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Scale-Invariant Quadratic Gravity and the Ghost Problem

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Abstract

In this thesis we investigate several phenomena in quantum gravity with a specific emphasis on scale-invariant models of quadratic gravity whose actions contain all three independent squares of the Riemann tensor. After discussing the different ways in which scale invariance can manifest and reviewing how spontaneous symmetry breaking may occur as a result of quantum effects, we marry these concepts by constructing a model of gravity and matter that dynamically generates the Planck and electroweak scales through the spontaneous breaking of scale symmetry, thus describing an origin for the very concept of mass. We also demonstrate that this same scale-invariant model describes a period of cosmic inflation that is consistent with modern observations. A simpler realization of this model with the same important features is then defined by including quantum effects that result from the traditionally neglected spin-2 ghost degrees of freedom that are inherently present in this type of theory. The second part of this work is devoted to studying the role of these spin-2 ghosts, which generically appear as negative norm states that threaten unitarity at the quantum level. We derive rigorous and novel covariant operator quantizations of both globally scale-invariant quadratic gravity in the phase of broken symmetry and of locally invariant conformal gravity in the unbroken phase. This leads us to establish the notion of "conditional unitary" wherein the broken phase theory is shown to be unitary up to very high energies, and grants a new perspective on the ghost problem in quantum gravity as a whole.

Zusammenfassung

In dieser Arbeit untersuchen wir verschiedene Phänomene der Quantengravitation mit besonderem Schwerpunkt auf skaleninvarianten Modellen der quadratischen Gravitation, deren Wirkungen alle drei unabhängigen Quadrate des Riemanntensors enthalten. Nach der Erörterung der verschiedenen Arten, wie sich Skaleninvarianz manifestieren kann, und der Überprüfung, wie spontane Symmetriebrechungen aufgrund von Quanteneffekten auftreten können, verbinden wir diese beiden Konzepte indem wir ein Modell der Gravitation und der Materie konstruieren, das dynamisch die Planck- und elektroschwache Skala durch die spontane Brechung der Skalensymmetrie erzeugt und somit auch den Ursprung für das grundlegende Konzept von Masse beschreibt. Wir zeigen auch, dass dieses skaleninvariante Modell eine Periode der kosmischen Inflation ermöglicht, die mit modernen Beobachtungen übereinstimmt. Eine einfachere Realisierung dieses Modells mit denselben wichtigen Eigenschaften wird dann durch die Einbeziehung von Quanteneffekten ermöglicht, die aus den üblicherweise vernachlässigten Freiheitsgraden eines Spin-2-Geistfeldes folgen, die in dieser Art von Theorien inhärent sind. Der zweite Teil dieser Arbeit ist der Untersuchung der Rolle dieser Spin-2-Geister gewidmet, die im Allgemeinen als negative Normzustände auftreten und somit die Unitarität der Quantentheorie bedrohen. Wir leiten rigoros neuartige kovariante Operatorquantisierungen sowohl der global skaleninvarianten quadratischen Gravitation in der Phase der gebrochenen Symmetrie als auch der lokal invarianten konformen Gravitation in der ungebrochenen Phase her. Dies führt uns dazu, den Begriff der "konditionalen Unitarität" einzuführen, worin sich die Theorie in der gebrochenen Phase bis zu sehr hohen Energien als unitär erweist, und gewährt somit eine neue gesamtheitliche Perspektive auf das Geistproblem in der Quantengravitation.

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Chapter 1

Introduction

Despite the overwhelming experimental success of the Standard Model (SM), it is well-known among theorists that the SM alone is far from providing a complete description of Nature. Several of the most important shortcomings of the SM stem from the very quantum field theoretical backbone that it is built on, namely, the hierarchy problem and the fact that the SM contains no description of the quantum nature of gravity. However, both of these issues (as well as many others) may be at least addressed, if not completely resolved, by the postulate that our universe is fundamentally scale-invariant.

The hierarchy problem refers to the incredible level of fine-tuning that is required to reconcile the large difference between the electroweak (EW) and Planck scales. There is actually no fine-tuning in the SM as it stands since the measured value of the Higgs mass, $m_H \approx 125$ GeV [5, 6], indicates that the SM is perturbative (specifically, it contains no Landau poles) up to the Planck scale [7–10]. However, issues may arise due to the fact that the Higgs, being the only fundamental scalar in the theory, receives radiative corrections to its mass $\delta m_H^2 \propto \Lambda_{\rm BSM}^2$ from loop diagrams involving heavy particles at the scale of new physics beyond the Standard Model (BSM), $\Lambda_{\rm BSM}$ [11]. Since the SM is certainly not a complete theory of everything, we can anticipate that some scale of new physics exists beyond what we are currently able to probe with experiment. This means that the only way to justify the measured mass of the Higgs boson in the SM framework is with a very unnatural (in the sense of [12]) fine-tuning of couplings that enforces precise cancellation of the troublesome radiative corrections and reproduces the values measured at low energies. Popular proposed resolutions to the hierarchy problem include: invoking large extra dimensions whose existence implies that the measured 4D Planck mass is actually an effective "scaled-up" version of the true, more natural extra-dimensional Planck mass [13–15], and supersymmetric extensions of the SM that posit the existence of fermionic (bosonic) superpartners for each boson (fermion) whose contributions to the total radiative corrections received by the Higgs precisely cancel as a result of the symmetry [16, 17] (though it should be noted that the most minimal of these models can come with a "little hierarchy problem" of their own [18, 19]).

In this work we will take a different approach to the hierarchy problem and assume it may instead be resolved through scale symmetry. When scale symmetry is linearly realized in a theory i.e. it is not spontaneously broken, the theory necessarily contains dimensionless constants only and is devoid of all fundamental scales. This implies that scale-invariant theories which attempt to describe the world as we know it must generate all the scales in physics including the electroweak scale, Planck scale, etc., as dynamical quantities that appear as a result of spontaneous symmetry breaking (SSB). In a scenario where all scales are dynamically generated quantities, quadratic divergences become mere artifacts of the regularization procedure that may be canceled with appropriate counter terms, meaning that the Higgs mass runs only logarithmically and is inherently stable under radiative corrections, thus suggesting a resolution to the hierarchy problem [20].

Studies of the SM renormalization group equations already seem to hint at scale invariance (SI) if the Higgs potential tends towards flatness at energies approaching the Planck mass [7, 21], and though the SM is not scale-invariant as it stands, the only term in its action that actually violates this symmetry is the massive parameter in the Higgs potential. This means that one may construct models that are able to dynamically generate this single parameter with only minimal extra field content, and many authors have written promising extensions to the SM in this spirit [22–27]. It is also natural to consider more complicated BSM models that account for neutrino masses with a scale-invariant realization of the neutrino option [28, 29] and suggest potential dark matter candidates that acquire their mass through the spontaneous breaking of scale symmetry [29–31]. SI as a fundamental principle is also well-motivated by cosmology, as it has the potential to shed light on the nature of dark energy and the cosmological constant (CC) [32–35], and to describe a period of inflation in the early universe that meshes nicely with experimental signatures [36–41]. Indeed, the most precise measurements performed by the Planck and BICEP/Keck collaborations [42–44] suggest a value of $n_s \approx .96$ for the scalar spectral index of cosmic microwave background (CMB) fluctuations, which is just barely removed from the scale-invariant value of $n_s = 1$.

Given that scale-invariant models are in principle valid up to arbitrary energies, it is also important to consider how they may be embedded into a theory of gravity as we approach the Planck scale, since this is where one expects gravitational interactions to start becoming relevant for particle physics. Theories that attempt to unify particle physics and gravity under the umbrella of SI have appeared in the literature for more than 50 years [45–50] and continue to be an active area of research [51–55]. The popularity of these kind of models stems in no small part from the fact that scale-invariant extensions of gravity tend to be renormalizable, in contrast to General Relativity (GR) which, despite its unprecedented success as a classical description of gravity, is power-counting non-renormalizable and thus cannot represent a complete description of quantum gravity. When GR is treated as an effective field theory, one encounters quantum corrections that depend on the three independent squares of the Riemann tensor [56] and it is thus natural to consider actions that contain these kind of terms already at tree-level. These theories are generally referred to as quadratic gravity (QG) and their full renormalizability was indeed demonstrated by Stelle in the seminal works [57, 58]. The important connection then follows from the fact that, as a result of its power-counting renormalizability, QG is easily interpreted as the most general scale-invariant description of gravity after the generation of an Einstein-Hilbert term through SSB.

When gravity is added to the picture, it also becomes important to distinguish between the cases of global SI and local SI i.e. conformal invariance. Except for a few niche examples, global SI in theories of particle physics also implies a local symmetry under the full conformal group, though this is not the case for theories of gravity. Demanding conformal invariance requires one to restrict the general action of scale-invariant QG to an action composed of only the squared Weyl tensor. This theory of conformal gravity (CG) was originally considered by Weyl and Bach more than 100 years ago [59, 60] and has remained interesting to theorists to this day thanks to its renormalizability and clear, aesthetically appealing interpretation as a gauge theory of the conformal group [61] which is reminiscent of the SM's formulation as a Yang-Mills gauge theory [62]. Even aside from these promising features, the CG action has a knack for appearing in theories even when it is not introduced from the start, perhaps most interestingly with respect to asymptotic safety [63–67] and 't Hooft's work on naturalness and the black hole information paradox [56, 68–70]. It should however be noted that the validity of CG-based theories is debated due to the ubiquitous conformal (trace) anomaly that is known to appear in scale-invariant theories [71, 72]. The conformal anomaly's role in quantum gravity was originally identified through a violation of the the conformal Ward identity by Duff and Capper while calculating corrections to the graviton propagator [73–75] and though such anomalies generally imply that the associated gauge theory is inconsistent [76], promising methods of reconciling the conformal anomaly have been proposed throughout the years [77–82] and its presence has not dissuaded authors from considering unified theories of CG and matter [83–97].

Despite the potential for scale-invariant QG to represent a consistent theory of quantum gravity thanks to its renormalizability and ability to resolve the hierarchy problem, theoretical problems arise due to the fact that its action contains four derivatives (two per Riemann tensor) acting on the metric. It has been known since the mid 1800's that classical theories with this derivative structure generically exhibit what is known as the Ostrogradsky instability [98], a feature that, after application of standard quantization procedures, leads to a Hilbert space containing quantum states with negative norm. This in turn leads to what is colloquially known as the ghost problem - a breakdown of unitarity and the usual interpretation of probability in quantum theory. After decades of study it has become clear that the ghost problem stems from the mathematical foundations of quantum field theory (QFT) itself and may not be easily overcome, however, there is good reason to believe that it may be resolved through a modification of the usual quantum prescription. Serious works with this goal in mind have appeared as early as 50 years ago the with the models of Lee and Wick [99, 100] and the work of Boulware, Horowitz, and Strominger [101], while a few promising resolutions have also been proposed in recent years; notable examples include the demonstration of ghost instability by Donoghue and Menezes [55, 102–104], Anselmi's fakeon prescription [105–108], as well as Bender and Mannheim's $\mathcal{PT}$ symmetric QFT [97, 109–119] (see also the similar ideas of Salvio and Strumia in [120, 121]). There are also ideas worth taking seriously that are based on the notion that general (non-scale-invariant) QG may be viewed as a truncated effective field theory that is part of a complete ghost-free theory containing an infinite tower of higher derivative terms [122]. In any case, the general consensus among experts in the field appears to be that the ghost problem may be resolved through a better understanding of quantum physics, which if true, would render scale-invariant QG a renormalizable, unitary, and thus quite satisfactory description of the quantum nature of gravity.

We will begin our investigations into all the ideas discussed above in Chapter 2 by precisely defining the various realizations of scale symmetry in physics, reviewing how SSB may be brought on by quantum effects through the Coleman-Weinberg (CW) mechanism, and presenting the concrete scale-invariant model established in [1] which dynamically generates the Planck and electroweak scales through the spontaneous breaking of scale symmetry. This same model was also shown to generate a viable period of cosmic inflation and this will be the focus of Chapter 3, where we will also present the work conducted in [2] that demonstrates some positive effects with respect to SSB and inflation that appear when spin-2 ghosts are present in a theory. Chapter 4 is devoted entirely to an understanding of the ghost problem in quantum gravity. After establishing a firm understanding of where the problem actually lies, we will review some of its promising resolutions mentioned above, and will conclude with the work performed in [3] and [4] where novel covariant operator quantizations were conducted for both globally scale-invariant QG in the broken phase of symmetry and conformal gravity in the unbroken phase, respectively. We will see that, with the full quantum versions of each theory in hand, we are able to establish a notion of "conditional unitarity" where the ghost problem is shown to occur only at energies near the Planck scale and generally gain a new understanding of the ghost problem in QG that we hope will pave the way for a fully satisfactory resolution in the future. We will conclude with a discussion of all our results in Chapter 5. Some mathematical details relevant to quantization may also be found in Appendix A, while Appendix B contains a derivation of the Lehmann–Symanzik–Zimmerman (LSZ) reduction formula in CG.

Throughout this work we will employ natural units where $c = \hbar = 1$ and when referencing the Planck mass, we will always use the reduced value $M_{\mathrm{Pl}} = 1/\sqrt{8\pi G_{\mathrm{N}}} = 2.435 \times 10^{18}$ GeV where G_{N} is Newton's constant. We will also use standard bracket notation for the (anti)symmetrization of indices, $X_{(\alpha}Y_{\beta)} = 1/2(X_\alpha Y_\beta + X_\beta Y_\alpha)$ and $X_{[\alpha}Y_{\beta]} = 1/2(X_\alpha Y_\beta - X_\beta Y_\alpha)$, and unless otherwise stated, we follow the conventions of Weinberg [123, 124] which include the metric signature $(-,+,+,+)$, $\Box = \partial_\alpha \partial^\alpha$, and the Riemann tensor sign $R_{\alpha\beta\gamma}{}^{\delta} = -\partial_\alpha \Gamma^{\delta}{}_{\beta\gamma} + \cdots$. We also note that many of the calculations performed in this work were greatly facilitated by the xAct [125, 126], xTras [127], and FieldsX [128] packages for Wolfram Mathematica.

Chapter 2

Scale Invariance

2.1 Scale, conformal, and Weyl symmetry

Before we begin with the analysis of a specific theory, it is important to establish some terminology regarding the symmetries that form the backbone of the models we will consider. Broadly speaking, the terms "scale invariance", "conformal invariance", and "Weyl invariance" are often used interchangeably in the literature to refer to the symmetry of a theory under a rescaling of spacetime coordinates or fields at either the global or local level. Though this usually does not cause too much unnecessary confusion in practice, it is important to be precise when considering multiple versions of what may be broadly referred to as scale invariance, as we will in what follows.

To begin laying the groundwork, we may define a scale transformation at the coordinate level as

$$x^\alpha \;\to\; x'^\alpha = \lambda x^\alpha \,, \tag{2.1}$$

where λ is an arbitrary parameter of the transformation that is constant in the case of global symmetry and spacetime-dependent ($\lambda = \lambda(x)$) when the transformation is local. When one considers the latter of these options in combination with the usual group of local Poincaré spacetime symmetries, it turns out that in all but a few niche cases (ex. the theory of elasticity in two dimensions [129]), one also finds an invariance under the full conformal group. As we already touched on in the Introduction, conformal symmetry as a basis for constructing theories in physics is interesting for a number of reasons, most notably because it may in some sense be considered the "maximal" amount of spacetime symmetry that a realistic physical theory can possess, due to the fact that it is the largest group of spacetime symmetries under which both the lightcone $\mathrm{d}s^2 = 0$ and the Yang-Mills EOMs are invariant [130].

Conformal transformations are at their core a particular type of diffeomorphism and are thus best understood in terms of infinitesimal coordinate transformations $x^\alpha \to x^\alpha + \epsilon\,\xi^\alpha$ where ϵ is an arbitrary infinitesimal parameter and ξ^α is a solution of the conformal Killing equations

$$\partial_{(\alpha}\xi_{\beta)} - \eta_{\alpha\beta}\partial_\gamma \xi^\gamma = 0\,. \tag{2.2}$$

The conformal algebra is generated by the fifteen unique solutions to these equations; the first ten being $\xi^\alpha = \{a^\alpha, b^\alpha{}_\beta x^\beta\}$ which correspond to translations and Lorentz transformations, and generate the complete Poincaré algebra. The remaining five solutions of (2.2) are given by $\xi^\alpha = \{cx^\alpha, d_\beta(\eta^{\alpha\beta}x^2 - 2x^\alpha x^\beta)\}$ and correspond to dilatations (scale transformations) and "special conformal transformations". The latter of these may be understood as a kind of inversion and represent the difference between the full conformal group and the group containing just Poincaré and local scale symmetries. All together, we may thus write a general conformal transformation as

$$x^\alpha \;\; \rightarrow \;\; x'^\alpha = x^\alpha + \epsilon\Big(a^\alpha + b^\alpha{}_\beta x^\beta + cx^\alpha + d_\beta\big(\eta^{\alpha\beta}x^2 - 2x^\alpha x^\beta\big)\Big)\,. \tag{2.3}$$

Under this operation, x'^α will always point in the same direction as x^α though it may have an arbitrarily different length, in contrast to a Poincaré transformation which conserves both length and direction.

The last piece of scale-invariant terminology that needs to be established is the notion of Weyl symmetry. Similarly to the familiar internal gauge symmetries of the SM, Weyl symmetry acts not on the spacetime coordinates, but directly on the fields as

$$\Phi(x) \;\; \rightarrow \;\; \Phi'(x) = \Omega^n \Phi(x)\,. \tag{2.4}$$

Here, Φ represents a general field in the theory, Ω is a dimensionless parameter of the transformation that may be constant or coordinate dependent (corresponding to global and local Weyl transformations respectively), and n varies depending on the field in question: $n = -1$ for scalars, $n = -3/2$ for fermions, $n = 0$ for vector bosons, and in $d = 4$ dimensions, $n = 2$ and $n = 8$ for the metric and its determinant respectively.

Despite the fact that conformal and Weyl transformations are distinctly different concepts (one group is not a subgroup of the other, as is sometimes confused), there is a crucial connection between the two operations. To see their relationship explicitly, we recall that conformal transformations are diffeomorphisms which act on the metric as

$$g_{\alpha\beta}(x) \;\; \rightarrow \;\; g'_{\alpha\beta}(x') = \frac{\partial x^\alpha}{\partial x'^\alpha}\frac{\partial x^\beta}{\partial x'^\beta} g_{\alpha\beta}(x) = \Omega^2(x')g_{\alpha\beta}(x') \tag{2.5}$$

for some function of the transformed coordinates $\Omega(x')$. Put simply, conformal transformations are a type of diffeomorphism that may be undone by an appropriate Weyl transformation and hence, Weyl invariance implies conformal invariance. The same type of relationship holds in the local and global cases and in practice it is often easier to employ Weyl invariance when performing analyses in quantum field theory where the natural objects to work with are the fields themselves. One should keep all of the discussion above in mind, though for the remainder of this work, we will generally use Weyl transformations in our calculations and will use "scale symmetry" to refer to the global case and "conformal" or "Weyl symmetry" for the local case, to keep the terminology separate.

