has the signature $(-,+,+,+)$.

Symmetrization and antisymmetrization of tensor indices is denoted by parentheses and brackets, respectively. Normalization is chosen so that the (anti)symmetrization has no effect on an already (anti)symmetric tensor. For example, we denote

$$A_{(\mu\nu)} = \frac{1}{2}(A_{\mu\nu} + A_{\nu\mu}),$$
$$A_{[\mu|\rho}B_{|\nu]}{}^{\rho} = \frac{1}{2}(A_{\mu\rho}B_{\nu}{}^{\rho} - A_{\nu\rho}B_{\mu}{}^{\rho}). \quad \text{(A1)}$$

We may also use the following notation,

$$A_{\mu\nu} + (\mu\leftrightarrow\nu) = A_{\mu\nu} + A_{\nu\mu},$$
$$A_{\mu\nu} - (\mu\leftrightarrow\nu) = A_{\mu\nu} - A_{\nu\mu}, \quad \text{(A2)}$$

if it is more convenient than the one with parentheses and brackets. This can be the case when $A_{\mu\nu}$ in (A2) is a long expression containing several terms. No normalization is included in this notation. This notation may also be used to denote (anti)symmetrization with respect to the exchange of functions.

APPENDIX B: THE CAYLEY-HAMILTON THEOREM

The Cayley-Hamilton theorem states that any square matrix A over a commutative ring is the root of its own characteristic polynomial, $P(A) = 0$. The characteristic

[8]Recently [2], it has been argued that conformal gravity is unitary, but its Hamiltonian is non-Hermitian. However, in order to achieve this, the gravitational field $g_{\mu\nu}$ would have to be anti-Hermitian; i.e., the metric would be purely imaginary.

polynomial is defined as $P(\lambda) = \det(\lambda I - A)$, where I is the unit matrix.

The Cayley-Hamilton theorem has a tensor form due to the well known relationship between matrices and linear transformations and rank 2 tensors on a vector space. Considering a tensor $A^\mu{}_\nu$ on a d-dimensional vector space, such as the tangent space of a d-dimensional smooth manifold, the Cayley-Hamilton theorem can be written as

$$\begin{aligned} P(A)^\mu{}_\nu &= -(d+1)\delta^\mu{}_{[\nu}A^{\rho_1}{}_{\rho_1}A^{\rho_2}{}_{\rho_2}\cdots A^{\rho_d}{}_{\rho_d]} \\ &= (A^d)^\mu{}_\nu + c_1(A^{d-1})^\mu{}_\nu + \ldots + c_{d-1}A^\mu{}_\nu \\ &\quad + c_d\delta^\mu{}_\nu = 0, \end{aligned} \tag{B1}$$

where the coefficients c_n are given as

$$c_n = (-1)^n A^{\mu_1}{}_{[\mu_1}A^{\mu_2}{}_{\mu_2}\cdots A^{\mu_n}{}_{\mu_n]}, \qquad n = 1,2,\ldots,d, \tag{B2}$$

and we denote the tensor $A^\mu{}_\nu$ to the mth power as

$$(A^m)^\mu{}_\nu = A^\mu{}_{\rho_1}A^{\rho_1}{}_{\rho_2}\cdots A^{\rho_{m-2}}{}_{\rho_{m-1}}A^{\rho_{m-1}}{}_\nu, \qquad m = 2,3,\ldots,d. \tag{B3}$$

We shall apply the Cayley-Hamilton theorem to a tensor field on the three-dimensional Riemannian manifold Σ_t. A tensor $A^i{}_j$ on a three-dimensional vector space satisfies

$$\begin{aligned} P(A)^i{}_j &= A^i{}_kA^k{}_lA^l{}_j - A^i{}_kA^k{}_jA - \frac{1}{2}A^i{}_j(A^k{}_lA^l{}_k - A^2) \\ &\quad - \frac{\delta^i{}_j}{6}(2A^k{}_lA^l{}_mA^m{}_k - 3A^k{}_lA^l{}_kA + A^3) = 0, \end{aligned} \tag{B4}$$

where $A = A^i{}_i$ denotes the trace.