2.2 The Coleman-Weinberg mechanism

There is one more crucial piece of theoretical background that must be established before getting into concrete calculations, which is related to the obvious fact that we do not observe a scale-invariant universe. This means that the only way to reconcile the scale-invariant picture with observation is to assume that scale invariance is spontaneously broken. In this section we will give a brief general overview of the "Coleman-Weinberg mechanism" that will eventually lead us to the spontaneous breakdown of scale symmetry and the resulting generation of physical scales. We will mostly follows the treatments in [76, 131], though the same type of discussion may be found in many nice reviews and in most good textbooks on QFT; see for example [132–135].

2.2.1 The quantum effective potential

The mathematical construction containing all of the physics that will be of interest to us in what follows is the quantum effective action, or more specifically, the one-loop quantum effective potential that is obtained from it via an expansion under the background field method [136–138]. The quantum effective action that we are after is a functional that, at the risk of oversimplifying, replaces the classical action in such a way that tree-level computations performed with it are able to account for loop-order interactions in the quantum theory.

One of the most important objects for practical applications in QFT is the correlation function, so we begin our derivations by considering a general theory described by a classical action $S[\phi]$ of some field(s) ϕ and the functional

$$Z[J_\phi] = \langle 0;\mathrm{out}|0;\mathrm{in}\rangle_J = \int \mathcal{D}\phi \exp\big(i(S[\phi] + \phi \cdot J_\phi)\big)\,, \tag{2.6}$$

which generates n-point correlation functions (vacuum-vacuum amplitudes) via successive functional derivatives with respect to some classical source (current) J_ϕ:

$$\begin{aligned} -iG(x_1,\cdots,x_n) &= \langle 0;\mathrm{out}|T\phi(x_1)\cdots\phi(x_n)|0;\mathrm{in}\rangle_{J_\phi=0} \\ &= \frac{1}{Z[0]}\prod^{n}\left(\frac{\delta}{\delta J_\phi(x_n)}\right)Z[J_\phi]\bigg|_{J_\phi=0}\,. \end{aligned} \tag{2.7}$$

The functional $Z[J_\phi]$ is non-perturbative and thus represents a sum of all connected and disconnected diagrams that contribute to the total amplitude, however, it does not distinguish between diagrams that differ by a permutation of vertices which contribute $N!$ times for each diagram with N connected components. This implies that the sum of all *connected* diagrams $W[J_\phi]$ is related to $Z[J_\phi]$ by the relation

$$Z[J_\phi] = \sum_{N=0}^{\infty}\frac{\big(iW[J_\phi]\big)^N}{N!} = \exp\big(iW[J_\phi]\big) \tag{2.8}$$

and may thus be derived from the complete generating functional with a simple logarithm.

Comparing the two descriptions of $Z[J_\phi]$ above, it is straightforward to see that $W[J_\phi]$ already resembles something like the quantum effective action that we are after, however, it is still unable to distinguish between connected diagrams that are related by vertex permutations and moreover, it is a functional of the arbitrary source J_ϕ. For practical purposes, it is much more convenient to describe a quantum theory in terms of a functional of the fields that represents a sum of all the one-particle-irreducible (1PI) diagrams. To this end, we consider a stationary point of the "effective action" $W[J_\phi]$,

$$\phi_J(x) = \frac{\delta W[J_\phi]}{\delta J_\phi(x)} = \frac{\langle 0; \mathrm{out}|\phi(x)|0; \mathrm{in}\rangle_J}{\langle 0; \mathrm{out}|0; \mathrm{in}\rangle_J}\,, \tag{2.9}$$

so that ϕ_J represents the vacuum expectation value (VEV) of the quantum operator corresponding to the classical ϕ in the presence of the source J_ϕ. Assuming that this expression is invertible, we may define $\bar{J}_\phi$ as the particular current that satisfies $\phi_J = \phi$ and perform a Legendre transform of $W[\bar{J}_\phi]$ to further define a quantum effective action with the desired properties,

$$\Gamma[\phi] = W[\bar{J}_\phi] - \phi \cdot \bar{J}_\phi\,. \tag{2.10}$$

Indeed, it is straightforward to show that

$$\frac{\delta \Gamma[\phi]}{\delta \phi(x)} = -\bar{J}_\phi(x) \tag{2.11}$$

and confirm that ϕ represents a stationary point of $\Gamma[\phi]$ in the absences of sources ($J_\phi = 0$). In short, ϕ solves the equations of motion derived from the action $\Gamma[\phi]$ which explicitly takes into account all of the quantum effects (includes contributions from all the 1PI diagrams) that result from the original classical action.

So far, everything above has been defined in a non-perturbative manner, however, in practice it is almost always necessary to expand the effective action in loops to reach any kind of tractable calculation. We will thus follow the original work of Coleman and Weinberg [11] and expand (2.10) using the background field method to arrive at an effective one-loop potential that is useful for practical application. This expansion may be derived after first separating the classical and quantum contributions to the effective potential by writing

$$\Gamma[\phi] = S[\phi] + \hbar K[\phi]\,, \tag{2.12}$$

where we have reinstated $\hbar$ to more easily denote the loop contributions contained in $K[\phi]$ which will be defined perturbatively below. In this form it is also easy to see that we recover the classical action exactly in the $\hbar \to 0$ limit as one should expect. We may now perform the actual perturbative expansion by replacing the original quantum field ϕ with

$$\phi \;\to\; \phi + \varphi\,, \tag{2.13}$$

where $\varphi(x)$ represents small quantum fluctuations around ϕ which should now be understood as a classical, approximately constant, background field. Combining (2.6), (2.8), (2.10), and (2.11) under the expansion above, we can arrive at

$$\exp\left(\frac{i}{\hbar}\Gamma[\phi]\right) = \int \mathcal{D}\varphi \exp\left[\frac{i}{\hbar}\left(S[\phi+\varphi] - \frac{\delta\Gamma[\phi]}{\delta\phi}\cdot\varphi\right)\right], \tag{2.14}$$

which allows us to express the effective potential in terms of an integral over the fluctuations φ,

$$\begin{aligned}\Gamma[\phi] &= S[\phi] - i\hbar\ln\left[\int \mathcal{D}\varphi \exp\left(-i\frac{\delta K[\phi]}{\delta\phi}\cdot\varphi + \frac{i}{2\hbar}\varphi\cdot\Omega[\phi]\cdot\varphi + \mathcal{O}(\varphi^3)\right)\right] \\ &= S[\phi] + \hbar K[\phi]\,,\end{aligned} \tag{2.15}$$

where $\Omega[\phi] = \delta^2 S[\phi]/\delta\phi^2$ is the Hessian of the classical action and we have used (2.12) to eliminate $\Gamma[\phi]$ on the right side of the expression.

Since $K[\phi]$ now appears on both sides, we may precisely define the quantum contributions to the effective action order by order in loops as

$$K[\phi] = K_{(\text{tree})}[\phi] + K_{(\text{1-loop})}[\phi] + K_{(\text{2-loop})}[\phi] + \cdots, \tag{2.16}$$

where $K_{(\text{tree})}[\phi] = 0$ and the higher orders may be solved for iteratively, though in practice is often sufficient to consider only the first order contribution given by

$$K_{(\text{1-loop})}[\phi] = -i\ln\int \mathcal{D}\varphi \exp\left(\frac{i}{2\hbar}\varphi\cdot\Omega[\phi]\cdot\varphi\right). \tag{2.17}$$

Finally, with this we may compute the integral and define the Coleman-Weinberg one-loop effective potential $U_{\text{CW}}(\phi)$ in terms of

$$\Gamma[\phi] = S[\phi] - V\big(U_{\text{CW}}(\phi) + \cdots\big) \tag{2.18}$$

where $V = \int \mathrm{d}^4x$ is the 4D spacetime volume and U_{CW} is not a functional but an ordinary function of ϕ that may be combined with the tree level mass and interactions terms in $S[\phi]$ to complete the entire effective potential $U_{\text{eff}}(\phi)$.

It is remarkable that all of the formal considerations above have led us to a Gaussian integral describing one-loop quantum effects that may actually be solved analytically. One may find more details on the specifics of solving such integrals, and on all of the other details glossed over in this section, in any QFT textbook (see for example [123]), so for the sake of brevity we will simply quote the result:

$$U_{\text{CW}}(\phi) = -\frac{i}{2}\ln\big[\,\mathrm{Det}\big(\Omega(x,y)\big)\big] = -\frac{i}{2}\mathrm{Tr}\big[\ln\big(\Omega(x,y)\big)\big]\,. \tag{2.19}$$

The determinant and trace here are understood to act in the functional sense on the kinetic Hessian operator $\Omega(x,y)$, which is usually the Klein-Gordon operator

$$\Omega(x,y) = \big(\Box + m^2 - i\epsilon\big)\delta^4(x-y) \tag{2.20}$$

or something similar, and may in principle be a matrix of kinetic operators when more than one field ϕ is present in the action. The trace is then most easily evaluated after Fourier transforming to momentum space yielding

$$U_{\rm CW}(\phi) = -\frac{i}{2}\int \frac{\mathrm{d}^4 p}{(2\pi)^4}\ln\left(p^2 + m^2 - i\epsilon\right) \tag{2.21}$$

when $\Omega(x, y)$ takes the form (2.20). Though this integral is obviously UV divergent, it is straightforward to remove the divergences via some regularization procedure, for example dimensional regularization [139]. We will see specific examples of effective potentials that result from this procedure in Sections 2.3.2 and 3.4.2.

2.2.2 Spontaneous symmetry breaking

The crux of the Coleman-Weinberg mechanism lies in a particular phenomenon that results from the one-loop effective potential derived above, namely, the spontaneous breaking of symmetry that may occur after including these quantum effects in the action. As opposed to explicit breaking which simply occurs when a term in a given action (or more precisely, the EOMs) does not respect the symmetry of the other terms, spontaneous breaking occurs when the ground state of a quantum system is degenerate and not individually invariant under the symmetries of the underlying theory. This behavior was first noted with respect to superconductors and later generalized in the QFT framework through Goldstone's theorem [136, 140, 141], which now plays a crucial role in our understanding of how gauge bosons acquire masses in the Standard Model via the Higgs mechanism [142–145]. It is often stated that spontaneous symmetry "breaking" is perhaps not the best nomenclature since the symmetries of a theory are not actually (explicitly) broken when SSB occurs, rather, they become non-linearly realized through so-called Nambu-Goldstone (NG) bosons when one expands around the potential minimum (ground state) thus obscuring the presence of the overall symmetry from a naive viewpoint.

There exists many formal descriptions of SSB, but it is perhaps best understood through a concrete example which we will now consider. For the sake of brevity we will only look at the case of spontaneously broken local symmetry here since it will have bearing on later chapters and will still demonstrate the most important aspects of general SSB that we will encounter for the global case later in the current chapter. Though this section is meant to serve as a brief review of its most important aspects, one should keep in mind that SSB is a very general phenomena that may occur with respect to global or local symmetries and that the Coleman-Weinberg process as a whole has been shown to respect gauge invariance in renormalizable theories when it is present [146, 147].

We follow [76, 148] and consider a classical action describing massless Abelian scalar electrodynamics,

$$S = \int \mathrm{d}^4 x\left(-\frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} - \frac{1}{2}\left(D_\alpha\Phi\right)^\dagger\left(D^\alpha\Phi\right) - U_0(\Phi)\right), \tag{2.22}$$

where $F_{\alpha\beta} = \partial_\alpha A_\beta - \partial_\beta A_\alpha$, $A_\alpha(x)$ is a $U(1)$ Abelian gauge field, $\Phi(x)$ is a complex scalar with a quartic self interaction potential $U_0(\Phi) = \lambda/4(\Phi^\dagger\Phi)^2$ parameterized by the dimensionless coupling constant λ, and $D_\alpha = \partial_\alpha - ieA_\alpha$ is the $U(1)$ covariant derivative with the coupling constant e. Naturally, this action is invariant under a local $U(1)$ symmetry which acts on the fields as

$$\Phi' = e^{ie\theta}\Phi \qquad\qquad A'_\alpha = A_\alpha - \partial_\alpha\theta\,, \tag{2.23}$$

where $\theta(x)$ is a local parameter of the transformation.

For the sake of argument let us now assume that, perhaps through some interactions with other unspecified fields, we calculate the one-loop effective potential for Φ and find that it takes the form $U_{\rm CW}(\Phi) = -(1/2)\mu^2(\Phi)\Phi^\dagger\Phi$ where $\mu(\Phi)$ is some massive field dependent parameter. Per our discussion in the last section, the classical potential in (2.22) may then be replaced with the effective potential

$$U_{\rm eff}(\Phi) = U_0(\Phi) + U_{\rm CW}(\Phi) = \frac{\lambda}{4}\big(\Phi^\dagger\Phi\big)^2 - \frac{\mu^2}{2}\Phi^\dagger\Phi\,, \tag{2.24}$$

to account for quantum effects that contribute at one-loop order. Though this potential is invariant under (2.23) for general Φ, it exhibits a crucial feature that is not present in the tree-level potential; it has a non-zero minimum when $\mu^2 > 0$:

$$\left.\frac{\partial U_{\rm eff}(\Phi)}{\partial\Phi}\right|_{\Phi=v_\Phi} = 0 \qquad \Rightarrow \qquad v_\Phi = \frac{\mu}{\sqrt{\lambda}}\,. \tag{2.25}$$

There are very important physical ramifications of this non-zero minimum. To see them, we reparameterize the two independent degrees of freedom (DOFs) in the complex Φ in terms of two real scalars by writing

$$\Phi = \big(h + v_\Phi\big)e^{\frac{i\chi}{v_\Phi}}\,, \tag{2.26}$$

where $\chi(x)$ corresponds to the phase of the original scalar and $h(x)$ represents fluctuations of its magnitude around the minimum of the potential. Plugging this into the action (2.22) with U_0 replaced by $U_{\rm eff}$, we find

$$\begin{aligned} S_{\rm eff} = \int {\rm d}^4x \bigg(&- \frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} - \frac{m_A^2}{2}A_\alpha A^\alpha - \frac{1}{2}\partial_\alpha h\partial^\alpha h - \frac{m_h^2}{2}h^2 \\ &- \frac{1}{2}\partial_\alpha\chi\partial^\alpha\chi + ev_\Phi A^\alpha\partial_\alpha\chi\bigg)\,, \end{aligned} \tag{2.27}$$

where we have identified the canonical masses

$$m_A = \frac{e\mu}{\sqrt{\lambda}} \qquad\qquad m_h = \sqrt{2}\mu\,. \tag{2.28}$$

From a naive perspective, one would say that the action (2.27) is obviously not invariant under $U(1)$ transformations due to the mass terms for A_α and h, however, it is straightforward to confirm that this symmetry does in fact hold if h is invariant and χ transforms non-linearly as

$$h' = h \qquad\qquad \chi' = \chi + e v_\Phi \theta \,. \tag{2.29}$$

This behavior is precisely what characterizes SSB and the role played by χ singles it out as an NG boson of the spontaneously broken $U(1)$ symmetry.

Going one step farther, it is instructive to fix the gauge symmetry in our theory to get a more precise picture of the field content. In particular, we may select the "unitary" gauge by writing

$$A_\alpha \;\to\; A_\alpha + \frac{1}{e v_\Phi}\partial_\alpha \chi \,, \tag{2.30}$$

which leaves us with the action

$$S_U = \int \mathrm{d}^4x \left(-\frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} - \frac{m_A^2}{2}A_\alpha A^\alpha - \frac{1}{2}\partial_\alpha h \partial^\alpha h - \frac{m_h^2}{2}h^2 \right) \tag{2.31}$$

and has the effect of completely removing χ from the spectrum, thus indicating that this field is unphysical (pure gauge). We note that χ differs in this way from the analogous NG boson that results from the breaking of a global rather than a local symmetry, which does indeed appear as a physical particle. A classic example of such a phenomena is the pion, which may be identified as the (pseudo) NG boson after the breaking of (approximate) global $SU(2)$ chiral symmetry in the SM. Some would thus not classify χ as a true NG boson in our setup since it is not physical and effectively just serves to give mass to the other particles, however, since it still serves to non-linearly preserve our underlying symmetry we will refer to it as such. We refer the reader to [76] for more formal details on SSB and the differences between the local and global cases.

Moving forward, we are now in a position to see the crucial feature that SSB in the present context does not add or subtract any DOFs from the original action, but simply reshuffles them; we started with a massless gauge boson and a massless complex scalar, $(2 + 2) = 4$ DOFs, and ended with a massive gauge boson and one massive real scalar, $(3 + 1) = 4$ DOFs. It should however be noted that, though the physical field content is more transparent in this gauge, it is a poor choice for many practical applications due to the fact that the photon propagator exhibits bad UV behavior and leads to divergent cross sections that cannot be cured with conventional renormalization techniques. In this respect it preferable to select either the Feynman or Landau gauge for example, where χ reenters the spectrum and improves the UV behavior. We will in fact see that this same type of phenomenon appear in conformal gravity in Section 4.7.

In summary, we have seen how to include quantum contributions into the analysis of a classical action by deriving its one-loop effective potential, and how these contributions may lead to a spontaneous breakdown of the symmetry present in that classical action, which in turn leads to the generation of mass terms for what were originally massless

DOFs. Though this has occurred with respect to local $U(1)$ symmetry in the short example above, we will now see how the same type of behavior may be exhibited by a more realistic globally scale-invariant theory of gravity and matter.

2.3 Dynamical generation of scales

2.3.1 Embedding the SM with gravity

We begin with the SM action which, as mentioned in the Introduction, is already nearly invariant under both global and local scale symmetry, with the only violating term coming from the Higgs potential. The pure Higgs part of the SM action is given by

$$S_{\mathrm{SM}} \supset S_H = \int \mathrm{d}^4x \sqrt{-g}\Big[-\frac{1}{2}(D_\alpha H)^\dagger(D^\alpha H) + \frac{\mu_H^2}{2}H^\dagger H - \frac{\lambda_H}{4}(H^\dagger H)^2\Big], \qquad (2.32)$$

where $H(x)$ is the SM Higgs doublet, μ_H is a massive constant that serves to define the EW scale and the mass of the radial component of the Higgs after SSB, and λ_H is the (dimensionless) Higgs quartic self-coupling constant [76]. It is straightforward to confirm that this expression is indeed only scale-invariant for $\mu_H = 0$.

In order to simultaneously realize the spontaneous breakdown of scale symmetry, generate masses for the SM neutrinos via a type-I seesaw, and realize an appropriate value for the EW scale using the neutrino option, we will also consider the BSM action

$$\begin{aligned} S_{\mathrm{BSM}} = \int \mathrm{d}^4x \sqrt{-g}\Big[&-\frac{1}{2}\big(D_\alpha\phi D^\alpha\phi + D_\alpha\sigma D^\alpha\sigma + i\bar{N}\not{D}N\big) \\ &-\frac{1}{4}\Big(\lambda_\phi\phi^4 + \lambda_\sigma\sigma^4 + \lambda_{\phi\sigma}\phi^2\sigma^2 + \big(\lambda_{H\phi}\phi^2 + \lambda_{H\sigma}\sigma^2\big)H^\dagger H\Big) \\ &-\frac{1}{2}\Big(\big(y_\phi\phi + y_\sigma\sigma\big)N^TCN + \big(y_H\bar{L}\tilde{H}(1+\gamma_5)N + \mathrm{h.c.}\big)\Big)\Big]. \end{aligned} \qquad (2.33)$$

Here, $\phi(x)$ and $\sigma(x)$ are real scalar fields that have quartic interactions with each other and the Higgs parameterized by the coupling constants λ_i. The fermionic portion of the action above describes the interactions of a family of right-handed sterile Majorana neutrinos $N(x)$ with the SM leptons $L(x)$, the Higgs ($\tilde{H} = i\sigma_2 H^*$), and the BSM scalars ϕ and σ. Though, naturally, there are minimal fermion-gravitational couplings built into the operator $\not{D} = \gamma^\alpha D_\alpha$ that may only be properly accounted for in the vierbein formalism [149], these will not play a role in the present analysis. We also note that flavor indices are suppressed in this action, however, the Yukawa couplings y_H, y_ϕ, and y_σ should, strictly speaking, be considered matrices in generation space even though they may simply be treated as real numbers for our purposes.

The last important piece of the present model is the gravitational part of the total action which, unlike the SM and BSM actions above, looks quite different if it is constructed on the basis of local or just global scale symmetry. We will focus on the global case for what follows and employ the following action which, assuming a metric-compatible and torsion-free connection, is given by a sum of the three independent contractions of squares of the Riemann tensor $R_{\alpha\beta\gamma\delta}$ and non-minimal couplings between the Ricci scalar R and the three non-gravitational scalars:

$$S_{\rm QG} = \int \mathrm{d}^4x\,\sqrt{-g}\Big[-\kappa C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} - \gamma R^2 + \frac{1}{2}\left(\beta_H H^\dagger H + \beta_\phi \phi^2 + \beta_\sigma \sigma^2\right)R\Big]\,, \quad (2.34)$$

where κ, γ, and the β_i are dimensionless coupling constants. We arrive at this specific parameterization of the action for quadratic gravity by rewriting the full Riemann square in terms of the Weyl tensor $C_{\alpha\beta\gamma\delta}$ using the identity $R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} = C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} + 2R_{\alpha\beta}R^{\alpha\beta} - 1/3R^2$ and dropping a multiple of the Gauß-Bonnet invariant

$$\mathcal{G} = -\frac{1}{4}\varepsilon^{\alpha\beta\mu\nu}\varepsilon^{\gamma\delta\rho\sigma}R_{\alpha\beta\gamma\delta}R_{\mu\nu\rho\sigma} = R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} - 4R_{\alpha\beta}R^{\alpha\beta} + R^2\,, \quad (2.35)$$

which is a total derivative, in order to eliminate the square Ricci tensor term [150]. Crucially, we do not include an Einstein-Hilbert term ($M_{\rm Pl}^2 R/2$) in the action (2.34) as its presence would violate scale symmetry. Though we have included the Weyl tensor term in the action for completeness, for the purposes of the present chapter we will always assume that the Weyl coupling constant κ is negligibly small so that its effects have no important bearing on our analyses of scale-invariant theories in the present context. However, in the next chapter we will relax this assumption and account for the gravitational DOFs that originate from the Weyl-squared term with general κ for comparison.

With all the considerations above, we may finally assemble the full action describing our model by summing (2.32–2.34):

$$S_{\rm SI} = S_H\big|_{\mu_H=0} + S_{\rm BSM} + S_{\rm QG}\,. \quad (2.36)$$

This action represents the most general functional that is invariant under the SM's $SU(3)_C\times SU(2)_L\times U(1)_Y$ gauge transformations, diffeomorphisms, and most importantly for the present discussion, global scale transformations (2.1). In what follows we will demonstrate explicitly how this symmetry of the classical action is spontaneously broken by loop effects à la Coleman(Gildener)-Weinberg [11, 151] and how these quantum effects are able to generate not only the Einstein-Hilbert and Higgs potential terms in the resulting effective action, but also light masses for the SM neutrinos.

2.3.2 The Planck mass

The presence of two extra scalars in the BSM action (2.33) turns out to be necessary to achieve our desired spontaneous breakdown of scale symmetry, however, this feature complicates matters with respect to the derivation of the one-loop effective potential following the original Coleman-Weinberg method which considers only a single scalar field. There is however a simple extension of this method that accounts for contributions from an arbitrary number of scalars known as the Gildener-Weinberg mechanism [151]. Though in principle, it is quite possible that both ϕ and σ might acquire a non-zero

VEV due to quantum effects, we will follow the previously mentioned work and assume for the sake of simplicity that the multi-field scalar potential has an approximately flat direction. We choose the flat σ direction i.e. $\phi \neq 0$ and $\sigma \approx 0$, which may be realized if the quartic couplings satisfy

$$\lambda_\phi \ll \lambda_{\phi\sigma} \qquad\qquad \lambda_\phi \ll \lambda_\sigma \,. \tag{2.37}$$

It is also necessary to assume that the Higgs couplings $\lambda_{H\phi}$, $\lambda_{H\sigma}$, and β_H are extremely suppressed in order to achieve a realistic neutrino option down the road, which requires $m_N \approx 10^7$ GeV, and to safely neglect contributions to the dynamically generated Planck mass from the Higgs VEV.

Under these assumptions, it becomes clear from the form of (2.34) that an Einstein-Hilbert term may indeed be generated if ϕ acquires a non-zero VEV v_ϕ, and that this same VEV may also generate the bare Higgs mass term $\mu_H^2 = -\lambda_{H\phi} v_\phi^2/2$ which will be required to spontaneously break EW symmetry and realize the Higgs mechanism. Furthermore, we can see from the Yukawa interactions in (2.33) that the Majorana neutrino acquires the mass $m_N = y_\phi v_\phi$ which in turn allows us to put an approximate value on the Yukawa coupling constant, $y_\phi \sim \sqrt{\beta_\phi}(m_N/M_{\text{Pl}}) \approx 10^{-10}$ for $\beta_\phi \approx 10^3$. Though there is some degree of fine-tuning involved when assuming small values for $\lambda_{H\phi}$, $\lambda_{H\sigma}$, and y_ϕ since there is no enhancement of symmetry associated with their vanishing, it should be noted that they are still in some sense natural since if one sets them strictly to zero, they will remain zero at all orders in perturbation theory (see also the discussion regarding enhanced Poincaré symmetry in scale-invariant theories in [152]).

With all the above considerations in mind, we may proceed with a derivation of the effective one-loop scalar potential as outlined in Section 2.2.1 by expanding each of the scalars in terms of quantum fluctuations around the classical backgrounds $\phi \neq 0$ and $\sigma = 0$, integrating out the fluctuations around these backgrounds, and employing dimensional regularization in the $\overline{\text{MS}}$ scheme [139, 153] to calculate U_{CW}. Then, after including the quartic tree-level contributions in (2.33), we find the effective potential

$$\begin{aligned} U_{\text{eff}}(R,\phi,\sigma) &= \frac{\lambda_\phi}{4}\phi^4 + \frac{\lambda_\sigma}{4}\sigma^4 + \frac{\lambda_{\phi\sigma}}{4}\phi^2\sigma^2 \\ &\quad + \frac{1}{64\pi^2}\left[m_\phi^4 \ln\left(\frac{m_\phi^2}{\mu^2}\right) + m_\sigma^4 \ln\left(\frac{m_\sigma^2}{\mu^2}\right)\right] + U_\Lambda \,, \end{aligned} \tag{2.38}$$

where U_Λ is an arbitrary constant whose role will addressed shortly, μ is the renormalization scale (that has absorbed a constant $-3/2$), and the effective scalar masses are defined as

$$m_\phi^2 = 3\lambda_\phi\phi^2 + \beta_\phi R \qquad\qquad m_\sigma^2 = \frac{\lambda_{\phi\sigma}}{2}\phi^2 + \beta_\sigma R \,. \tag{2.39}$$

Naturally, the integration that yields this potential also produces divergent terms that may be absorbed into λ_ϕ, β_ϕ, and γ as part of the renormalization process. We also note that these results are in full agreement with calculations of the same type of effective potential in [154–156], though for completeness, it should be pointed out that we have made the simplifications $\beta_\phi \approx \beta_\phi - 1/6$ and $\beta_\sigma \approx \beta_\sigma - 1/6$ since we will eventually find that $\beta_\phi \gtrsim 10^2$ and since β_σ turns out to play only a negligible role in our analyses. In fact, due to its vanishing VEV, the scalar σ ends up playing no further role for our purposes and we will thus suppress it in all further calculations.

Moving forward, we recast (2.38) in a more convenient form by making the safe assumptions that $\beta_\phi R < 3\lambda_\phi \phi^2$ and $\beta_\sigma R < (1/2)\lambda_{\phi\sigma}\phi^2$ so that the effective potential may be expanded in powers of R as

$$U_{\text{eff}}(R, \phi) = U_{(0)}(\phi) + U_{(1)}(\phi)R + U_{(2)}(\phi)R^2 + \mathcal{O}(R^3)\,, \tag{2.40}$$

where the ϕ-dependent terms are given by

$$U_{(0)}(\phi) = \frac{\lambda_\phi}{4}\phi^4 + \frac{\phi^4}{64\pi^2}\left[9\lambda_\phi^2 \ln\left(\frac{3\lambda_\phi\phi^2}{\mu^2}\right) + \frac{\lambda_{\phi\sigma}^2}{4}\ln\left(\frac{\lambda_{\phi\sigma}\phi^2}{2\mu^2}\right)\right] + U_\Lambda \tag{2.41}$$

$$U_{(1)}(\phi) = \frac{\phi^2}{64\pi^2}\left[6\beta_\phi\lambda_\phi\left(\ln\left(\frac{3\lambda_\phi\phi^2}{\mu^2}\right) + \frac{1}{2}\right) + \beta_\sigma\lambda_{\phi\sigma}\left(\ln\left(\frac{\lambda_{\phi\sigma}\phi^2}{2\mu^2}\right) + \frac{1}{2}\right)\right] \tag{2.42}$$

$$U_{(2)}(\phi) = \frac{1}{64\pi^2}\left[\beta_\phi^2\left(\ln\left(\frac{3\lambda_\phi\phi^2}{\mu^2}\right) + \frac{3}{2}\right) + \beta_\sigma^2\left(\ln\left(\frac{\lambda_{\phi\sigma}\phi^2}{2\mu^2}\right) + \frac{3}{2}\right)\right]. \tag{2.43}$$

Following the discussion in Section 2.2.2, we may now solve for the VEV v_ϕ under the simplifying assumption that R is negligibly small, though non-zero, compared to ϕ:

$$\left.\frac{\partial U_{\text{eff}}(0,\phi)}{\partial\phi}\right|_{\phi=v_\phi} = 0 \qquad \Rightarrow \qquad v_\phi = \mu e^{-f_\phi}\,, \tag{2.44}$$

where we have defined the dimensionless functions of the couplings[1]

$$f_\phi = \frac{1}{g_\phi}\left[\frac{9\lambda_\phi^2}{256\pi^2}\left(\ln(3\lambda_\phi) - \ln\left(\frac{\lambda_{\phi\sigma}}{2}\right)\right) + \frac{\lambda_\phi}{16}\right] + \frac{1}{2}\ln\left(\frac{\lambda_{\phi\sigma}}{2}\right) + \frac{1}{4} \tag{2.45}$$

$$g_\phi = \frac{36\lambda_\phi^2 + \lambda_{\phi\sigma}^2}{512\pi^2}\,. \tag{2.46}$$

With the VEV in hand, we are able to determine an explicit value for U_Λ, which is now included in (2.41), by allowing it to assume the role of a zero-point energy density that is fixed in order to avoid an explicit breaking of scale symmetry by the R-independent leading-order contribution $U_{(0)}(\phi)$,

$$U_{\text{eff}}(0, v_\phi) = 0 \qquad \Rightarrow \qquad U_\Lambda = -g_\phi v_\phi^4\,. \tag{2.47}$$

Finally, the VEV also fixes a value for the dynamically generated Planck mass which follows from (2.42) and a simple identification with the last term in (2.34):

$$M_{\text{Pl}}^2 = \beta_\phi v_\phi^2 + 2U_{(1)}(v_\phi)\,. \tag{2.48}$$

[1] The function g_ϕ in fact corresponds to the β-function for the coupling λ_ϕ in the absence of y_ϕ.

It important to reinforce the fact that in the present scheme where v_ϕ depends on the renormalization scale μ, the measured value of M_{Pl} does also.

Before we continue with more analysis of the model at hand, the role of the negative zero-point energy density U_Λ deserves further discussion. Its presence is required as a direct consequence of the spontaneous breakdown of scale symmetry, despite the fact that it is in essence nothing more than a constant that results in an explicit, though super-soft, breaking of scale invariance at tree level. Even though our choice to include U_Λ allows us to remedy the cosmological constant problem in this way, it is important to acknowledge that it is not possible to determine the exact value of the zero-point energy within the framework of QFT in flat spacetime. To comprehensively address the cosmological constant problem, one must also consider gravitational quantum fluctuations and include contributions from the Weyl tensor term in the action (2.34). As previously mentioned, the role of gravitational DOFs will be investigated in detail in the coming chapters where we will address this issue again, though a complete resolution to the CC problem is beyond the scope of this work. For now, we will proceed with our analyses of the scale-invariant theory at hand.

2.3.3 Neutrino masses and the EW scale

The principle reason that we have included right-handed Majorana neutrinos in the BSM action (2.33) is to demonstrate how scale-invariant models are able to generate not only the Planck and EW scales, but also light masses for the SM neutrinos through a type-I seesaw. This mechanism, originally laid out by Minkowski, Gell-Mann, and others [48, 157, 158], describes a simple way to naturally introduce small SM neutrino masses, which are forbidden by gauge symmetry in the bare SM, in the presence of additional heavy sterile Majorana neutrinos. The basic premise is based on introducing a Majorana neutrino such as ours where $m_N \gg m_L$ so that the full neutrino mass matrix has the eigenvalues

$$m_\pm = \frac{1}{2}\left(m_N \pm \sqrt{m_N^2 + m_L^2}\right) \qquad \text{where} \qquad m_+ \approx m_N \qquad m_- \approx -\frac{m_L^2}{m_N}\,, \tag{2.49}$$

and the determinant $m_+ m_- = -m_L^2$, where $m_L = y_H v_H$ is the off-diagonal mass term that is generated from the last term in (2.33) i.e. by Higgs-neutrino Yukawa couplings after the spontaneous breaking of EW symmetry, and thus sits at approximately the EW scale for natural values of y_H. When this situation is realized, the physical masses of the sterile and SM neutrinos, m_+ and m_- respectively, form a "seesaw" where the fixed value of the determinant means that a larger value for m_+ forces a smaller value for m_-. This mechanism applies to the present model in a similar way to the original formulation with the important caveat being that instead of introducing the heavy Majorana mass by hand (which would violate scale symmetry), it has been generated by dynamical effects and is related to the VEV of ϕ.

In order to generate a satisfactory Higgs potential, via a mechanism that will be addressed shortly, we assume that the Majorana mass takes the relatively natural and

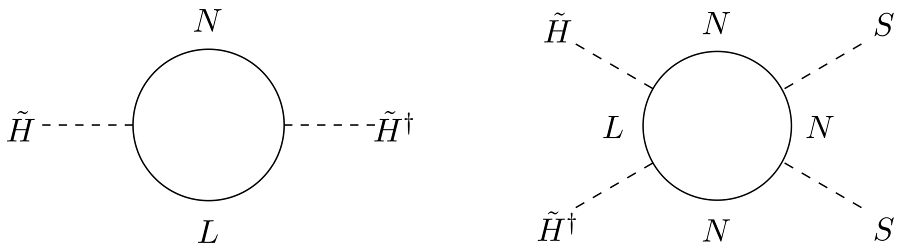


Figure 2.1: Neutrino contributions to the Higgs mass (left) and portal coupling (right).

phenomenologically viable value of $m_N \approx 10^7$ GeV and parameterize it in terms of $M_{\rm Pl}$ as

$$m_N = y_\phi v_\phi = y_\phi M_{\rm Pl} \left(\beta_\phi + \frac{2U_{(1)}(v_\phi)}{v_\phi^2} \right)^{-1/2} , \tag{2.50}$$

where $U_{(1)}$ is given in (2.42). We have written m_N in this way because, in the parameter space that we consider where v_ϕ sits just below the Planck scale and $\beta_\phi \gtrsim 10^2 \gg 2U_{(1)}(v_\phi)/v_\phi^2$, it allows us to put an approximate bound on y_ϕ:

$$y_\phi \approx \frac{m_N \beta_\phi^{1/2}}{M_{\rm Pl}} \approx 10^{-12} \beta_\phi^{1/2} . \tag{2.51}$$

It should be noted that this small value of y_ϕ does not constitute a fine-tuning and is natural in the sense of 't Hooft [12] since a $U(1)_{B-L}$ symmetry is acquired as y_ϕ goes to zero. Furthermore, for $v_H = 246$ GeV and $y_H \approx 10^{-4}$, we find that the type-I seesaw functions as advertised and leads to a physical SM neutrino mass of $m_- \sim y_H^2 v_H^2 / m_N \approx 0.1$ eV.

The inclusion of heavy right-handed neutrinos has an important bearing on not only the SM neutrinos, but also on the Higgs sector via Brivio's "neutrino option" [159–161] (see also [162]). This mechanism takes into account loop corrections to the Higgs mass term, $-\mu_H^2 H^\dagger H$, that arise from the diagram Fig. 2.1 (left) and asserts that these corrections actually form the dominant contribution to the total value in the parameter space described above. This means that in the neutrino option paradigm, one can write $\mu_H^2 \sim \Delta\mu_H^2 \approx 2(125 \text{ GeV})^2$ where

$$\Delta\mu_H^2 \sim \frac{y_H^2 m_N^2}{4\pi^2} \tag{2.52}$$

is the finite (renormalization-scale-dependent) part of the contribution [163–166].

Just as in the basic type-I seesaw, the original formulation of the neutrino option introduces m_N at tree level and thus violates classical scale invariance, however, it is also possible to embed the neutrino option into a scale-invariant theory such as the one at hand where m_N is generated dynamically, as demonstrated in [28, 167]. In this extension, one necessarily has a strictly vanishing contribution $\Delta\mu_H^2 = 0$ before the spontaneous breaking of scale symmetry and finds the VEV-dependent value $\Delta\mu_H^2 \sim y_H^2 y_\phi^2 v_\phi^2/4\pi^2$ after SSB, in line with our previous assertions. It is also important to account for radiative corrections to the dimensionless coupling $\lambda_{H\phi}$ that originate from the second diagram in Fig. 2.1 (right) in this scenario,

$$\Delta\lambda_{H\phi} \sim \frac{y_H^2 y_\phi^2}{16\pi^2}\,, \tag{2.53}$$

which, similarly to the Higgs mass parameter, must constitute the dominant portion of $\lambda_{H\phi}$ for the neutrino option to work as intended.

With all of the previous discussions in mind, we can finally see the first appealing feature of scale-invariant theories, namely, that dynamical breaking of SI can lead to the unified emergence of all the important energy scales in physics through a cascading effect that begins with the non-zero VEV of ϕ. This is not the end of the story however, because as we will see in the next chapter, the same effective potential that spontaneously breaks scale symmetry can also constitute an inflationary potential that leads to predictions well within modern experimental bounds.