APPENDIX C: REMOVING THE AUXILIARY VARIABLES

We show that the Hamiltonian formalism where the Lagrange multiplier λ^{ij} and its conjugated momentum p^λ_{ij} are included as canonical variables is equivalent to the formalism presented in Sec. IV. If the canonical variables λ^{ij} and p^λ_{ij} are included, we obtain the extra primary constraints

$$\Pi^{ij} = p^{ij} - \sqrt{h}\lambda^{ij} \approx 0, \qquad p^\lambda_{ij} \approx 0. \tag{C1}$$

Each of these constraints has a nonvanishing Poisson bracket with one other constraint,

$$\{\Pi^{ij}(x), p^\lambda_{kl}(y)\} = -\delta^{(i}_k\delta^{j)}_l\sqrt{h}\delta(x-y). \tag{C2}$$

Thus Π^{ij} and p^λ_{ij} are second-class constraints. Second-class constraints become strong equalities when we replace the canonical Poisson bracket with the Dirac bracket (4.71). The matrix (4.72) for the second-class constraints $\phi_a = (\Pi^{ij}, p^\lambda_{ij})$ is given by the Poisson brackets (C2) in the cross-diagonal form $M(x,y) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\sqrt{h}\delta(x-y)$, where 0 and 1 denote the nine-dimensional zero and unit matrices, respectively. The inverse matrix has the form $M^{-1}(x,y) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\frac{1}{\sqrt{h}}\delta(x-y)$, and the Dirac bracket is defined as

$$\begin{aligned} &\{f_1(x), f_2(y)\}_{\mathrm{D}} \\ &= \{f_1(x), f_2(y)\} - \int_{\Sigma_t} d^3z\frac{1}{\sqrt{h}}\{f_1(x), \Pi^{ij}(z)\}\{p^\lambda_{ij}(z), f_2(y)\} \\ &\quad + \int_{\Sigma_t} d^3z\frac{1}{\sqrt{h}}\{f_1(x), p^\lambda_{ij}(z)\}\{\Pi^{ij}(z), f_2(y)\}. \end{aligned} \tag{C3}$$

Then we set the constraints (C1) to zero strongly and eliminate the variables λ^{ij} and p^λ_{ij} by substituting

$$\lambda^{ij} = \frac{p^{ij}}{\sqrt{h}}, \qquad p^\lambda_{ij} = 0. \tag{C4}$$

The Dirac bracket (C3) modifies the Poisson bracket if one of the arguments depends on λ^{ij} and the other argument depends on h_{ij}, p^{ij} or p^λ_{ij}. Otherwise the Dirac bracket is equivalent to the Poisson bracket. Since we have solved the constraints everywhere as (C4), none of the arguments can depend on λ^{ij} or p^λ_{ij}. Thus the Dirac bracket (C3) is equivalent to the Poisson bracket

$$\{f_1(x), f_2(y)\}_{\mathrm{D}} = \{f_1(x), f_2(y)\}, \tag{C5}$$

for any arguments f_1 and f_2 that depend on the remaining variables N, N^i, h_{ij}, K_{ij} and their canonically conjugated momenta p_N, p_i, p^{ij}, $\mathcal{P}^{ij}$. Therefore, introducing the Dirac bracket and imposing the second-class constraints strongly is equivalent to substituting (C4) and removing the auxiliary variables λ^{ij} and p^λ_{ij} from the system.

We can now see that it is unnecessary to include the Lagrange multiplier λ^{ij} and its conjugated momentum as extra canonical variables. We can directly identify $\sqrt{h}\lambda^{ij}$ as the canonical momentum p^{ij} conjugate to h_{ij} and hence avoid the inclusion of extra canonical variables. This is a general feature of the Hamiltonian formulation of higher-derivative theories (see e.g. [42]).