Chapter 3

Inflation

Prior to the introduction of inflationary theory, simple big bang models struggled to resolve several well-known problems in cosmology. Most notable are the horizon and flatness problems which describe a lack of explanation for the facts that the universe appears to be in nearly perfect isotropy at large scales and that it must have began with a very particular curvature radius to remain as flat as we currently observe it. In an attempt to resolve yet another problem regarding the lack of magnetic monopoles in the context of Grand Unified Theories, Alan Guth proposed that the very early universe may have gone through a period of rapid spatial expansion [168] which, as is often the case with the best theories in physics, ended up being able to resolve the previously mentioned problems while also providing an explanation for yet another puzzle, the origin of large-scale structure in our universe. However, it was soon realized that Guth's "old inflation" had its own problems related to the reemergence of inhomogeneities and an inability to generate the necessary amount of reheating after inflation. In order to avoid these issues, Linde, Albrecht, and Steinhardt introduced the concept of "new inflation" [169–171], or "slow-roll" inflation as it is more commonly referred to today, which represents a key component in our modern understanding of early universe cosmology. We will explicitly demonstrate how inflation may be incorporated into the scale-generating model established in the last chapter, but before we do, it is important that we nail down the basics of slow-roll inflationary theory.

3.1 Slow-roll inflation

There are countless excellent reviews on inflation, though for the present discussion we will follow [124, 172] and begin by considering the basic inflationary action

$$S_{\text{inf}} = \int \mathrm{d}^4x\,\sqrt{-g}\left(\frac{M_{\text{Pl}}^2}{2}R - \frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - U_{\text{inf}}(\phi)\right), \tag{3.1}$$

which couples the Einstein-Hilbert action to a real scalar $\phi(x)$ known as the "inflaton", with the potential $U_{\text{inf}}(\phi)$. Naturally, the dynamics of this cosmological theory are

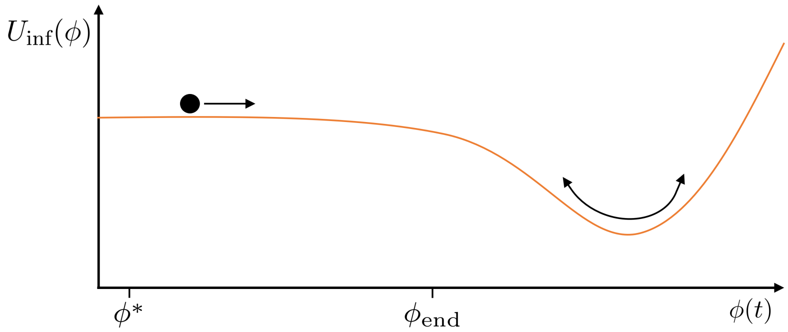


Figure 3.1: A graphical representation of the slow-roll scenario. As the inflaton evolves in time, it slowly rolls down its approximately flat (constant) potential before finally oscillating around its true minimum. The inflationary period is identified with the flat part of the evolution that begins at some unknown time, proceeds through the time of CMB horizon exit corresponding to $\phi^* = \phi(t^*)$, and concludes at $\phi_{\text{end}} = \phi(t_{\text{end}})$. A period of reheating occurs during the oscillation where the energy that was stored in the inflaton potential is transferred to SM fields, dark matter, etc.

governed by the Einstein equations where the metric is assumed to be the flat Friedmann-Lemaître-Robertson-Walker (FLRW) metric [173–177],

$$g_{\alpha\beta}\mathrm{d}x^\alpha \mathrm{d}x^\beta = -\mathrm{d}t^2 + a(t)^2\big(\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2\big)\,, \tag{3.2}$$

where $a(t)$ is the scale function that describes the expansion of space over time. Under the assumption of approximate spatial isotropy where $\phi(x) = \phi(t)$, we may focus on the time evolution controlled by the (00) component of the Einstein equations ($G_{00} = M_{\text{Pl}}^{-2} T_{00}$) which, paired with the inflaton EOM, yields the two dynamical equations

$$H^2 - \frac{1}{3M_{\text{Pl}}^2}\left(\frac{1}{2}\dot{\phi} + U_{\text{inf}}(\phi)\right) = 0 \qquad\qquad \ddot{\phi} + 3H\dot{\phi} + U'_{\text{inf}}(\phi) = 0\,, \tag{3.3}$$

where $H(t) = \dot{a}(t)/a(t)$ is the Hubble function.

For inflation to successfully resolve all of the previously mentioned issues, it is necessary for space to expand at an exponential rate for a brief period of time before entering a period of slower expansion that follows a power law. This type of behavior is well described by the standard model of cosmology in terms of a cosmological constant dominated era followed the matter and radiation dominated eras of the early universe whose appearance signal the end of inflation. The main idea behind slow-roll inflation is that the inflaton potential takes an approximately flat (constant) value that mimics a cosmological constant for just enough time to generate the desired exponential expansion before eventually acquiring its true minimum and dumping all of the energy that was stored in the inflaton into a reheating of the universe (see Figure 3.1).

We may quantify this behavior using the EOMs derived above by combing them and taking a time derivative to find the relation

$$\dot{H} = -\frac{1}{2M_{\text{Pl}}^2}\dot{\phi}^2\,, \tag{3.4}$$

while noting that the desired exponential expansion ($a(t) \sim e^{Ht}$) may only occur for an approximately constant Hubble rate where $|\dot{H}| \ll H^2$. Under this approximation, (3.3) and (3.4) imply the slow-roll conditions

$$\dot{\phi}^2 \ll \left|U_{\text{inf}}(\phi)\right| \qquad\qquad \left|\ddot{\phi}\right| \ll H\left|\dot{\phi}\right|. \tag{3.5}$$

The first of these conditions is just the statement that the scalar's potential must dominate over its kinetic energy in order to properly mimic a cosmological constant, while the second simply expresses the assumption that the rolling is indeed "slow" i.e. it ensures that the kinetic energy $\dot{\phi}$ changes only negligibly during an expansion time $1/H$. It is useful to re-express these conditions in terms of the dimensionless slow-roll parameters

$$\epsilon(\phi) = \frac{M_{\text{Pl}}^2}{2}\left(\frac{U_{\text{inf}}'(\phi)}{U_{\text{inf}}(\phi)}\right)^2 \qquad\qquad \eta(\phi) = M_{\text{Pl}}^2 \frac{U_{\text{inf}}''(\phi)}{U_{\text{inf}}(\phi)}\,, \tag{3.6}$$

that take values $\epsilon \ll 1$ and $|\eta| \ll 1$ during inflation and signify its end as they approach unity, as may be easily derived from inserting the conditions (3.5) into the EOMs (3.3). These same relations also imply that the approximately constant Hubble parameter during inflation is given by $H^2 \approx U_{\text{inf}}/(3M_{\text{Pl}}^2)$. The final piece of the slow-roll paradigm is a quantification of the amount of time that inflation is actually taking place. This is usually expressed in terms of the number of e-folds N_e, which is defined as the log of the change in scale factor during inflation,

$$N_e = \ln\left(\frac{a(t_{\text{end}})}{a(t^*)}\right) = \int_{t^*}^{t_{\text{end}}} \mathrm{d}t H \approx -\frac{1}{M_{\text{Pl}}^2}\int_{\phi^*}^{\phi_{\text{end}}} \mathrm{d}\phi \frac{U_{\text{inf}}(\phi)}{U_{\text{inf}}'(\phi)}\,, \tag{3.7}$$

where t^* marks the time of CMB horizon exit and t_{end} marks the end of inflation.

There is a wide range of diverse theories in the literature (see [178] for a nearly comprehensive list) that all lead, at least in some approximation, to a period of slow-roll inflation as described above. Indeed, as we will see in the coming sections this is even true of theories based on quadratic gravity as opposed to GR and in theories with more than one scalar field. At the end of the day, what actually distinguishes between different theories of slow-roll inflation is the form of their inflationary potentials. Once a potential is established, one may determine the parameters (3.6) and (3.7), which in turn enter directly into predictions for a few key observables that are constrained by experiment.

Inflationary observables are related to primordial quantum fluctuations of the inflaton that get stretched to macroscopic scales during inflation and "frozen in" after leaving the horizon. These fluctuations form the seeds for structure formation during the matter and radiation dominated eras, and lead to tiny anisotropies in the CMB. Measurements of these anisotropies by the Planck and BICEP/Keck collaborations are what then allow us to put strong bounds on several observables related to the power spectrum of gravitational perturbations produced during inflation [43, 44]. Gauge invariant scalar perturbations of the comoving curvature, denoted as $\mathcal{R}$, are of particular interest since their power spectrum (spectral function) $P_s(k)$ is fully determined by the form of the inflationary potential [179]. This spectrum is defined in terms of the ensemble average of the scalar perturbations,

$$\left\langle \mathcal{R}(t,\boldsymbol{k})\mathcal{R}(t,\boldsymbol{k}')\right\rangle = (2\pi)^3\delta(\boldsymbol{k}+\boldsymbol{k}')P_s(k)\,, \tag{3.8}$$

where $\boldsymbol{k}$ is the 3D comoving wavevector and $k = |\boldsymbol{k}|$ is the associated wavenumber. Provided that the scalar perturbations follow Gaussian statistics, P_s contains all the relevant physical information describing them[1]. Straightforward derivations of the relation above may be found in the works cited at the beginning of this section [124, 172].

Considering the fact that P_s scales with volume, it is convenient to define the dimensionless power spectrum $\Delta_s(k) = k^3/(2\pi^2)P_s(k)$ which may be expressed as

$$\Delta_s(k) = A_s\left(\frac{k}{aH}\right)^{n_s-1}\,, \tag{3.9}$$

where A_s is the spectral amplitude and n_s is the spectral index, each of which are directly related to the inflationary potential through the slow-roll parameters (3.6) as follows,

$$A_s = \frac{U_{\rm inf}}{24\pi^2\epsilon M_{\rm Pl}^4} \qquad\qquad n_s = 1 - 6\epsilon + 2\eta\,. \tag{3.10}$$

Both of these objects effectively appear as observables in the measured spectrum Δ_s when one considers its dependence on k since the amplitude may be expressed in terms of the value of the potential during inflation, leaving the spectral index to quantify the k-dependence. This has important implications since for $n_s = 1$, the power spectrum becomes completely k-independent and thus, scale-invariant.

It is also straightforward to derive an expression for the power spectrum related to tensor fluctuations produced during inflation (primordial gravitational waves), Δ_t, following the same type of procedure summarized above. However, partly due to the fact that their amplitude is generally much smaller than the scalar spectral amplitude (and the fact that a tensor spectral index has not even been observed up to this point), it is usually more instructive to report their contribution in terms of the scalar-to-tensor ratio

$$r = \frac{2\Delta_t^2}{\Delta_s^2} = 16\epsilon\,, \tag{3.11}$$

where the factor of two in the numerator accounts for the two independent polarizations of massless gravitational waves.

With this establishment of the basics of slow-roll inflationary theory and a general understanding of the observables that it predicts, we may now proceed with a more detailed analysis of how they fit into the scale-invariant picture we are considering.

[1] We do not consider the possibility of non-Gaussianities in this work since they are highly suppressed in single-field inflationary models and no evidence for their existence has yet been reported [180, 181].

3.2 The inflationary action

In the last chapter we demonstrated how SSB in the scale-invariant theory that we presented can lead to the unified emergence of all the important energy scales in the SM and we hinted that the scalar ϕ may serve an additional role, beyond contributing to SSB, as an inflaton. To begin pursuing this topic we begin with some necessary assumptions regarding the model. It has already been noted that the Higgs couplings $\lambda_{H\phi}$, $\lambda_{H\sigma}$, and β_H must be very suppressed in order for the neutrino option to function correctly and so that the Higgs VEV does not contribute in any significant way to the generated Planck mass. When adding inflation into the picture, it is necessary to specify these requirements more precisely and further assume that $\beta_H R \ll \lambda_{H\phi}\phi^2$ during inflation, so that the Higgs plays no relevant role in our inflationary setup. We also stated previously that $\beta_\phi R < 3\lambda_\phi\phi^2$ and $\beta_\sigma R < (1/2)\lambda_{\phi\sigma}\phi^2$ must be satisfied in order to safely expand the effective potential (2.38) in powers of R. These requirements are naturally also important for inflationary calculations and it is straightforward to confirm they hold by approximating the Ricci scalar during inflation as $R = 12H^2$ where H is the Hubble parameter.

In light of all the considerations above, we find that the part of the effective (Jordan frame) action obtained in Sections 2.3.1 and 2.3 that is relevant for inflation is given by

$$S^J_{\text{eff}} = \int \mathrm{d}^4x \sqrt{-g_J}\left(\frac{M_{\text{Pl}}^2}{2}A(\phi)R_J - B(\phi)R_J^2 - \frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - U_{(0)}(\phi)\right), \tag{3.12}$$

where M_{Pl} takes the dynamically generated value in (2.48) and "J" denotes quantities evaluated using the original Jordan frame metric. Here we have also defined the functions

$$A(\phi) = \frac{1}{M_{\text{Pl}}^2}\left(\beta_\phi\phi^2 + 2U_{(1)}(\phi)\right) \qquad\qquad B(\phi) = \gamma - U_{(2)}(\phi) \tag{3.13}$$

which depend on the effective potential contributions $U_{(1)}$ and $U_{(2)}$ given in (2.42) and (2.43). It should be noted that similar actions with a priori arbitrary functions A, B, and U_{eff} have been investigated for purely phenomenological purposes in the past [182–186], however, in our case these functions are restricted to their forms above through the effective potential.

So far, the R^2 term in the action has not played a significant role in our analyses, however, it has very important effects related to inflation that must be accounted for. These effects stem from an additional scalar degree of freedom that comes hidden inside this term, which may be exposed by transforming our action to the Einstein frame. This transformation is achieved by first introducing an auxiliary field χ with mass dimension two and making the replacement

$$R_J^2 \;\; \rightarrow \;\; 2R_J\chi - \chi^2 \tag{3.14}$$

in the action (3.12). It is important to note that the physical content of the theory is unaltered by this replacement since the original action may be recovered by simply integrating χ out with its EOM. With this, we need only change field variables and rewrite the action in terms of the Weyl rescaled metric $g^E_{\mu\nu} = \Omega^2 g^J_{\mu\nu}$ where

$$\Omega^2(\phi,\chi) = A(\phi) - \frac{4}{M_{\rm Pl}^2} B(\phi)\chi\,, \tag{3.15}$$

to arrive at the Einstein frame action

$$S^E_{\rm eff} = \int \mathrm{d}^4x\,\sqrt{-g_E}\bigg(\frac{M_{\rm Pl}^2}{2}\big(R_E - 6\Omega^{-2}\partial_\alpha\Omega\partial^\alpha\Omega\big) - \frac{1}{2}\Omega^{-2}\partial_\alpha\phi\partial^\alpha\phi - U_E(\phi,\chi)\bigg)\,. \tag{3.16}$$

Here, U_E simply denotes the scalar potential in the Einstein frame that is found by collecting all the non-kinetic terms left over after the transformation,

$$U_E(\phi,\chi) = \frac{M_{\rm Pl}^4\left(U_{(0)}(\phi) + B(\phi)\chi^2\right)}{\left(M_{\rm Pl}^2 A(\phi) - 4B(\phi)\chi\right)^2}\,. \tag{3.17}$$

It is easy to see that, due to the Weyl rescaling and the resulting second term in (3.16), χ is in fact a propagating scalar field in the Einstein frame. This scalar DOF is referred to as the "scalaron" [187, 188], whose canonically normalized form is given by

$$S = \sqrt{\frac{3}{2}} M_{\rm Pl} \ln\left|\Omega^2\right|\,. \tag{3.18}$$

With this definition, the Einstein frame action describing the coupled ϕ-scalaron system becomes

$$S^E_{\rm eff} = \int \mathrm{d}^4x\,\sqrt{-g_E}\bigg(\frac{M_{\rm Pl}^2}{2}R_E - \frac{1}{2}\left(\partial_\alpha S\partial^\alpha S + e^{-\Sigma(S)}\partial_\alpha\phi\partial^\alpha\phi\right) - U_E(\phi,S)\bigg)\,, \tag{3.19}$$

where $\Sigma(S) = \sqrt{2}S/(\sqrt{3}M_{\rm Pl})$, and the potential U_E, which is now a function of ϕ and S, is given by

$$U_E(\phi,S) = e^{-2\,\Sigma(S)}\left(U_{(0)}(\phi) + \frac{M_{\rm Pl}^4}{16B(\phi)}\left(A(\phi) - e^{\Sigma(S)}\right)^2\right)\,. \tag{3.20}$$

3.3 Inflationary predictions

3.3.1 The valley approximation

The fact that the scalar potential (3.20) depends on two independent scalars makes a naive investigation of the resulting CMB observables complicated, and though multifield inflationary techniques exist [189], there is a simpler approach that we will employ here. Similarly to the simplification of the CW potential that is based on the assumptions (2.37), it is possible to approximate (3.20) in terms of a single scalar field if the potential exhibits a clear valley structure i.e if it possesses a flat direction in field space that mimics the form of a standard single field slow-roll potential. As demonstrated on the similar

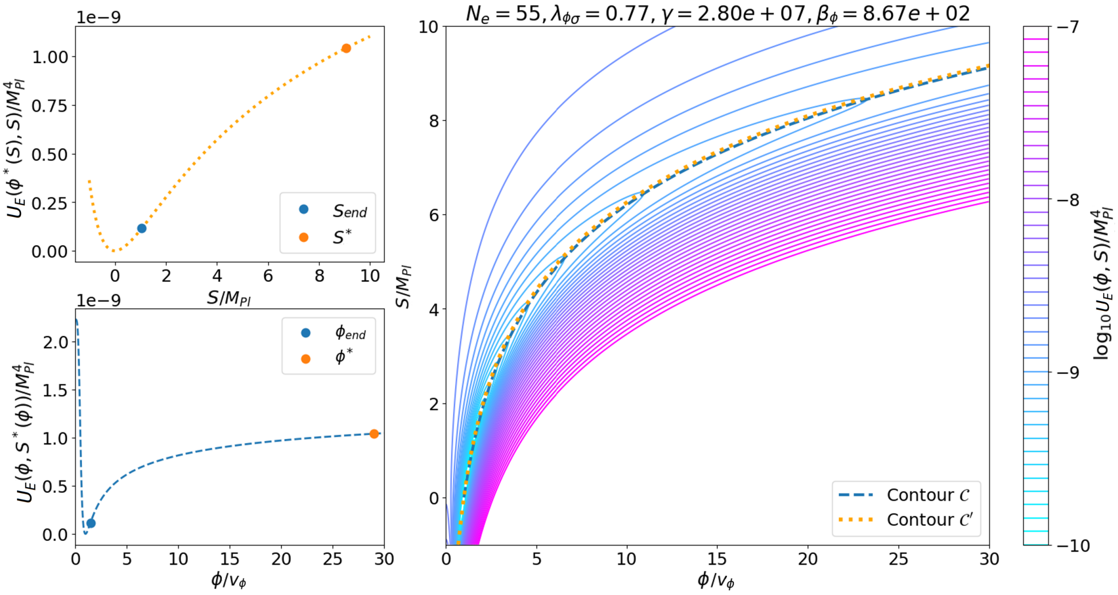


Figure 3.2: 1D inflaton potentials (left) resulting from the contours defined in (3.21) and (3.30) which are displayed on top of the plot of the full 2D potential (3.20) (right), all corresponding to the benchmark point #3 in Table 3.1.

model studied in [37], classical trajectories with a wide range of initial conditions do indeed converge to just such a valley contour provided that there is a large hierarchy between the eigenvalues of the scalar mass matrix. In other words, provided that one scalar is much heavier than the other, the heavier scalar will stabilize the potential and allow it to be approximated in terms of only the lighter scalar, which will in turn exhibit slow-roll evolution along the contour. Moving forward we will assume that this kind of mass hierarchy is realized in our scalar sector and investigate two possible realizations of the valley structure based on varying regions of parameter space[2].

The first possibility for our single field contour, which we will call $\mathcal{C}$, is defined by eliminating the scalaron S in favor of ϕ,

$$\mathcal{C} = \{\phi, \tilde{S}(\phi)\}\,, \tag{3.21}$$

where $\tilde{S}$ is the local extremum in the scalaron direction when $\phi > v_\phi$:

$$\left.\frac{\partial U_E(\phi, S)}{\partial S}\right|_{S=\tilde{S}(\phi)} = 0 \qquad \Rightarrow \qquad \tilde{S}(\phi) = \sqrt{\frac{3}{2}} M_{\rm Pl} \ln\left(A(\phi) + \frac{16B(\phi)U_{(0)}(\phi)}{M_{\rm Pl}^4 A(\phi)}\right)\,. \tag{3.22}$$

[2]Here we will present only the key results pertaining to the valley approximation used in this study. More details on the numerical analysis and scanning of parameter space may be found in the appendix of [1].

The valley structure displayed in Figure 3.2 indicates that the approximation $S = \tilde{S}(\phi)$ is good one provided that

$$\frac{m_S^2}{H_{\text{inf}}^2} \gg 1\,, \tag{3.23}$$

where H_{inf} is the Hubble scale during inflation. In other words, motion in the scalaron direction (away from $\mathcal{C}$) can be neglected in this regime during the slow-roll phase.

The inflationary potential along $\mathcal{C}$ is obtained from inserting (3.22) into the multifield potential (3.20),

$$U_{\text{inf}}(\phi) = U_E(\phi, \tilde{S}(\phi)) = \frac{M_{\text{Pl}}^4 U_{(0)}(\phi)}{M_{\text{Pl}}^4 A(\phi)^2 + 16B(\phi)U_{(0)}(\phi)}\,. \tag{3.24}$$

Naturally, we must replace the scalaron in the rest of the action (3.19) as well, which leads to a modification of the scalar kinetic terms,

$$\partial_\alpha \tilde{S} \partial^\alpha \tilde{S} + e^{-\Sigma(\tilde{S})} \partial_\alpha \phi \partial^\alpha \phi = F^2(\phi) \partial_\alpha \phi \partial^\alpha \phi\,, \tag{3.25}$$

where we have defined the shorthands

$$F^2(\phi) = \frac{1}{\big(1 + 4G(\phi)\big)A(\phi)} \left[1 + \frac{3M_{\text{Pl}}^2\Big(\big(1 + 4B(\phi)\big)A'(\phi) + 4G'(\phi)A(\phi)\Big)^2}{2\big(1 + 4G(\phi)\big)A(\phi)}\right] \tag{3.26}$$

$$G(\phi) = \frac{4B(\phi)U_{(0)}(\phi)}{M_{\text{Pl}}^2 A^2(\phi)}\,. \tag{3.27}$$

Finally, with all the considerations above, we may write the complete effective action for inflation along $\mathcal{C}$,

$$S_{\text{inf}}^E = \int \mathrm{d}^4x \sqrt{-g_E} \left(\frac{M_{\text{Pl}}^2}{2} R_E - \frac{1}{2} F^2(\phi) \partial_\alpha \phi \partial^\alpha \phi - U_{\text{inf}}(\phi) \right), \tag{3.28}$$

where one may obtain a canonically normalized inflaton $\hat{\phi}$ by computing

$$\hat{\phi}(\phi) = \int_{v_\phi}^{\phi} \mathrm{d}x F(x)\,. \tag{3.29}$$

The second contour possibility, $\mathcal{C}'$, is obtained in an analogous way to the first except with the roles of ϕ and S swapped,

$$\mathcal{C}' = \{\tilde{\phi}(S), S\}\,, \tag{3.30}$$

and should be employed in the case that the condition (3.23) is violated. The local minima $\tilde{\phi}(S)$ and the resulting single field inflationary potential may then be solved for in the same way as for contour $\mathcal{C}$,

$$\left.\frac{\partial U_E(\phi,S)}{\partial \phi}\right|_{\phi=\tilde{\phi}(S)} = 0 \qquad\qquad U'_{\text{inf}}(S) = U_E(\tilde{\phi}(S),S)\,. \tag{3.31}$$

Naturally, the field normalization that replaces (3.26) in this case takes an analogous form as well.

$$F^2(S) = 1 + e^{-\Sigma(S)}\left(\frac{\partial\tilde{\phi}(S)}{\partial S}\right)^2 . \tag{3.32}$$

3.3.2 CMB observables

Concrete predictions for the CMB observables introduced in Section 3.1 depend on all of the free parameters in the present model and a thorough scan over all the reasonable values for them has been carried out for each contour $\mathcal{C}$ and $\mathcal{C}'$ (see [1] for more details on this scan). Interestingly, though perhaps not surprisingly, it turns out the choice of contour has little bearing on the numerical predictions for CMB observables; in other words, the model is effectively insensitive to which scalar (ϕ or S) plays the role of inflaton (see Table 3.1 for a confirmation of this fact). We will thus move forward assuming that the condition (3.23) holds and that $\phi(\tilde{S})$ acts as the inflaton following the contour $\mathcal{C}$. Additionally, we note that though ϕ may be normalized using (3.29), it is perhaps simpler to derive expressions for inflationary parameters using the original ϕ to avoid yet another rewriting of the inflationary action.

With the considerations above, one finds that the slow-roll parameters are given by the analytic expressions

$$\epsilon(\phi) = \frac{M_{\text{Pl}}^2}{2F^2(\phi)}\left(\frac{U'_{\text{inf}}(\phi)}{U_{\text{inf}}(\phi)}\right)^2 \qquad\qquad \eta(\phi) = \frac{M_{\text{Pl}}^2}{F^2(\phi)}\left(\frac{U''_{\text{inf}}(\phi)}{U_{\text{inf}}(\phi)} - \frac{F'(\phi)}{F(\phi)}\frac{U'_{\text{inf}}(\phi)}{U_{\text{inf}}(\phi)}\right), \tag{3.33}$$

and that the number of e-folds may be expressed as

$$N_e = \int_{\phi^*}^{\phi_{\text{end}}} \frac{F^2(\phi)}{M_{\text{Pl}}^2}\frac{U_{\text{inf}}(\phi)}{U'_{\text{inf}}(\phi)}\,, \tag{3.34}$$

where ϕ^* is the value of ϕ at the time of CMB horizon exit and ϕ_{end} is the value of ϕ at the end of the inflationary period i.e. when $\max\{\epsilon(\phi=\phi_{\text{end}}), |\eta(\phi=\phi_{\text{end}})|\} = 1$. Finally, the observable scalar power spectrum amplitude A_s, scalar spectral index n_s, and tensor-to-scalar ratio r are determined by the parameters (3.33) up to first order in the usual way as

$$A_s = \frac{U^*_{\text{inf}}}{24\pi^2\epsilon^* M_{\text{Pl}}^4} \qquad\qquad n_s = 1 + 2\eta^* - 6\epsilon^* \qquad\qquad r = 16\epsilon^*\,, \tag{3.35}$$

where the quantities with an asterisk are evaluated at $\phi = \phi^*$.

			Contour $\mathcal{C}$					Contour $\mathcal{C}'$				
#	β_ϕ	γ	ϕ^*/μ	$\phi_{\rm end}/\mu$	n_s	r	A_s	S^*/μ	$S_{\rm end}/\mu$	n_s	r	A_s
1	1.01×10^2	5.24×10^8	0.11	0.09	0.967	0.004	3.032	4.75	0.83	0.965	0.004	3.088
2	5.69×10^2	1.68×10^8	0.45	0.11	0.972	0.010	3.041	13.46	2.02	0.972	0.010	3.075
3	8.67×10^2	2.80×10^7	2.56	0.13	0.973	0.034	3.038	23.46	2.74	0.973	0.034	3.040

Table 3.1: Representative benchmark points for both choices of contour $\mathcal{C}$ and $\mathcal{C}'$ where $\lambda_{\phi\sigma} = 0.77$, $\lambda_\phi = 0.005$, $\beta_\sigma = 1$, and $N_e = 55$ are fixed for all points.

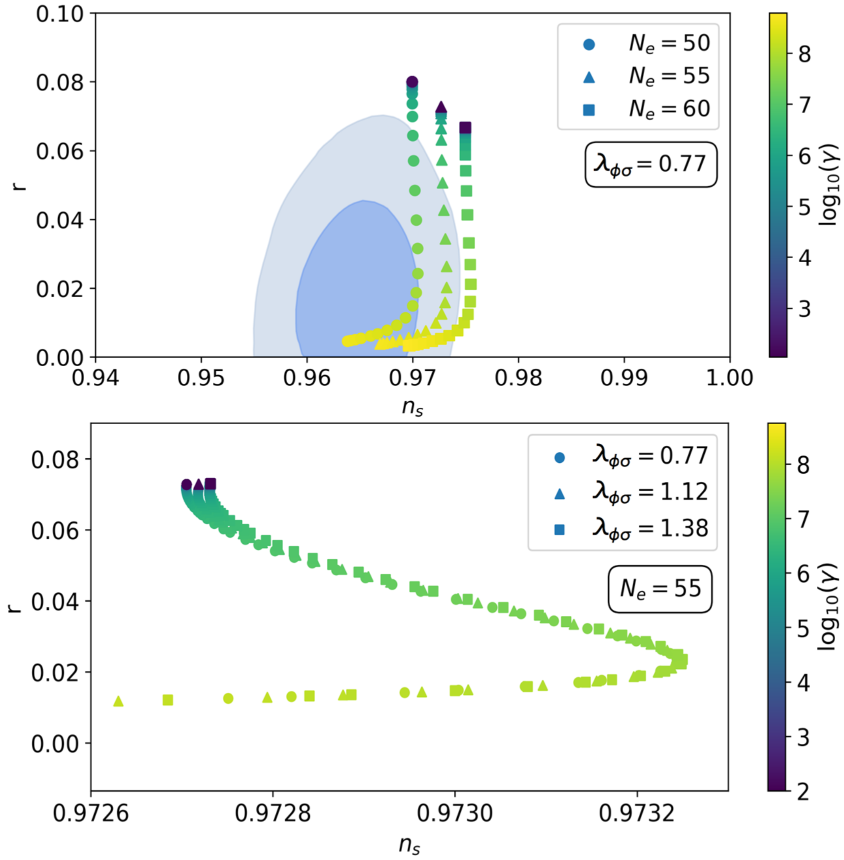


Figure 3.3: Predictions for the scalar spectral index n_s vs. the tensor-to-scalar ratio r that satisfy the constraint (3.36) with varying e-folds N_e (top) and varying $\lambda_{\phi\sigma}$ (bottom), where $\beta_\sigma = 1$ and $\lambda_\phi = 0.005$ for all points. Planck TT,TE,EE+lowE+lensing+BK15 68% and 95% CL regions taken from [43, 44] are indicated by the blue regions in the top panel.

The observables above are constrained by the latest Planck mission data [42, 43] and are determined by the values of the couplings $\lambda_\phi, \lambda_{\phi\sigma}, \beta_\phi, \beta_\sigma, \gamma$, as well as the renormalization scale μ whose value is fixed through the experimentally determined value of $M_{\rm Pl}$ and its definition in (2.48). Additionally, as a result of choosing the flat direction towards σ when calculating the effective potential in Section 2.3 (see (2.37)), λ_ϕ and β_σ turn out to be essentially irrelevant for inflation, so we set them to the realistic values $\lambda_\phi = 0.005$ and $\beta_\sigma = 1$. We also assume the well-established value of $N_e \approx 50 - 60$ e-folds from CMB horizon exit until the end of inflation, allowing us to further constrain the parameter space spanned by $\lambda_{\phi\sigma}$, β_ϕ, and γ so that

$$\ln\left(10^{10} A_s\right) = 3.044 \pm 0.014 \tag{3.36}$$

is satisfied in line with the Planck data [42, 43]. This rather stringent constraint may be used to effectively remove one free parameter from the model, so we thus eliminate β_ϕ in favor of γ and take $\gamma_{\max} \approx 10^9$. All of the parameter dependence in this model may then be nicely expressed in the n_s–r plane as displayed in Figure 3.3. Interestingly, it turns out that the lower end (larger γ) of the predictions displayed there end up corresponding to those of R^2 Starobinsky inflation [190–192], while the upper end (smaller γ) enters the regime of linear chaotic inflation [193–195], implying that the present model somehow interpolates between the two theories.

With our results in hand, it is worthwhile to take a moment and compare them to other works on inflation in scale-invariant models. Some studies such as [29, 39, 96, 196–200] do not explicitly obtain their inflationary potential from the Coleman-Weinberg mechanism as we do, though others employ similar strategies [37, 40, 201–206]. The most similar of these are [203, 204] but there are still key differences between the derivations of their potentials and ours. Whereas we demonstrate the spontaneous breakdown of SI in the original Jordan frame action, then go to the Einstein frame to derive our potential, both of the above mentioned works implicitly assume that scale invariance is broken in order to perform a Weyl rescaling to the Einstein frame where they then employ the Gildener-Weinberg approach and encounter symmetry breaking. Though in practice one often finds physical equivalence between the Jordan and Einstein frames, it is important to remember that this is not always strictly the case, particularly when the metric enters as quantum mechanical DOF [207, 208]. In the present case based on the action (2.36) (where we have assumed a vanishingly small Weyl curvature coupling κ), gravity is indeed treated classically and the possible inequivalence is of no concern, however, it is important to avoid making assumptions about SSB when gravitational DOFs enter the discussion, as they will in the next section.

3.4 Inflation with spin-2 ghosts

In the previous sections we have assumed that $\kappa \approx 0$ so that contributions from the Weyl tensor may be neglected, as is very commonly done for semi-classical treatments of quadratic gravity. The principle reason that the Weyl tensor term is so often swept under the rug is that, due to the fourth-order derivatives of the metric inside, it propagates massive spin-2 DOFs in addition to the standard massless graviton. The trouble with these extra massive DOFs is that they are "ghosts" which enter with a relative minus sign on their kinetic term in the action and represent a serious threat to unitarity when gravity enters into the quantum picture. However, as we will see shortly, they may also present positive phenomenological features. The next chapter in this work will be devoted to an in-depth look at the role of these extra gravitational DOFs and how unitarity may be established in their presence, so for the time being we will set this issue aside and look at how the scale-invariant picture changes when they are allowed to propagate.

3.4.1 The "minimal" action

To begin, we recall that in the $\kappa \approx 0$ version of our scale-invariant model, it was necessary to introduce two BSM scalars in order to successfully achieve dynamical generation of the Planck mass. As we saw, the first of these scalars, ϕ, ends up playing the additional role of inflaton while the massless σ does not play much of a role beyond helping to generate the required one-loop effective potential. One may then naturally wonder if including σ in the picture is necessary since other scalars also exist in the theory, however, it turns out that neither the scalaron S nor the Higgs can generate the required scale symmetry breaking potential, even though they may lead to satisfactory inflationary potentials independently of the present scale-invariant setup [190–192, 209].

As we have already alluded to, there are additional DOFs coming from the gravitational part of the action that may in fact fill the role of σ when the Weyl coupling κ is allowed to take a natural value. To see this explicitly, we consider the following "minimal" version of the action (2.36) where scale-invariant quadratic gravity is coupled only to ϕ,

$$S_{\mathrm{SImin}} = \int \mathrm{d}^4x\,\sqrt{-g}\bigg(-\frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - \frac{\lambda}{4}\phi^4 - \kappa C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} - \gamma R^2 + \frac{\beta}{2}\phi^2 R\bigg)\,. \tag{3.37}$$

As before, this action is invariant under infinitesimal local diffeomorphisms in addition to the global scale transformations

$$g_{\alpha\beta} \;\to\; \Omega^2 g_{\alpha\beta} \qquad\qquad \phi \;\to\; \Omega^{-1}\phi\,, \tag{3.38}$$

where Ω is a constant. Naturally, one may also include Higgs interactions and BSM fields such as heavy right-handed neutrinos in this picture to recreate the same kind of results displayed in Section 2.3, but in this section we will focus on just the gravity-dilaton(inflaton) action above that is "minimal" in the sense that it contains no additional scalar σ and not in the sense that this extra physics is not being discussed.

To derive the effective one-loop potential for this theory, we proceed as we did previously by expanding the dynamical fields in our theory as quantum perturbations around classical backgrounds. For the scalar this means writing

$$\phi \;\to\; \phi + \varphi\,, \tag{3.39}$$

where $\phi \approx$ const. for the purposes of deriving the effective potential. As our goal now is to put gravity on the same footing as the other fields in our theory, we perform an analogous expansion of the metric,

$$g_{\alpha\beta} \;\to\; \eta_{\alpha\beta} + h_{\alpha\beta}\,, \tag{3.40}$$

where $\eta_{\alpha\beta}$ is the Minkowski metric and $h_{\alpha\beta}(x)$ is a small quantum perturbation. Under these expansions, the part of the action (3.37) that is quadratic in the fluctuations $h_{\alpha\beta}$ and φ is given by

$$\begin{aligned} S^{(0)}_{\mathrm{SImin}} = \int \mathrm{d}^4x \Bigg[& \frac{1}{2}\varphi(\Box - 3\lambda\phi^2)\varphi - \frac{\kappa}{6}h^{\alpha\beta}\Big(3\Box^2 h_{\alpha\beta} - 6\Box\partial_\beta\partial^\gamma h_{\alpha\gamma} + 2\partial_\alpha\partial_\beta\partial_\gamma\partial_\delta h^{\gamma\delta} \\ & - \eta_{\alpha\beta}\Box\big(\Box h_\beta{}^\beta - 2\partial_\beta\partial_\gamma h^{\beta\gamma}\big)\Big) - \gamma h^{\alpha\beta}\Big(\partial_\alpha\partial_\beta\partial_\gamma\partial_\delta h^{\gamma\delta} \\ & + \eta_{\alpha\beta}\Box\big(\Box h_\beta{}^\beta - 2\partial_\beta\partial_\gamma h^{\beta\gamma}\big)\Big) + \frac{\beta}{8}h^{\alpha\beta}\Big(8\phi\big(\partial_\alpha\partial_\beta - \Box\eta_{\alpha\beta}\big)\varphi \\ & + \phi^2\Big(\Box h_{\alpha\beta} - 2\partial_\beta\partial^\gamma h_{\alpha\gamma} - \eta_{\alpha\beta}\big(\Box h_\beta{}^\beta - 2\partial_\beta\partial_\gamma h^{\beta\gamma}\big)\Big)\Big)\Bigg], \end{aligned} \tag{3.41}$$

where we have integrated by parts and omitted terms related to the tree-level cosmological constant generated by ϕ.