APPENDIX D: CALCULATION OF POISSON BRACKETS FOR THE HAMILTONIAN CONSTRAINT $\mathcal{H}_0$

Because of the simple p^{ij} dependence of the Hamiltonian constraint $\mathcal{H}_0$, namely the term $2p^{ij}K_{ij}$, we have the following Poisson brackets between the metric and $\mathcal{H}_0[\xi]$:

$$\{h_{ij}(x),\mathcal{H}_0[\xi]\}=2\xi(x)K_{ij}(x),$$
$$\{h^{ij}(x),\mathcal{H}_0[\xi]\}=-2\xi(x)K^{ij}(x),$$
$$\{\sqrt{h}(x),\mathcal{H}_0[\xi]\}=\xi(x)\sqrt{h}K(x),$$
$$\left\{\frac{1}{\sqrt{h(x)}},\mathcal{H}_0[\xi]\right\}=-\xi(x)\frac{K}{\sqrt{h}}(x). \tag{D1}$$

The rest of the Poisson brackets differ depending on which of the couplings are switched on. In particular, including the R^2 term into the Lagrangian (2.1), i.e., $\beta\neq 0$, alters the kinetic part of the Hamiltonian significantly.

1. Weyl gravity: $\alpha\neq 0$, $\beta=\gamma=0$ in (2.1)

First we consider the cases where the curvature-squared part of the action (2.1) is the Weyl action ($\alpha\neq 0$, $\beta=\gamma=0$). The Einstein-Hilbert action and the cosmological constant can be included or excluded, since they do not alter the kinetic part of the Hamiltonian constraint. The Hamiltonian constraint is given in (4.65). When the cosmological constant and/or the Einstein-Hilbert action are not present in the action, one simply sets $\Lambda=0$ and/or $\kappa^{-1}=0$ in the following results.

a. Poisson brackets between the canonical variables and the Hamiltonian constraint

The Poisson bracket between K_{ij} and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ reads as

$$\{K_{ij}(x),\mathcal{H}_0[\xi]\}=\xi(x)\left(-\frac{\mathcal{P}_{ij}}{\alpha\sqrt{h}}+{}^{(3)}R_{ij}+K_{ij}K\right)(x)+D_{ij}\xi(x). \tag{D2}$$

We shall denote the symmetrized second-order covariant derivative as $D_{ij}=D_{(i}D_{j)}$ and later the symmetrized higher-order covariant derivatives similarly as $D_{ijk}=D_{(i}D_jD_{k)}$, etc.

The Poisson bracket between the momentum $\mathcal{P}^{ij}$ and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ is obtained as

$$\{\mathcal{H}_0[\xi],\mathcal{P}^{ij}(x)\}=\xi(x)\left[2p^{ij}+\mathcal{P}^{ij}K+h^{ij}\mathcal{P}^{kl}K_{kl}-\frac{\sqrt{h}}{\kappa}(K^{ij}-h^{ij}K)\right]+4\alpha\sqrt{h}D_k(\xi C^{k(ij)}{}_{\boldsymbol{n}})(x). \tag{D3}$$

The Poisson bracket between the momentum p^{ij} and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ is very complicated. It can be obtained after a quite laborious calculation as

$$\{\mathcal{H}_0[\xi],p^{ij}(x)\}=E^{ij}_{(0)}\xi(x)+E^{ijk}_{(1)}D_k\xi(x)+E^{ijkl}_{(2)}D_{kl}\xi(x), \tag{D4}$$

where we have defined the three coefficient tensor densities $E^{i_1\cdots i_{2+I}}_{(I)}$ $(I=0,1,2)$ as

$$\begin{aligned}E^{ij}_{(0)}={}&-\frac{1}{\alpha\sqrt{h}}\left(\mathcal{P}^i_k\mathcal{P}^{jk}-\frac{1}{4}h^{ij}\mathcal{P}_{kl}\mathcal{P}^{kl}\right)+D_kD^{(i}\mathcal{P}^{j)k}-\frac{1}{2}h^{ij}D_{kl}\mathcal{P}^{kl}-\frac{1}{2}D^kD_k\mathcal{P}^{ij}-\mathcal{P}^{kl}K_{kl}K^{ij}-\frac{1}{2}\sqrt{h}h^{ij}\Lambda\\&+\frac{\sqrt{h}}{2\kappa}\left[{}^{(3)}R^{ij}+2K^i{}_kK^{jk}-2K^{ij}K-\frac{1}{2}h^{ij}({}^{(3)}R+K_{ij}K^{ij}-K^2)\right]\\&+\alpha\sqrt{h}\Big[2C^i{}_{kl\boldsymbol{n}}C^{jkl}{}_{\boldsymbol{n}}+C_{kl}{}^i{}_{\boldsymbol{n}}C^{klj}{}_{\boldsymbol{n}}-\frac{1}{2}h^{ij}C_{klm\boldsymbol{n}}C^{klm}{}_{\boldsymbol{n}}-2D_kK_l{}^{(i}C^{j)lk}{}_{\boldsymbol{n}}-2D_kK_l{}^{(i|}C^{kl|j)}{}_{\boldsymbol{n}}-2K_l{}^{(i}D_kC^{j)lk}{}_{\boldsymbol{n}}\\&-2K_l{}^{(i|}D_kC^{kl|j)}{}_{\boldsymbol{n}}-2K_{kl}D^kC^{l(ij)}{}_{\boldsymbol{n}}-2(2D_lK^l{}_k-D_kK)C^{k(ij)}{}_{\boldsymbol{n}}\Big],\end{aligned} \tag{D5}$$

$$E^{ijk}_{(1)}=D^{(i}\mathcal{P}^{j)k}+2h^{k(i}D_l\mathcal{P}^{j)l}-h^{ij}D_l\mathcal{P}^{kl}-\frac{3}{2}D^k\mathcal{P}^{ij}-2\alpha\sqrt{h}(K_l{}^{(i}C^{j)lk}{}_{\boldsymbol{n}}+K_l{}^{(i|}C^{kl|j)}{}_{\boldsymbol{n}}+K^k{}_lC^{l(ij)}{}_{\boldsymbol{n}}) \tag{D6}$$

and

$$E^{ijkl}_{(2)}=h^{i(k}\mathcal{P}^{l)j}+h^{j(k}\mathcal{P}^{l)i}-\frac{1}{2}h^{ij}\mathcal{P}^{kl}-h^{kl}\mathcal{P}^{ij}+\frac{\sqrt{h}}{2\kappa}(h^{ij}h^{kl}-h^{i(k}h^{l)j}). \tag{D7}$$

In Weyl gravity, the Poisson bracket between $\mathcal{Q}$ and $\mathcal{H}_0[\xi]$ requires the trace of the Poisson bracket between p^{ij} and $\mathcal{H}_0[\xi]$. It can be obtained from (D4) as

$$\begin{aligned}\{\mathcal{H}_0[\xi], p^{ij}(x)\}h_{ij}(x) = &-\xi(x)\left[\frac{\mathcal{P}_{ij}\mathcal{P}^{ij}}{4\alpha\sqrt{h}} + \frac{1}{2}D_iD_j\mathcal{P}^{ij} + \frac{1}{2}D^iD_i\mathcal{P} + \mathcal{P}^{ij}K_{ij}K + \frac{3}{2}\sqrt{h}\Lambda + \frac{\sqrt{h}}{4\kappa}({}^{(3)}R - K_{ij}K^{ij} + K^2)\right.\\ &\left. + \alpha\sqrt{h}\left(2D_iC^{ijk}{}_{\boldsymbol{n}}K_{jk} - \frac{1}{2}C_{ijk\boldsymbol{n}}C^{ijk}{}_{\boldsymbol{n}}\right)\right](x) - D_i\xi(x)\left(\frac{3}{2}D^i\mathcal{P} + 2\alpha\sqrt{h}C^{ijk}{}_{\boldsymbol{n}}K_{jk}\right)(x)\\ &+ D_{ij}\xi(x)\left(\frac{1}{2}\mathcal{P}^{ij} - h^{ij}\mathcal{P} + \frac{\sqrt{h}h^{ij}}{\kappa}\right)(x).\end{aligned} \tag{D8}$$

The Poisson bracket between $\mathcal{Q}$ and $\mathcal{H}_0[\xi]$ will be obtained in the next subsection, D 1 b.

b. Poisson brackets between the Hamiltonian constraints and with the other constraints