As mentioned at the beginning of this section, the graviton $h_{\alpha\beta}$ in the action above actually contains additional DOFs beyond the standard massless spin-2 graviton due to the four-derivative nature of quadratic gravity. We may expose these DOFs by performing a York decomposition of the full gravitational perturbation as

$$h_{\alpha\beta} = \bar{h}_{\alpha\beta} + \partial_\alpha V_\beta + \partial_\beta V_\alpha + \left(\partial_\alpha\partial_\beta - \frac{1}{4}\eta_{\alpha\beta}\Box\right)a + \frac{1}{4}\eta_{\alpha\beta}h_\gamma{}^\gamma\,, \tag{3.42}$$

where $\bar{h}_{\alpha\beta}(x)$ is a transverse-traceless tensor mode ($\partial_\beta\bar{h}_\alpha{}^\beta = \bar{h}_\alpha{}^\alpha = 0$), $V(x)$ is a transverse vector mode ($\partial_\alpha V^\alpha = 0$), and $h_\alpha{}^\alpha(x)$ and $a(x)$ are independent scalar modes [210]. After rewriting these scalars in terms of the gauge-invariant quantity

$$S = h_\alpha{}^\alpha - \Box a\,, \tag{3.43}$$

which corresponds to the quantum fluctuations of the scalaron (3.18) defined in the last section, we see from the decomposed action

$$\begin{aligned} S^{(0)}_{\mathrm{SImin}} = \int \mathrm{d}^4x \bigg(& \frac{1}{2}\varphi(\Box - m_\phi^2)\varphi - \frac{\kappa}{2}\bar{h}^{\alpha\beta}\Box(\Box - m_h^2)\bar{h}_{\alpha\beta} \\ & - \frac{9\gamma}{16}S\Box(\Box - m_S^2)S - \frac{3\beta\phi}{4}\varphi\Box S\bigg)\,, \end{aligned} \tag{3.44}$$

that the decomposition (3.42) actually amounts to a gauge fixing in the gravitational sector, as all of the quadratic terms containing V_α, $h_\alpha{}^\alpha$, and a cancel out identically.

In the action (3.44) above, we have identified the ϕ-dependent masses

$$m_\phi^2 = 3\lambda\phi^2 \qquad m_S^2 = \frac{\beta}{12\gamma}\phi^2 \qquad m_h^2 = \frac{\beta}{4\kappa}\phi^2\,, \tag{3.45}$$

and we restate that for the purposes of deriving the effective potential, ϕ should be considered an approximately constant (classical) background field. Though ϕ's value is as of yet unspecified, its VEV v_ϕ that will be derived in what follows will fix these masses up to the renormalization scale.

3.4.2 The effective potential

The effective potential containing contributions from the scalar and tensor sectors may now be derived using standard Coleman-Weinberg techniques [11]. As before, this involves integrating out the fluctuations $\Phi_A = \{\varphi, S, \bar{h}_{\alpha\beta}\}$ and since the part of the functional integral that is quadratic in Φ_A is Gaussian, we find that the one-loop contributions amount to

$$\begin{aligned} U_{\rm CW}(\phi, \eta_{\alpha\beta}) &= -\frac{i}{2}\ln\left[\mathrm{Det}\left(\frac{\delta^2 S_{\rm quad}}{\delta\Phi^A\delta\Phi^B}\right)\right] \\ &= -\frac{i}{2}\ln\left[\mathrm{Det}M\right] - \frac{i}{2}\ln\left[\mathrm{Det}\Big(\delta_{\alpha\beta\gamma\delta}\Box\big(-\Box + m_h^2\big)\Big)\right], \end{aligned} \tag{3.46}$$

where we have used the shorthand $\delta_{\alpha\beta\gamma\delta} = \frac{1}{2}(\eta_{\alpha\gamma}\eta_{\beta\delta} + \eta_{\alpha\delta}\eta_{\beta\gamma})$. Though the dependence on $\eta_{\alpha\beta}$ in the potential above is similar to the background dependence on ϕ, it should be obviously understood and we will suppress it moving forward.

The first term in (3.46) describes the off-diagonal scalar sector with the Hessian matrix

$$M = \begin{pmatrix} -\frac{9\gamma}{8}\Box\left(\Box - m_S^2\right) & -\frac{3}{4}\beta\phi\Box \\ -\frac{3}{4}\beta\phi\Box & \Box - m_\phi^2 \end{pmatrix}, \tag{3.47}$$

where the log can be rewritten using the standard "$\ln\mathrm{Det} = \mathrm{Tr}\ln$" trick as

$$\ln(\mathrm{Det}M) = \mathrm{Tr}\big[\ln\big(\Box - m_+^2\big)\big] + \mathrm{Tr}\big[\ln\big(\Box - m_-^2\big)\big] + \cdots \tag{3.48}$$

with the "$\cdots$" representing irrelevant constant terms that are independent of ϕ. Here we have identified the mass eigenvalues of the matrix M,

$$m_\pm^2 = \frac{1}{2}\left(m_\phi^2 + (1+6\beta)m_S^2\right) \pm \frac{1}{2}\sqrt{\left(m_\phi^2 + (1+6\beta)m_S^2\right)^2 - 4m_\phi^2 m_S^2}\,, \tag{3.49}$$

which agree with the values of the Einstein frame mass eigenstates calculated in [51]. With this we may next rewrite the trace in (3.48) as a sum of the momentum space eigenvalues of the operators $\ln\big(\Box - m_\pm^2\big)$ and evaluate the resulting expression using dimensional regularization under $\overline{\rm MS}$ [139, 153] to yield

$$U_{\rm scal}(\phi) = -\frac{i}{2}\sum_{j=\pm}\int\frac{\mathrm{d}^4p}{(2\pi)^4}\ln\left(p^2 + m_j^2\right) = \sum_{j=\pm}\frac{1}{64\pi^2}m_j^4\left[\ln\left(\frac{m_j^2}{\mu^2}\right) - \frac{3}{2}\right]. \tag{3.50}$$

This sum over mass eigenstates then represents the one-loop contribution to the effective potential from the scalar sector, where μ is the renormalization scale and divergent terms have been absorbed into the renormalized constant λ.

Contributions from the tensor sector may be calculated in a similar fashion, starting by rewriting the last term in (3.46) as

$$\ln\left[\mathrm{Det}\Big(\delta_{\alpha\beta\gamma\delta}\Box\big(-\Box + m_h^2\big)\Big)\right] = \mathrm{Tr}\big[\ln\big(\delta_{\alpha\beta\gamma\delta}\big(\Box - m_h^2\big)\big)\big] + \cdots\,, \tag{3.51}$$

where the $\mathrm{Tr}\ln(-\Box)$ term has been relegated to the "$\cdots$" since it is independent of ϕ, leaving only the massive (ghostly) term to contribute in this sector. It is important to note that there is no troublesome minus sign related to the ghost in this context since it has been associated with the massless inverse propagator. This in turn implies that the ghost contributes to the effective potential just as a normal particle would, a fact which is consistent with the calculation of the quartic beta function β_λ [51]. With this we may transition to momentum space which, due to the tensorial nature of the inverse spin-2 propagator, requires that we write

$$\bar{h}^{\alpha\beta}\delta_{\alpha\beta\gamma\delta}\bar{h}^{\gamma\delta} = \bar{h}^{\alpha\beta}P^{(2)}_{\alpha\beta\gamma\delta}\bar{h}^{\gamma\delta}\,, \tag{3.52}$$

where we have used the transverse-traceless nature of $\bar{h}_{\alpha\beta}$ to write its contribution in terms of the purely spin-2 projection operator defined by

$$P^{(2)}_{\alpha\beta\gamma\delta} = \frac{1}{2}\big(\theta_{\alpha\gamma}\theta_{\beta\delta} + \theta_{\alpha\delta}\theta_{\beta\gamma}\big) - \frac{1}{d-1}\theta_{\alpha\beta}\theta_{\gamma\delta} \qquad \theta_{\alpha\beta} = \eta_{\alpha\beta} - \frac{p_\alpha p_\beta}{p^2}\,, \tag{3.53}$$

as outlined in [211]. This rewriting allows us to correctly count the five DOFs expected from a massive spin-2 field in four dimensions, which is confirmed by noting

$$\mathrm{Tr}\big(P^{(2)}_{\alpha\beta\gamma\delta}\big) = \delta^{\alpha\beta\gamma\delta}P^{(2)}_{\alpha\beta\gamma\delta} = \frac{1}{2}(d+1)(d-2)\,. \tag{3.54}$$

With all of the above considerations, dimensional regularization may be carried out under $\overline{\mathrm{MS}}$ just as in the scalar sector and we find that the massive spin-2 contribution to the effective potential is given by

$$\begin{aligned} U_h(\phi) &= -\frac{i}{2}\lim_{d\to 4}\left[\mu^{4-d}\int\frac{\mathrm{d}^d p}{(2\pi)^d}\frac{1}{2}(d+1)(d-2)\ln\left(\frac{p^2+m_h^2}{p^2}\right)\right] \\ &= \frac{5}{64\pi^2}m_h^4\left[\ln\left(\frac{m_h^2}{\mu^2}\right) - \frac{1}{10}\right]. \end{aligned} \tag{3.55}$$

Our final step is assemble the entire effective potential,

$$U_{\mathrm{eff}}(\phi) = \frac{\lambda}{4}\phi^4 + U_{\mathrm{scal}}(\phi) + U_h(\phi) + U_\Lambda\,, \tag{3.56}$$

which includes the tree-level quartic term, one-loop contributions from the scalar and tensor sectors, and the arbitrary constant background U_Λ which, just as in the previous study, is a free parameter that we will tune to ensure that the classical zero-point energy vanishes when scale invariance is broken spontaneously.

To see this breaking in the present model, we first write (3.56) in the form

$$U_{\mathrm{eff}}(\phi) = g_\phi\left(2\ln\left(\frac{\phi^2}{\mu^2}\right) + f_\phi - 1\right)\phi^4 + U_\Lambda\,, \tag{3.57}$$

where similarly to (2.45, 2.46), f_ϕ and g_ϕ are combinations of the dimensionless coupling constants λ, κ, γ, and β given by

$$\begin{aligned} f_\phi = \frac{\beta^2}{g_\phi}\Bigg[&\frac{1}{36864\pi^2\gamma^2\kappa^2}\left(45\gamma^2\left(\ln\left(\frac{12\kappa}{\beta}\right)+\ln(\lambda)-\frac{7}{5}\right)\right. \\ &\left.+\kappa^2\left(\ln\left(\frac{36\gamma}{\beta}\right)+\ln(\lambda)\right)\right)+\frac{\lambda}{16\beta^2}\Bigg]+\frac{1}{2}\ln(3\lambda)-\frac{1}{2} \end{aligned} \tag{3.58}$$

$$g_\phi = \frac{1}{18432\pi^2}\left[\beta^2\left(\frac{1}{\gamma^2}+\frac{45}{\kappa^2}\right)+1296\lambda^2\right]. \tag{3.59}$$

With this, the VEV of ϕ may be identified as the minimum of this potential in the usual way:

$$\left.\frac{\partial U_{\text{eff}}(\phi)}{\partial\phi}\right|_{\phi=v_\phi} = 0 \qquad \Rightarrow \qquad v_\phi = \mu e^{-f_\phi}\,. \tag{3.60}$$

Thus, due to the non-zero value of v_ϕ, we find that scale invariance has indeed been broken spontaneously in this setup where no contribution from an additional σ-like scalar is present. In the previous chapter we saw how σ is required to successfully realize SSB when gravity is treated classically, however, the massive spin-2 ghost now very naturally fills the same role when gravity is included in the quantum picture. Though this is a novel consideration, it should be noted that in retrospect, this type of phenomena may have been anticipated from analysis of the renormalization group equations in this type of model where it is also possible to account for a dynamical solution to the cosmological constant problem [51, 212].

With the above value of v_ϕ in hand, we may also address the cosmological constant problem in our more simplistic method where U_Λ is fixed according to

$$U_{\text{eff}}(v_\phi) = 0 \qquad \Rightarrow \qquad U_\Lambda = -g_\phi v_\phi^4\,. \tag{3.61}$$

To reiterate the discussion at the end of the Section 3.3.2; deriving the effective potential and establishing SSB in the Jordan frame as we have done here ensures that when the cosmological constant is canceled by U_Λ in this way, it will remain zero after we go to the Einstein frame.

Finally, the dynamically generated value of the Planck mass in this setup may be identified in terms of what will become the canonical Einstein term as

$$M_{\text{Pl}}^2 = \beta v_\phi^2\,. \tag{3.62}$$

This expression may be contrasted with (2.48) which contains extra contributions proportional to $U_{(1)}(v_\phi)$ that originate from our expansion in powers of the classical Ricci scalar. This kind of expansion is unnecessary in the present theory where gravitational contributions have been accounted for in the effective potential, thus implying that the extra term in (2.48) is implicitly included in the present value of v_ϕ. It should however be noted that, even though an expansion in terms of R is no longer necessary when gravity is treated quantum mechanically, there is still the additional expansion of the metric in terms of the graviton that essentially takes its place.

3.4.3 Inflationary predictions

We saw in Sections 3.2 and 3.3 that the same potential which spontaneously breaks scale symmetry may also represent a satisfactory inflationary potential and the situation is no different here. Many of the considerations that were employed previously naturally apply here as well, so we will gloss over many of the details of deriving inflationary predictions that have already been stated, however, we may still proceed from our derivation of the effective potential by using it to assemble the one-loop effective action in the Jordan frame,

$$S^J_{\rm eff} = \int \mathrm{d}^4x\,\sqrt{-g}\Big(-\frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - \kappa C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} - \gamma R^2 + \frac{\beta}{2}\phi^2 R - U_{\rm eff}(\phi)\Big)\,. \quad (3.63)$$

With this, we may transform to the Einstein frame by introducing and auxiliary field that exposes the *classical* scalaron buried in R^2 and performing a Weyl rescaling to yield

$$S^E_{\rm inf} = \int \mathrm{d}^4x\,\sqrt{-g}\Big(-\frac{1}{2}F^2(\phi)\partial_\alpha\phi\partial^\alpha\phi - \kappa C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} + \frac{M^2_{\rm Pl}}{2}R - U_{\rm inf}(\phi)\Big)\,, \quad (3.64)$$

where $F(\phi)$ is a function that quantifies the modification to the kinetic term for ϕ brought on by the Weyl rescaling,

$$F^2(\phi) = \frac{1}{\big(1+4A(\phi)\big)B(\phi)}\left[1 + \frac{3M^2_{\rm Pl}\Big(\big(1+4A(\phi)\big)B'(\phi) + 4A'(\phi)B(\phi)\Big)^2}{2\big(1+4A(\phi)\big)B(\phi)}\right]\,, \quad (3.65)$$

and A and B are additional functions of the scalar field,

$$A(\phi) = \frac{4\gamma U_{\rm inf}(\phi)}{B^2(\phi)M^4_{\rm Pl}} \qquad\qquad B(\phi) = \frac{\beta\phi^2}{M^2_{\rm Pl}}\,. \quad (3.66)$$

One may note that the scalaron is not present in the action (3.64), which is simply due to the fact that the effective potential in the Einstein frame exhibits a valley structure just as was discuss in detail in Section 3.3.1, thus allowing us to eliminate it from the action in favor of ϕ provided that the scalaron is heavy enough to stabilize the associated contour during slow roll. For the easy comparison of results, we assume that the mass hierarchy works out in this fashion for the scalars in this model as well, thus leading us to the inflationary potential

$$U_{\rm inf}(\phi) = \frac{M^4_{\rm Pl}U_{\rm eff}(\phi)}{\beta^2\phi^4 + 16\gamma U_{\rm eff}(\phi)}\,. \quad (3.67)$$

This potential allows us to compute predictions for the scalar power spectrum amplitude A_s, the scalar spectral index n_s, and the tensor-to-scalar ratio r defined in (3.35), in terms of the slow-roll parameters (3.35, 3.34). These predictions are displayed in Figure 3.4 where we have also accounted for additional small corrections to the tensor-to-scalar ratio with the replacement

$$r \;\to\; r\left(1 + \frac{2H^2}{m_h^2}\right)^{-1} \approx r\left(1 + \frac{2U_{\rm inf}(\phi^*)}{3M^2_{\rm Pl}m_h^2}\right)^{-1}\,, \quad (3.68)$$

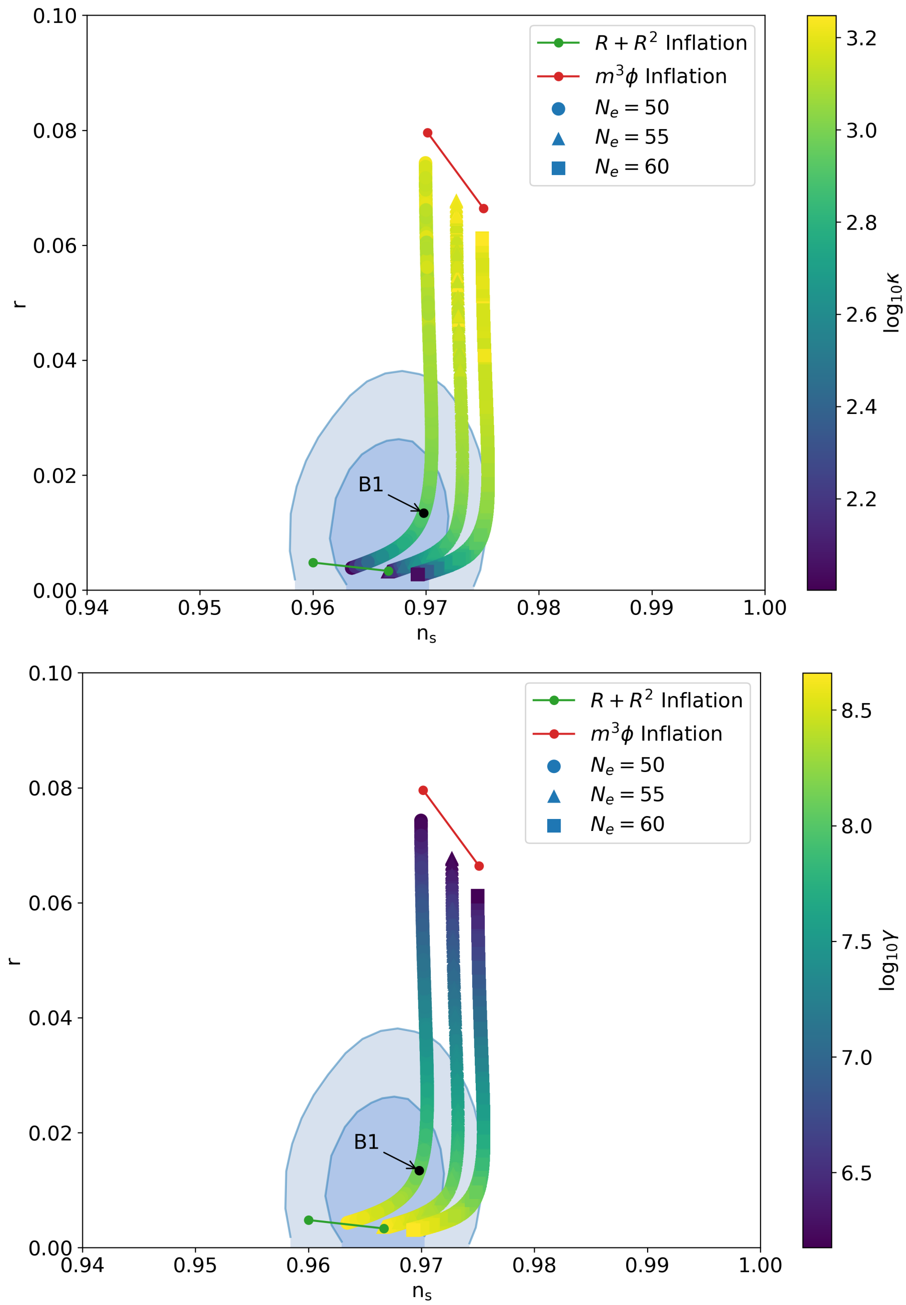


Figure 3.4: Predictions for the scalar spectral index n_s vs. the tensor-to-scalar ratio r that satisfy the constraint (3.36) for a range of e-folds N_e, with varying coupling constants in the ranges (3.69). Planck TT,TE,EE+lowE+lensing+BK15 68% and 95% CL regions taken from [43, 44] are indicated by the blue regions in each panel. Representative predictions from the Starobinsky model [190–192] (green) and linear inflation [193–195] (red) are also included for easy comparison.

as suggested in [212]. These corrections arise from classical non-CW effects that are known to appear when considering the Weyl tensor term in a de Sitter background [213–215].