Poisson brackets between the Hamiltonian constraint and the other constraints are then determined by using the previous results for the canonical variables . The Poisson bracket between the constraints $\mathcal{P}$ and $\mathcal{H}_0[\xi]$ is a sum of the constraints $\mathcal{P}$ and $\mathcal{Q}$,

$$\{\mathcal{P}(x), \mathcal{H}_0[\xi]\} = \mathcal{P}^{ij}(x)\{h_{ij}(x), \quad \mathcal{H}_0[\xi]\} - h_{ij}(x)\{\mathcal{H}_0[\xi], \mathcal{P}^{ij}(x)\} = -\xi(x)(\mathcal{Q} + \mathcal{P}K)(x), \tag{D9}$$

where $\mathcal{Q}$ is defined by (4.67). The Poisson bracket between the constraints $\mathcal{Q}$ and $\mathcal{H}_0[\xi]$ is a sum of constraints only in the case of pure Weyl gravity. If the cosmological constant and/or Einstein-Hilbert term are included into the action, the Poisson bracket between $\mathcal{Q}$ and $\mathcal{H}_0[\xi]$ is not a sum of constraints. We then obtain the Poisson bracket as

$$\begin{aligned}\{\mathcal{Q}(x), \mathcal{H}_0[\xi]\} = &\, 2p^{ij}(x)\{h_{ij}(x), \mathcal{H}_0[\xi]\} - 2\{\mathcal{H}_0[\xi], p^{ij}(x)\}h_{ij}(x) + \mathcal{P}^{ij}(x)\{K_{ij}(x), \mathcal{H}_0[\xi]\} - \{\mathcal{H}_0[\xi], \mathcal{P}^{ij}(x)\}K_{ij}(x)\\ &+ \frac{2}{\kappa}(\{\sqrt{h}(x), \mathcal{H}_0[\xi]\}K(x) + \sqrt{h}K_{ij}(x)\{h^{ij}(x), \mathcal{H}_0[\xi]\} + \sqrt{h}h^{ij}(x)\{K_{ij}(x), \mathcal{H}_0[\xi]\})\\ = &\, \xi\mathcal{H}_0 + \xi D^iD_i\mathcal{P} + 3D_i\xi D^i\mathcal{P} + 2D^iD_i\xi\mathcal{P} - \xi\frac{2}{\kappa\alpha}\mathcal{P} + \xi\sqrt{h}\left[4\Lambda + \frac{3}{\kappa}({}^{(3)}R - K_{ij}K^{ij} + K^2)\right],\end{aligned} \tag{D10}$$

where we have omitted the arguments (x) for brevity. The first five terms are the known constraints, but rest of the terms are not constraints. As shown, for pure Weyl gravity with $\Lambda = 0$ and $\kappa^{-1} = 0$ the result (4.30) consists of the first four terms which are all constraints. The extra terms that are not constraints are a result of the fact that adding the cosmological constant or the Einstein-Hilbert action into Weyl gravity, breaks the conformal symmetry.

Finally, we determine the Poisson bracket of the Hamiltonian constraint with itself,

$$\begin{aligned}\{\mathcal{H}_0[\xi], \mathcal{H}_0[\eta]\} &= \int_{\Sigma_t} d^3x[\{\mathcal{H}_0[\xi], p^{ij}(x)\}\{h_{ij}(x), \mathcal{H}_0[\eta]\} + \{\mathcal{H}_0[\xi], \mathcal{P}^{ij}(x)\}\{K_{ij}(x), \mathcal{H}_0[\eta]\} - (\xi\leftrightarrow\eta)]\\ &= \int_{\Sigma_t} d^3x[F^i_{(1)}D_i\xi\eta + F^{ij}_{(2)}D_{ij}\xi\eta + 4\alpha\sqrt{h}D_i(\xi C^{i(jk)}{}_{\boldsymbol{n}})D_{jk}\eta - (\xi\leftrightarrow\eta)],\end{aligned} \tag{D11}$$

where we denote

$$F^i_{(1)} = 2D^j\mathcal{P}^{ik}K_{jk} + 4D_j\mathcal{P}^{jk}K^i{}_k - 2D_j\mathcal{P}^{ij}K - 3D^i\mathcal{P}^{jk}K_{jk} - 4C^i{}_{jk\boldsymbol{n}}\mathcal{P}^{jk} + 4\alpha\sqrt{h}C^{ijk}{}_{\boldsymbol{n}}{}^{(3)}R_{jk} \tag{D12}$$

and

$$F^{ij}_{(2)} = -2p^{ij} + 4\mathcal{P}^{(i|k}K^{|j)}{}_k - 2\mathcal{P}^{ij}K - 3h^{ij}\mathcal{P}^{kl}K_{kl}. \tag{D13}$$

It is noteworthy that this Poisson bracket is insensitive to the presence of Einstein-Hilbert or cosmological constant parts of the action. This means that the result for the Poisson bracket between Hamiltonian constraints does not contain the Hamiltonian constraint itself, but rather consists of other constraints. In obtaining (D12), we used the fact that the terms involving a product of three K_{ij} turn out to be equal to the covariant divergence of the characteristic polynomial (B4) of K_{ij}:

$$C^{ijk}{}_{\boldsymbol{n}}K_{jl}K^{l}{}_{k}+K^{i}{}_{j}C^{jkl}{}_{\boldsymbol{n}}K_{kl}-C^{ijk}{}_{\boldsymbol{n}}K_{jk}K=-D_{j}P(K)^{ij}=0. \quad \text{(D14)}$$

Integrating by parts enables us to write the Poisson bracket between Hamiltonian constraints as

$$\{\mathcal{H}_0[\xi],\mathcal{H}_0[\eta]\}=\int_{\Sigma_t}d^3x(\xi D_i\eta-D_i\xi\eta)G^i, \quad \text{(D15)}$$

where we denote

$$G^i=-F^i_{(1)}+D_jF^{ij}_{(2)}+4\alpha\sqrt{h}C^{ijk}{}_{\boldsymbol{n}}{}^{(3)}R_{jk}=h^{ij}[\mathcal{H}_j+2\mathcal{P}(D^kK_{jk}-D_jK)]. \quad \text{(D16)}$$

The second- and third-order derivatives of the test functions cancel. This is because $F^{ij}_{(2)}$ is symmetric and $C_{ijk\boldsymbol{n}}$ inherits the cyclic property of the Weyl tensor:

$$C_{ijk\boldsymbol{n}}+C_{kij\boldsymbol{n}}+C_{jki\boldsymbol{n}}=0 \quad \Rightarrow \quad C_{(ijk)\boldsymbol{n}}=0. \quad \text{(D17)}$$

The Ricci identity was used in obtaining the coefficient of the first-order derivatives of the test functions in (D15), and the Riemann tensor was written in terms of the Ricci tensor since the three-dimensional Weyl tensor is zero, (3.24).

Finally, we may write the Poisson bracket between Hamiltonian constraints as a sum of the momentum and $\mathcal{P}$ constraints,

$$\{\mathcal{H}_0[\xi],\mathcal{H}_0[\eta]\}=\Phi[\xi\vec{D}\eta-\eta\vec{D}\xi]+2\mathcal{P}[(\xi D_i\eta-\eta D_i\xi)h^{ij}(D^kK_{jk}-D_jK)], \quad \text{(D18)}$$

where the gradient vector $\vec{D}\xi$ is defined as $(\vec{D}\xi)^i=h^{ij}D_j\xi$.

Substituting the test functions $\xi=\delta(x-y)$ and $\eta=N$ gives the Poisson bracket between $\mathcal{H}_0(x)$ and $\mathcal{H}_0[N]$ as a sum of the constraints $\mathcal{H}_i$ and $\mathcal{P}$,

$$\{\mathcal{H}_0(x),\mathcal{H}_0[N]\}=(2D^iN+ND^i)\times[\mathcal{H}_i+2\mathcal{P}(D^jK_{ij}-D_iK)](x). \quad \text{(D19)}$$

2. Curvature-squared gravity: $\alpha\neq 0,\ \beta\neq 0,\ \gamma=0$

We consider the case when both the Weyl tensor squared and scalar curvature squared terms are included in the Lagrangian (2.1). The Einstein-Hilbert action and the cosmological constant may be included or excluded, since they do not alter the kinetic part of the Hamiltonian constraint. The Hamiltonian constraint is given in (4.81). When the cosmological constant and/or the Einstein-Hilbert action are not present in the action, one simply sets $\Lambda=0$ and/or $\kappa^{-1}=0$ in the following results.