Just as in the previous analysis, the parameter space has been constrained so as to produce results which fit within the latest experimental data from the Planck satellite mission [43, 44], which includes an assumption that inflation lasts for $N_e \approx 50 - 60$ e-folds and that the scalar power spectrum amplitude satisfies $\ln\big(10^{10} A_s\big) = 3.044 \pm 0.014$. These requirements result in a viable parameter space spanned by the ranges

$$\lambda = 0.005 \qquad \beta \in [10^3, 10^4] \qquad \gamma \in [10^3, 10^9] \qquad \kappa \in [10^2, 10^{3.25}]\,, \tag{3.69}$$

which guarantee that the logarithms such as $\ln(\phi^*/v_\phi)$ which appear in the inflationary potential do not grow to non-perturbative values during inflation. In other words, the choice of ranges above ensure the one-loop potential represents a good approximation during inflation, which further implies that any additional unaccounted for RG-running effects are negligible. To get a better feeling for the best case situation at hand, we have also singled out a representative benchmark point corresponding to the values

$$\mathrm{B1}: \;\lambda = 0.005 \qquad \beta = 5.62 \times 10^2 \qquad \gamma = 1.22 \times 10^8 \qquad \kappa = 837\,, \tag{3.70}$$

which is labeled as "B1" in both plots of Figure 3.4.

Special focus has been put on the higher derivative coupling constants κ and γ in Figure 3.4 by indicating their ranges with color gradients in order to better illustrate the effects of including general C^2 and R^2 terms in the action. In this form it is clear that there is a large subset of the parameter space (3.69) that rests within even the most stringent Planck and BICEP/Keck constraints over the full range of possible e-folds. Interestingly, just as was pointed out in the last inflationary analysis, the present theory seems to interpolate very nicely between the analogous results of Starobinsky [190–192] and linear chaotic inflation [193–195], as we have pointed out explicitly in this set of plots.

It is also instructive to get an order of magnitude estimate for the masses of the gravitational fields in our theory. This is easily done by setting $\phi = v_\phi$ in the relations (3.45) which, after also taking the benchmark values (3.70) for the coupling constants, yields the numerical values

$$m_S \approx 10^{14}\,\mathrm{GeV} \qquad\qquad m_h \approx 10^{17}\,\mathrm{GeV}\,, \tag{3.71}$$

which we note do not change by more than about an order of magnitude for any of the parameter combinations in (3.69). As is made clear in Figure 3.4, higher values of γ correspond to lower values of m_S which in turn correspond to lower values of r. Smaller r is not only preferable from a phenomenological point of view, but it also means that the ghost mass will be relatively larger since $m_h^2 \propto 1/\kappa$. This all amounts to a novel consideration in scale-invariant models, namely, that a very heavy ghost is simultaneously able to aid in generating all the important scales in physics through SSB and is able to generate a low value for the tensor-to-scalar ratio in line with modern observations.

There is even more to the story however, as it turns out that a very heavy spin-2 ghost is not only phenomenologically preferred, but is strictly theoretically necessary for the present kind of model to be considered viable. In the following chapters we will demonstrate this fact explicitly by deriving a limit on the energy of interactions in quadratic gravity that may be considered perturbatively unitarity, which corresponds precisely to the mass of the ghost. For now we may simply state that, luckily for the current analysis, all the energy scales associated with inflation (which usually have a maximum of approximately 10^{15} GeV [178]) sit well below the mass of the ghost.

Chapter 4

The Ghost Problem

So far we have seen the most intriguing features of scale-invariant theories on display, but have glossed over what is perhaps the biggest theoretical roadblock standing in the way of their widespread adoption – the issue of establishing unitarity in their gravitational sectors. We will begin to tackle this topic here after first introducing the Ostrogradsky instability and ghost problem with a concrete mechanical example, being careful to distinguish between the classical and quantum levels. Though they are of course related, it is important to distinguish between the theoretical issues that present themselves in each regime as, naturally, there are relevant quantum mechanical phenomena which have no classical counterpart. We will also introduce the notion of conditional unitarity that was established in [3] and review some of the most promising resolutions to the ghost problem that have appeared in recent literature.

Once we have a good idea of the problem that we are facing, we will see exactly how it presents itself in theories of scale-invariant quadratic gravity. This involves establishing a novel quantization of the theory in the covariant operator formalism that will follow after an introduction to the general process. We will perform such a quantization on both globally scale-invariant QG after SSB (where a massive ghost will appear) and on locally invariant conformal gravity (which presents a massless ghost) in order to compare and contrast how the ghost problem appears in both theories.

4.1 The Ostrogradsky instability

To begin, let us consider the following action describing the motion of a time-dependent 3D "coordinate" $\boldsymbol{z}(t)$,

$$S_{\mathrm{OI}} = \int \mathrm{d}t \bigg(-\frac{1}{2\omega^2}\ddot{\boldsymbol{z}}^2 + \frac{1}{2}\dot{\boldsymbol{z}}^2 - V\big(\boldsymbol{z}\big) \bigg) \,. \tag{4.1}$$

This action exhibits an Ostrogradsky instability due to the fact that it is fourth-order in derivatives, and may thus serve as a toy model of classical quadratic gravity for our purposes. Actions like (4.1) have been well-studied in the past and are known as Pais-Uhlenbeck (PU) oscillators [216].

Though it is possible to investigate the Ostrogradsky instability directly from (4.1) in its fourth-order form, it is more convenient to first transform the action into an equivalent second-order form so that the instability may be analyzed in a more familiar language. This is achieved via the introduction of an auxiliary "coordinate" $\boldsymbol{y}(t)$ and the action

$$S_{\text{OIaux}} = \int \mathrm{d}t \biggl(-\sqrt{m}\ddot{\boldsymbol{z}} \cdot \boldsymbol{y} + \frac{m\omega^2}{2}\boldsymbol{y}^2 + \frac{1}{2}\dot{\boldsymbol{z}}^2 - V(\boldsymbol{z}) \biggr) . \tag{4.2}$$

We may integrate $\boldsymbol{y}$ out of this action using its equation of motion, $\boldsymbol{y} = 1/(\sqrt{m}\omega^2)\ddot{\boldsymbol{z}}$, and find that (4.2) is physically equivalent to (4.1). It is also instructive to further redefine $\boldsymbol{z}$ as

$$\boldsymbol{z} = \sqrt{m}(\boldsymbol{x} - \boldsymbol{y}) \tag{4.3}$$

in order to obtain the equivalent diagonalized action

$$S_{\text{OIdiag}} = \int \mathrm{d}t \biggl(\frac{m}{2}\bigl(\dot{\boldsymbol{x}}^2 - \dot{\boldsymbol{y}}^2 + \omega^2\boldsymbol{y}^2\bigr) - V\bigl(\boldsymbol{x} - \boldsymbol{y}\bigr) \biggr) , \tag{4.4}$$

where we have neglected total derivatives.

In this form we see a crucial feature of higher derivative theories made manifest – they generally propagate more degrees of freedom than one might naively assume from looking at only the bare fourth-order action. The appearance of these additional independent DOFs may be understood in terms of a Cauchy problem wherein the additional derivatives (as compared to the standard two) imply that more independent initial conditions are required to solve the equations of motion. Moreover, the separated DOFs appear with opposite sign kinetic terms. We refer to the coordinate with a canonically negative kinetic term (here $\boldsymbol{y}$) as a ghost. It is also important to note that the mass term for the ghost in (4.4) is also negative as compared to that of a healthy particle, thus distinguishing this scenario from a tachyonic instability. As we will see in later sections, the scenario presented above serves as a direct analogy to quadratic gravity after SSB where the four derivatives that act on the metric may be rewritten to describe a "healthy" massless spin-2 field (the graviton) and massive spin-2 ghost.

With the second-order version of our toy theory established, the precise nature of the classical Ostrogradsky instability becomes clear. From (4.4), we may derive the equations of motion

$$m\frac{\mathrm{d}^2\boldsymbol{x}}{\mathrm{d}t^2} = -\nabla_{\boldsymbol{x}}V \qquad\qquad m\frac{\mathrm{d}^2\boldsymbol{y}}{\mathrm{d}t^2} = \nabla_{\boldsymbol{y}}V - m\omega^2\boldsymbol{y} , \tag{4.5}$$

and note that, due to the sign of the $\boldsymbol{y}$ kinetic term, the force $\nabla_{\boldsymbol{y}}V$ has the opposite sign as the force $-\nabla_{\boldsymbol{x}}V$. This feature is the root of the instability, which may be seen even more explicitly by writing $V(\boldsymbol{z}) = V(|\boldsymbol{x} - \boldsymbol{y}|)$ per the definition (4.3). This leads to the relation

$$\nabla_{\boldsymbol{x}}V = -\nabla_{\boldsymbol{y}}V = \frac{\boldsymbol{x} - \boldsymbol{y}}{|\boldsymbol{x} - \boldsymbol{y}|}V' , \tag{4.6}$$

where $V' = \mathrm{d}V/\mathrm{d}|\boldsymbol{x}-\boldsymbol{y}|$, which indicates that if the force $-\nabla_{\boldsymbol{x}}V$ is a restoring force, then $\nabla_{\boldsymbol{y}}V$ is necessarily an anti-restoring force leading to a run-away instability in $\boldsymbol{y}$. Of course we must also consider the restoring force originating from the mass term since if $m\omega^2|\boldsymbol{y}| > |\nabla_{\boldsymbol{y}}V|$ for some finite range of values of $|\boldsymbol{y}|$, then the runaway of $\boldsymbol{y}$ may be avoided. We also note that this behavior exists for large class of different potentials and that it has been shown that it is possible to avoid the run-away instability with several different specific potentials [217–219].

It is instructive to further analyze the behavior of this system in the Hamiltonian formalism as it will serve as a nice link to the quantum version of the problem. The classical Hamiltonian for the Pais-Uhlenbeck system described above is given by

$$\mathcal{H} = \frac{1}{2m}\left(\boldsymbol{p}^2 - \boldsymbol{q}^2\right) - \frac{m\omega^2}{2}\boldsymbol{y}^2 + V\left(|\boldsymbol{x}-\boldsymbol{y}|\right), \tag{4.7}$$

where the canonical momentum for each coordinate is defined in the conventional manner as $\boldsymbol{p} = m\dot{\boldsymbol{x}}$ and $\boldsymbol{q} = -m\dot{\boldsymbol{y}}$. Naturally, the total energy of this system is conserved, however, some rather atypical phenomena can occur due to the fact that the ghost's contribution to the total energy is negative.

As an example, consider a scenario where the ghost sits at rest at the origin and the healthy coordinate runs toward the ghost with some impact parameter $\boldsymbol{x} = \{-a, b, 0\}$, $\dot{\boldsymbol{x}} = \{v, 0, 0\}$. Assuming the $1/r$ gravity-style potential $V(|\boldsymbol{x}-\boldsymbol{y}|) = G/|\boldsymbol{x}-\boldsymbol{y}|$, the coordinates' trajectories are uniquely determined and if a is large enough that this gravitational potential energy may be neglected, the initial energy $E_{\text{in}} \simeq (1/2)mv^2$ of the healthy particle corresponds to the approximate total energy. After some finite $t > 0$, the healthy coordinate scatters off the ghost as a free particle, while the ghost begins simple harmonic motion. This would be a very standard situation if not for the relative minus sign between the healthy and ghost parts of the Hamiltonian. A pathology can appear due to this relative minus when the outgoing energy of the healthy coordinate, E_{out}, exceeds the (conserved) total energy due to the ghost's negative contribution. Even in the case where stable motion is achieved (E_{out} is fixed at a finite value) and the ghost does not run away, an outside observer witnesses $\boldsymbol{x}$ scatter off a stationary $\boldsymbol{y}$ with a greater velocity than it approached with. It is precisely this *classical* pathology that we refer to as the Ostrogradsky instability.

4.2 Quantum states with negative norm

4.2.1 Classical correspondence and the vacuum

The classical pathology we have just seen appear in fourth-order systems becomes more subtle and complicated when viewed through the lens of quantum mechanics. The quantum system corresponding to (4.7) may be described by the Schrödinger equation

$$i\frac{\partial\Psi(\boldsymbol{x},\boldsymbol{y},t)}{\partial t} = \mathcal{H}\Psi(\boldsymbol{x},\boldsymbol{y},t), \tag{4.8}$$

where $\Psi(\boldsymbol{x}, \boldsymbol{y}, t)$ is a wave function that satisfies $|\langle\Psi|\Psi\rangle|^2 > 0$ and

$$\mathcal{H} = -\frac{1}{2m}\left(\nabla_{\boldsymbol{x}}^2 - \nabla_{\boldsymbol{y}}^2\right) - \frac{m\omega^2}{2}\boldsymbol{y}^2 + V\left(|\boldsymbol{x} - \boldsymbol{y}|\right) \tag{4.9}$$

is the Hamiltonian operator corresponding to the classical expression (4.7). We may safely assume that this quantum system approaches the Pais-Uhlenbeck model in the classical limit, though it is important to stress that there exists a non-zero probability that the energy of the outgoing healthy particle may now take an arbitrarily large value even if no run-away instability is present. This Schrödinger picture quantization thus fails to define a non-pathological quantum system, reflecting the pathology of its classical counterpart. This quantum version of the pathology that we established in the last section is not the end of the story however.

In the Heisenberg picture of quantum mechanics, where one constructs time-independent state operators and relegates all time-dependence into operators that act on those states, we may define a quantum system that reinterprets the ghostly phenomena in a manner that has no classical correspondence. For the sake of the simplifying the present argument, let us consider the free theory case with $V = 0$ and focus on the ghost with the harmonic oscillator EOM $\ddot{\boldsymbol{y}} + \omega^2\boldsymbol{y} = 0$ and asymptotic solution

$$y_j^{\mathrm{as}}(t) = \frac{1}{\sqrt{2m\omega}}\left(\hat{a}_j e^{-i\omega t} + \hat{a}_j^\dagger e^{i\omega t}\right)\,, \tag{4.10}$$

where $\hat{a}_j$ and $\hat{a}_j^\dagger$ are creation and annihilation operators for the ghost state and $j = 1, 2, 3$ stands for the three spatial components of $\boldsymbol{y}$. Using the definition of the momentum $q_j = -m\dot{y}_j$ along with the canonical equal-time commutation relations $[y_j(t), q_k(t')]|_{t=t'} = i\delta_{jk}$, we may derive the ghost commutator

$$\left[\hat{a}_j, \hat{a}_k^\dagger\right] = -\delta_{jk} \tag{4.11}$$

and find that it appears with a relative minus when compared to the analogous relation for the healthy particle. The free Hamiltonian operator for the ghost part of the system is determined from the Heisenberg equation

$$\dot{y}_j^{\mathrm{as}} = i\left[\mathcal{H}_0, y^{\mathrm{as}}\right] \tag{4.12}$$

and given by

$$\mathcal{H}_0 = -\frac{\omega}{2}\sum_j\left(\hat{a}_j\hat{a}_j^\dagger + \hat{a}_j^\dagger\hat{a}_j\right) = -\omega\sum_j\left(\hat{a}_j\hat{a}_j^\dagger + \frac{1}{2}\right)\,. \tag{4.13}$$

Other than the uncharacteristic minus sign that appears in the commutation relation (4.11), all of the above is standard procedure for quantization in the Heisenberg picture, however, there is an often overlooked ambiguity that plays a crucial role when quantizing a ghostly particle. There are in fact two possibilities for how one might define the ground state (vacuum) of the quantum theory,

$$\hat{a}_j |0\rangle_+ = 0 \qquad \text{or} \qquad \hat{a}_j^\dagger |0\rangle_- = 0\,. \tag{4.14}$$

When quantizing a healthy particle in the Heisenberg picture, the first of these options is selected based on the requirement that all energy eigenstates must be positive, however, for a ghost, the choice is not so clear due to the classically negative kinetic energy of the particle. It is important to look at each possibility with care, to which end we note that selection of an annihilation operator also fixes the creation operator and defines the excited n-particle states as

$$|n\rangle_+ = \frac{1}{\sqrt{n!}}\big(\hat{a}_j^\dagger\big)^n |0\rangle_+ \qquad \text{or} \qquad |n\rangle_- = \frac{1}{\sqrt{n!}}\big(\hat{a}_j\big)^n |0\rangle_- \,. \tag{4.15}$$

Using the relation (4.11), we can calculate the inner product of these states,

$${}_+\big\langle n'\big|n\big\rangle_+ = (-1)^n \delta_{nn'} \qquad \text{or} \qquad {}_-\big\langle n'\big|n\big\rangle_- = \delta_{nn'}\,, \tag{4.16}$$

and derive the energy eigenstates associated with each vacuum

$$\mathcal{H}_0 |n\rangle_+ = (n+1/2)\,\omega\,|n\rangle_+ \qquad \text{or} \qquad \mathcal{H}_0 |n\rangle_- = -(n+1/2)\,\omega\,|n\rangle_- \,. \tag{4.17}$$

We thus find that it is in fact the second choice of vacuum, $|0\rangle_-$, that maintains classical correspondence and an equivalency to the Schrödinger picture (positive norm and negative energy eigenvalues), however, we argue that this feature should not take precedence over maintaining positive energy eigenvalues.

We can see that choosing the standard Heisenberg vacuum definition does not directly resolve the ghost problem but rather moves the troublesome ghostly minus sign from the energy eigenvalues to the inner product metric (4.16). It is thus still natural to wonder whether anything is gained by selecting $|0\rangle_+$ since it removes the classical correspondence and association with the Schrödinger picture, however, there is an important corollary related to the $i\epsilon$ prescription in QFT that indicates this is the only logical choice for quantization in the presence of a ghost. To see this explicitly we may consider the propagator

$${}_\pm\langle 0|T y_j^{\rm as}(t) y_k^{\rm as}(t')|n\rangle_\pm = \theta(t-t')\,{}_\pm\langle 0|y_j^{\rm as}(t) y_k^{\rm as}(t')|n\rangle_\pm + (t \leftrightarrow t')\,, \tag{4.18}$$

and employ the identity

$$\theta(t) = \frac{i}{2\pi}\int \mathrm{d}E \frac{e^{-iEt}}{E+i\epsilon} \tag{4.19}$$

to rewrite it as

$${}_\pm\langle 0|T y_j^{\rm as}(t) y_k^{\rm as}(t')|n\rangle_\pm = -\delta_{jk}\frac{i}{2\pi m}\int \mathrm{d}E \frac{e^{-iE(t-t')}}{E^2-\omega^2 \pm i\epsilon}\,. \tag{4.20}$$

If we repeat the process above for the healthy particle, we will arrive at almost the same expression for that propagator with the only differences being the leading minus sign and, crucially, the fact that the two particles only share the same pole structure when the ghost is quantized using $|0\rangle_+$. With the choice $|0\rangle_+$ ($|0\rangle_-$), the pole is located on the lower (upper) half complex plane for positive energy $E = \omega$ and is located on the upper (lower) half complex plane for negative energy. It should also be mentioned that this in turn implies that the negative energy state propagates forward in time and corresponds to a violation of causality for the $|0\rangle_-$ vacuum.