a. Poisson brackets between the canonical variables and the Hamiltonian constraint

The Poisson bracket between K_{ij} and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ reads as

$$\{K_{ij}(x),\mathcal{H}_0[\xi]\}=\xi(x)\left[-\frac{\mathcal{G}_{ijkl}\mathcal{P}^{kl}}{\alpha\sqrt{h}}+{}^{(3)}R_{ij}+K_{ij}K-\frac{1}{2}h_{ij}({}^{(3)}R-K_{ij}K^{ij}+K^2)\right](x)+D_{ij}\xi(x). \quad \text{(D20)}$$

The Poisson bracket between the momentum $\mathcal{P}^{ij}$ and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ is obtained as

$$\{\mathcal{H}_0[\xi],\mathcal{P}^{ij}(x)\}=\xi(x)\left[2p^{ij}+\mathcal{P}^{ij}K+h^{ij}\mathcal{P}^{kl}K_{kl}+\mathcal{P}(K^{ij}-h^{ij}K)-\frac{\sqrt{h}}{\kappa}(K^{ij}-h^{ij}K)\right](x)+4\alpha\sqrt{h}D_k(\xi C^{k(ij)}{}_{\boldsymbol{n}})(x). \quad \text{(D21)}$$

The Poisson bracket between the momentum p^{ij} and the Hamiltonian constraint $\mathcal{H}_0[\xi]$ is obtained via a similar calculation as in the case with $\beta=0$. We obtain it as

$$\{\mathcal{H}_0[\xi],p^{ij}(x)\}=E^{ij}_{(0)}\xi(x)+E^{ijk}_{(1)}D_k\xi(x)+E^{ijkl}_{(2)}D_{kl}\xi(x), \quad \text{(D22)}$$

where we have defined the three coefficient tensor densities $E^{i_1\cdots i_{2+I}}_{(I)}$ $(I=0,\,1,\,2)$ as

$$E^{ij}_{(0)} = -\frac{1}{\alpha\sqrt{h}}\left(\mathcal{P}^i{}_k\mathcal{P}^{jk} - \frac{\alpha+3\beta}{9\beta}\mathcal{P}^{ij}\mathcal{P} - \frac{1}{4}h^{ij}\mathcal{P}^{kl}\mathcal{G}_{klmn}\mathcal{P}^{mn}\right) + D_kD^{(i}\mathcal{P}^{j)k} - \frac{1}{2}h^{ij}D_kD_l\mathcal{P}^{kl} - \frac{1}{2}D^kD_k\mathcal{P}^{ij} - \frac{1}{2}D^{ij}\mathcal{P}$$
$$+\frac{1}{2}h^{ij}D^kD_k\mathcal{P} - \mathcal{P}^{kl}K_{kl}K^{ij} - \frac{1}{2}\mathcal{P}^{ij}({}^{(3)}R - K_{kl}K^{kl} + K^2) + \frac{1}{2}\mathcal{P}^{(3)}R^{ij} - \mathcal{P}K^i{}_kK^{jk} + \mathcal{P}K^{ij}K - \frac{1}{2}\sqrt{h}h^{ij}\Lambda$$
$$+\frac{\sqrt{h}}{2\kappa}\left[{}^{(3)}R^{ij} + 2K^i{}_kK^{jk} - 2K^{ij}K - \frac{1}{2}h^{ij}({}^{(3)}R + K_{ij}K^{ij} - K^2)\right]$$
$$+\alpha\sqrt{h}\Big[+2C^i{}_{kl\boldsymbol{n}}C^{jkl}{}_{\boldsymbol{n}} + C_{kl}{}^i{}_{\boldsymbol{n}}C^{klj}{}_{\boldsymbol{n}} - \frac{1}{2}h^{ij}C_{klm\boldsymbol{n}}C^{klm}{}_{\boldsymbol{n}} - 2D_kK_l{}^{(i}C^{j)lk}{}_{\boldsymbol{n}} - 2D_kK_l{}^{(i|}C^{kl|j)}{}_{\boldsymbol{n}} - 2K_l{}^{(i}D_kC^{j)lk}{}_{\boldsymbol{n}}$$
$$-2K_l{}^{(i|}D_k{}^{kl|j)}{}_{\boldsymbol{n}} - 2K_{kl}D^kC^{l(ij)}{}_{\boldsymbol{n}} - 2C^{k(ij)}{}_{\boldsymbol{n}}(2D_lK^l{}_k - D_kK)\Big], \tag{D23}$$

$$E^{ijk}_{(1)} = D^{(i}\mathcal{P}^{j)k} + 2h^{k(i}D_l\mathcal{P}^{j)l} - h^{ij}D_l\mathcal{P}^{kl} - \frac{3}{2}D^k\mathcal{P}^{ij} - D^{(i}\mathcal{P}h^{j)k} + h^{ij}D^k\mathcal{P} - 2\alpha\sqrt{h}(K_l{}^{(i}C^{j)lk}{}_{\boldsymbol{n}} + K_l{}^{(i|}C^{kl|j)}{}_{\boldsymbol{n}} + K^k{}_lC^{l(ij)}{}_{\boldsymbol{n}}) \tag{D24}$$

and

$$E^{ijkl}_{(2)} = h^{i(k}\mathcal{P}^{l)j} + h^{j(k}\mathcal{P}^{l)i} - \frac{1}{2}h^{ij}\mathcal{P}^{kl} - h^{kl}\mathcal{P}^{ij} + \frac{1}{2}\mathcal{P}(h^{ij}h^{kl} - h^{i(k}h^{l)j}) + \frac{\sqrt{h}}{2\kappa}(h^{ij}h^{kl} - h^{i(k}h^{l)j}). \tag{D25}$$

b. Poisson bracket between the Hamiltonian constraints

We determine the Poisson bracket between Hamiltonian constraints:

$$\{\mathcal{H}_0[\xi], \mathcal{H}_0[\eta]\} = \int_{\Sigma_t} d^3x[F^i_{(1)}D_i\xi\eta + F^{ij}_{(2)}D_{ij}\xi\eta + 4\alpha\sqrt{h}D_i(\xi C^{i(jk)}{}_{\boldsymbol{n}})D_{jk}\eta - (\xi\leftrightarrow\eta)], \tag{D26}$$

where we denote

$$F^i_{(1)} = 2D^j\mathcal{P}^{ik}K_{jk} + 4D_j\mathcal{P}^{jk}K^i{}_k - 2D_j\mathcal{P}^{ij}K - 3D^i\mathcal{P}^{jk}K_{jk} - 4C^i{}_{jk\boldsymbol{n}}\mathcal{P}^{jk} - 2D^j\mathcal{P}K^i{}_j + 2D^i\mathcal{P}K + 4\alpha\sqrt{h}C^{ijk}{}_{\boldsymbol{n}}{}^{(3)}R_{jk} \tag{D27}$$

and

$$F^{ij}_{(2)} = -2p^{ij} + 4\mathcal{P}^{(i|k}K^{|j)}{}_k - 2\mathcal{P}^{ij}K - 3h^{ij}\mathcal{P}^{kl}K_{kl} + 2\mathcal{P}(h^{ij}K - K^{ij}). \tag{D28}$$

We again integrate by parts to obtain (D15), but now with $G^i = h^{ij}\mathcal{H}_j$. Thus the result is given solely by the momentum constraint:

$$\{\mathcal{H}_0[\xi], \mathcal{H}_0[\eta]\} = \int_{\Sigma_t} d^3x(\xi D_i\eta - \eta D_i\xi)h^{ij}\mathcal{H}_j = \Phi[\xi\vec{D}\eta - \eta\vec{D}\xi]. \tag{D29}$$

This result has the same form as in the Hamiltonian structure of general relativity. Finally, we obtain

$$\{\mathcal{H}_0(x), \mathcal{H}_0[N]\} = 2D^iN\mathcal{H}_i + ND^i\mathcal{H}_i. \tag{D30}$$

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