When considering a theory that contains both ghosts and healthy particles it is thus necessary to assign creation and annihilation operators so that the vacuum corresponds to positive energies (whether the norm is negative or not) as this is the only way to guarantee the $i\epsilon$ prescription remains consistent for renormalized Feynman diagrams that contain both species of particle (as suggested by Stelle [57] and Salvio [150]). This prescription is crucial for proving absolute convergence of integrals over the internal momenta and it also plays a key role in showing the existence of the $\epsilon \to 0^+$ limit [220] (see also [221, 222]). In short, we must give precedence to the $|0\rangle_+$ choice of vacuum since it is the one that yields healthy propagators.

4.2.2 Probability interpretation

There is an important corollary to the discussion above regarding the interpretation of probability in the presence of negative norm states that should also be addressed. The notion of probability in QFT is inherently related to the pseudo-unitarity of the S-matrix, which is expressed through the relation

$$S^\dagger S = SS^\dagger = \mathbb{1}\,, \tag{4.21}$$

and comes by virtue of the assumption that the asymptotic "in" and "out" states in a theory form orthonormal bases on the Hilbert space [223]. We also note that, since the S-matrix is simply given by $S = \mathbb{1}$ in the absence of interactions, it is often convenient to parameterize it in terms of the transfer matrix T as

$$S = \mathbb{1} + iT\,, \tag{4.22}$$

so that all non-trivial interactions are described by T. By plugging this expansion into the identity (4.21), we arrive at an expression of the optical theorem,

$$T^\dagger T = i\big(T^\dagger - T\big)\,, \tag{4.23}$$

which implies a fundamental relationship between tree-level interactions and loop-order diagrams.

An understanding of how these considerations define the notion of probability in QFT is best achieved by example. Consider a theory containing an unstable particle Φ that may decay into some other particle ϕ through the interaction term $\mathcal{L}_{\text{int}} \supset g\Phi\phi\phi$ where

g is a real coupling constant. The decay process $\Phi \to \phi\phi$ governed by this interaction term may be described in the S-matrix language by writing

$$S\,|\Phi\rangle = |\Phi\rangle + i\big(g\,C_1\,|\phi\phi\rangle + g^2 C_2\,|\Phi\rangle\,\big)\,, \tag{4.24}$$

where $|\Phi\rangle$ is state vector associated with the particle Φ and $|\phi\phi\rangle$ corresponds to the two particle end state after decay, while C_1 and C_2 are non-zero complex constants that quantify the tree-level decay and one-loop correction to the inverse Φ propagator (one-loop forward amplitude), respectively. With this we apply the standard Born rule (see the later discussion around (4.45)) to interpret the quantities

$$P_{\rm decay} = |g\,C_1|^2 \qquad\qquad P_{\rm live} = |1 + ig^2 C_2|^2 = 1 - 2g^2\,\mathrm{Im}(C_2) + \mathcal{O}(g^3) \tag{4.25}$$

as the probabilities that Φ will decay or continue to propagate.

If both possible end states have positive norms ($\langle\Phi|\Phi\rangle = \langle\phi\phi|\phi\phi\rangle = 1$), then by pseudo-unitarity of the S-matrix (4.21) we may write

$$1 = \langle\Phi|\Phi\rangle = \langle\Phi|S^\dagger S|\Phi\rangle = P_{\rm decay} + P_{\rm live}\,. \tag{4.26}$$

We thus find a logical interpretation of probability where $0 < P_{\rm decay} < 1$ and $0 < P_{\rm live} < 1$. Moreover, the norm of the original Φ has decreased after the interaction as a result of the particle's possible decay,

$$\big|\big\langle\tilde\Phi\big|\tilde\Phi\big\rangle\big|^2 < 1 \qquad \text{where} \qquad \big|\tilde\Phi\big\rangle = (1 + ig^2 C_2)\big|\Phi\big\rangle\,, \tag{4.27}$$

as one should expect. It may also be noted that (4.26) grants a realization of the optical theorem (4.23) through the relation

$$|C_1|^2 = 2\,\mathrm{Im}(C_2)\,, \tag{4.28}$$

which further indicates that $\mathrm{Im}(C_2) > 0$.

This clear interpretation becomes obscured when Φ is a ghost with negative norm ($\langle\Phi|\Phi\rangle = -1$)). The analogous calculation in this case looks like

$$-1 = \langle\Phi|\Phi\rangle = \langle\Phi|S^\dagger S|\Phi\rangle = -1 + g^2|C_1|^2 + 2g^2\,\mathrm{Im}(C_2) = P_{\rm decay} - P_{\rm live}\,. \tag{4.29}$$

Since $P_{\rm decay} > 0$ by the definition (4.25), this implies that $P_{\rm live} > 1$ and that the norm of Φ *increases* after the interaction,

$$\big|\big\langle\tilde\Phi\big|\tilde\Phi\big\rangle\big|^2 > 1\,. \tag{4.30}$$

Needless to say, this behavior makes it impossible to interpret quantum probability in the standard fashion since, taking the above literally, one encounters a process where there is more than a 100% chance to find Φ after its own "decay". The situation is complicated even further by noting that the optical theorem now takes the form $|C_1|^2 = -2\,\mathrm{Im}(C_2)$, so that one must require $\mathrm{Im}(C_2) < 0$. Though there may be some small room for interpretation since the above process is still valid in the sense that C_1 and C_2 may actually be calculated in terms of Feynman diagrams, it is still tricky to reconcile the complete picture including the probability interpretation when ghosts are present in a quantum theory.

4.3 Conditional unitarity

As we have just seen in detail, the quantum version of the Ostrogradsky instability that we refer to as the ghost problem is much more complicated than the pathology related to negative kinetic energy that is present in classical fourth-order systems. When quantization is carried out in the Heisenberg picture, we are actually free to define the vacuum in such a way that the energy eigenvalues come out positive, but this comes at the cost of dealing with an indefinite metric on the ghostly inner product space (4.16). Though this allows us to consistently compute Feynman diagrams, the presence of the indefinite metric means that the standard way of defining probability via pseudo-unitarity of the S-matrix is not well-defined and in this sense leads to a violation of unitarity in scattering events. However, this fact does not mean that it is impossible to make statements about quantum probability when ghosts are present in a theory.

Turning back to the classical system described in Section 4.1 for a moment, we recall that in the region of phase space where the restoring force on the ghost that originates from its mass term $-m\omega^2\boldsymbol{y}$ is stronger than the anti-restoring force from the potential $V(|\boldsymbol{x}-\boldsymbol{y}|)$, it is possible to maintain stable motion with no run-away behavior despite the *apparent* violation of energy conservation with respect to the healthy particle. This is especially true in the physically realistic case where $V(r)$ approaches zero as $r \to \infty$ i.e. the asymptotic limit of a scattering event. In this stable region of phase space, we might also make the observation that if ω is large enough, the healthy particle is only able to excite the ghost very slightly after scattering so that the interaction becomes approximately elastic.

This feature of apparent elasticity has important ramifications for the quantum version of the theory, as originally introduced in [3]. When the $|0\rangle_+$ vacuum is employed, the energy eigenvalues of the ghost states are not only positive but, since they are quantized, separated by an energy gap ω. This means that it is not possible to excite the ghost at all whenever the energy of the incoming healthy particle is less than ω, a fact that promotes the approximate classical elasticity to an exact statement in the quantum theory. In the language of operator-based QFT this statement goes (informally) as follows: given a theory where the Fock space is spanned by a basis of both healthy and ghost states that exhibit an indefinite inner product metric, and where the associated positive energy eigenvalues are separated by a gap (ω), we may choose a basis spanned by the total four-momentum eigenstates $|p_T\rangle$ and find that the subspace spanned by the states that satisfy

$$-p_T^2 < \omega^2\,, \tag{4.31}$$

is positive-definite and that the S-matrix is fully unitary on this subspace. Put simply, when interaction energies are below the threshold of the ghost's energy gap, the ghosts remain in their ground state and it becomes possible to define a consistent notion of quantum probability, thus achieving "conditional unitarity". Naturally, the ghost may still be virtually excited and run in loops even when the condition (4.31) is satisfied, but this has no bearing on unitarity since it is only the scalar products between excited on-shell states that are relevant for proving unitarity, provided of course that the S-matrix is represented by a pseudo unitarity operator ($S^\dagger S = \mathbb{1}$) on the full space.

In the coming chapters we will elaborate on how the points introduced in our toy models, in particular the notion of conditional unitarity, are relevant for fourth-order scale-invariant quadratic gravity. However, before getting into these specific models, it will be instructive to first review some of the more interesting works that have attempted to address the ghost problem in recent years.

4.4 Promising resolutions

4.4.1 Lee-Wick-based models

The first well-established attempt to make sense of fourth-order quantum field theories was put forward by Lee and Wick in the late 60's in an attempt to resolve the hierarchy problem [99, 100] (see also [224]), and is based on the simple notion that the regulator in the Pauli-Villars (PV) regularization scheme might actually correspond to the mass of a physical degree of freedom. In standard PV regularization [225], one considers modified propagators that follow from replacements like

$$\frac{1}{p^2 - i\epsilon} \rightarrow \frac{1}{p^2 - i\epsilon} - \frac{1}{p^2 + \Lambda^2 - i\epsilon}, \tag{4.32}$$

where Λ is a (large) fictitious mass scale. Modifying the propagator in this fashion allows one to modulate UV divergences at large momenta while maintaining the ability to recover the original propagator in the $\Lambda \to \infty$ limit.

The idea that a PV-style propagator might arise naturally without being introduced as a calculational tool is obviously theoretically appealing, however, the relative minus sign in (4.32) indicates the presence of a ghost state with mass Λ. This naturally leads to all of the issues described in the last section that cannot be removed by taking the $\Lambda \to \infty$ limit when Λ is a physical and not a fictitious scale. Though Lee and Wick included proofs for unitarity and renormalizability in their original papers, the validity of their theory as a QFT has been debated since its inception, with criticisms[1] that include the potential violation of Lorentz invariance [226–228], as well as difficulties constructing the non-perturbative formulation of the theory [229].

Perhaps most importantly however, are the theory's issues related to its modification of the $i\epsilon$ prescription [230, 231]. Computing sensible loop integrals in the presence of ghostly propagators is actually a very non-trivial process. This is because the negative sign in the ghost propagator leads to another relative minus in the sign of the residue of the associated pole, thus shifting the pole off the real axis in such a manner that the standard $i\epsilon$ prescription leads to a propagator that describes modes which grow exponentially in time. Lee and Wick, with some input from Cutkosky [224], were able to get around this unacceptable feature by proposing a modified contour that instead

[1] It should be noted that Lee-Wick theory is also tricky to implement in non-Abelian gauge theories for the same reasons that PV regularization loses its validity in that context [123].

allows one to derive a propagator with the required exponentially damped modes, but at the cost of introducing violations of microcausality at the order $\Delta t \sim 1/M$. While this might seem rather unappealing, it should be stressed that maintaining microcausality need not be considered a requirement for a physical theory in the same way that unitarity is, provided of course that causality is eventually recovered on macroscopic scales. The real issue with the Lee-Wick approach is that, broadly speaking, the $i\epsilon$ prescription is not truly a "free parameter" to be altered at will, provided that one desires to stay within the bounds of established QFT[2].

Moreover, the Lee-Wick solution rests on a demonstration that the ghost mass, and thus also necessarily the ghost itself, becomes complex after including radiative corrections. This complexification lead Lee and Wick to conclude that their ghost is stable since it takes complex energy values and may thus not decay into standard particles with purely real energies. The important corollary to this demonstration is that, thanks to simple energy conservation, the complex ghost may also not be created through the collisions of ordinary particles, thus preserving unitary in scattering events. Lee and Wick demonstrated this feature by computing the ghost's one-loop amplitude which was found to have a vanishing imaginary part. As a result of the optical theorem (4.23), this implies that the associated cross section must also vanish. We will address this concept in more detail shortly, but it should first be noted that evidence has recently come to light that it may in fact be possible to create Lee-Wick ghosts through the collisions of standard particles if complex energy conservation is properly accounted for [232], thus indicating yet another reason why the Lee-Wick solution should be taken with a grain of salt. Despite all its potential issues, Lee-Wick theory is still an active area of research in the context of BSM physics (see for example [233–235]) though it is of particular interest to us simply due to the interesting potential solutions to the ghost problem that it has inspired.

Unstable ghosts

There is another potential route to establishing unitarity in the presence of ghosts that rests not on the assertion that they cannot be created as in Lee-Wick theory, but rather on the idea that they may decay into standard particles. In this case, proofs established by Veltman in [236] may imply that ghosts do not belong to the asymptotic spectrum of physical states, thus allowing unitarity to be established using standard methods.

This concept forms a basis for the work of Donoghue and Menezes [55, 102–104], which is the first contemporary potential solution to the ghost problem that we will review here. The authors consider a fourth order action of the form

$$S_{\mathrm{DM}} = \int \mathrm{d}^4x \left(-\frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi - \frac{1}{2M^2}\Box\phi\Box\phi + \frac{\kappa}{2}\Box\phi\big(\phi^2 + \chi^2\big) \right), \tag{4.33}$$

[2]The origin of the standard $i\epsilon$ prescription may be traced back to the definition of the θ-function given in (4.19) [223]. We thank Jisuke Kubo for illuminating discussions on this topic and Lee-Wick theory in general.

where $\phi(x)$ is a real scalar whose interactions with another real scalar $\chi(x)$ are parameterized by the massive coupling constant κ. This action serves as a handy toy model of quadratic gravity as it possesses the same kind of derivative interactions and propagates both a standard massless mode and a massive ghost mode, a feature that is made evident by the propagator

$$D(p) = \frac{i}{p^2 - i\epsilon} - \frac{i}{p^2 + M^2 - i\epsilon}\,, \tag{4.34}$$

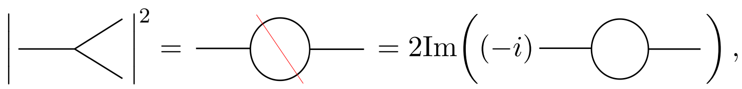
which includes factors of $i\epsilon$ per the standard prescription and may be compared with the PV-regulated propagator (4.32).

It is interesting to point out that after transforming to coordinate space and separating the propagator in terms of modes that propagate forward and backward in time with the appropriate θ-functions, one encounters the required exponential decay associated with the massive ghostly modes as well as the feature that these modes imply a flow of positive energy backwards in time. Naturally, this is related to the usual overall minus sign attached to the ghost propagator and implies the same type of microcausality violations encountered in Lee-Wick theories. We will not get into the details of microcausality violation here (these are nicely explained [103]), since for our current purposes, we are most interested in the demonstration of unitarity to all orders that follows from Veltman's prescription of only including contributions from stable particles in the perturbative unitarity sum. The authors use these ideas to assert that one should only consider diagrams that do not include ghosts in the external states, while still allowing them to appear as virtual particles that run in loops. With this notion, the proof of unitarity in the present theory then relies on Cutkosky's cutting rules [237] to evaluate discontinuous bubble diagrams.

A basic understanding of the cutting rules employed in this context may come from the optical theorem (4.23), which as we have seen, is itself an expression of the pseudo-unitarity of the S-matrix. If we consider a matrix element constructed from the optical theorem between arbitrary states $\langle b|$ and $|a\rangle$, we arrive at an expression of the cutting equation,

$$\sum_c \langle b|T^\dagger|c\rangle\ \langle c|T|a\rangle = i\big(\,\langle b|T^\dagger|a\rangle - \langle b|T|a\rangle\,\big)\,, \tag{4.35}$$

which when interpreted in terms of diagrams, states that the sum over all possible cuts that split the original diagram into tree-level diagrams involving stable external states is equivalent to the imaginary part of a loop diagram amplitude [223]. The simplest example of such a relationship involving a self-energy loop diagram may be expressed schematically as



(4.36)

which relates directly to the toy model realization of the optical theorem found in (4.28). This kind of relation between loop-order diagrams and the tree-level graphs used to construct them allows for much simpler calculations and is implemented through the cutting rules which state that one may replace internal propagators to the left of a cut in a Feynman integral according to

$$-\frac{i}{p^2+m^2-i\epsilon} \;\rightarrow\; 2\pi\delta(p^2+m^2)\,, \tag{4.37}$$

while propagators to the right are replaced using the complex conjugate of the above. One may understand the validity of making such a replacement by roughly equating it to the "1" that appears on the left side of (4.35) i.e. $\sum_c |c\rangle\langle c| = \mathbb{1} \leftrightarrow \delta(p^2+m^2)$.

In [103], Donoghue and Menezes use these cutting rules to demonstrate that the toy model for QG described by (4.33) is unitarity (satisfies (4.35)) to all orders in perturbation theory if one does not include cuts through internal ghost lines in the sum. Unlike the unitarity proof in Lee-Wick QED, all of these calculations are completed using the standard $i\epsilon$ prescription, though the authors note that the Lee-Wick contour may be used to recover the same answers in the narrow-width approximation where the ghost is treated as stable. Though their work is based around a scalar toy model and does not address the role of gauge symmetry, it is probably safe to assume that their proof may be extended so as to preserve the relevant Ward identities in QG, given that the same kind of calculation has been performed in Lee-Wick QED.

There are however two crucial assumptions related to their unitarity proof that may be called into question. The first is the fact that the instability of ghostly modes has not been explicitly demonstrated in QG for general matter couplings. In the toy model described above, the instability is obvious due to the $\phi\chi$ interactions (which are both real fields), however, in the original Lee-Wick papers it is specifically pointed that the ghosts acquire an effective complex mass term due to the radiative corrections introduced by fermion loops, meaning that the ghosts must actually be complex [100]. There is still however reason to expect that complex spin-2 ghosts would still decay to standard particles in line with [232]. The second and perhaps more questionable assumption in [103] is that Veltman's prescription of excluding unstable states from the unitarity sum still applies in the presence of ghosts. As demonstrated in Section 4.2.2, ghost decay leads to issues with defining quantum probability in the standard fashion and calculations of diagrams based on the optical theorem alone are not enough to see the pathological norm-increasing behavior that may result from ghost decay. Donoghue and Menezes also specifically note that it is tricky to reinterpret their work in the canonical operator formalism where these issues are made the most apparent. To summarize, this kind of demonstration of unitarity through ghost decay should certainly be considered a strong step forward towards a general solution to the ghost problem in QG, though more work still needs to be done in terms of reconciling Veltman's ideas with the decay of ghosts before it might be considered a complete solution.

The fakeon prescription

There is another Lee-Wick-based[3] potential solution to the ghost problem in QG that is worth taking the time to review. Anselmi's "fakeon" prescription [105–108] is at its core a completely new quantization procedure that stands as an alternative to the usual Feynman prescription. This new prescription does not completely replace standard methods, but rather adds an additional option that allows for some particles to be quantized differently than others. The basic procedure for each case proceeds according to

$$\text{Feynman:} \qquad iD(p) = \pm\frac{1}{p^2+m^2} \;\;\rightarrow\;\; \pm\frac{1}{p^2+m^2-i\epsilon} \simeq \pm\delta(p^2+m^2) \tag{4.38}$$

$$\text{fakeon:} \qquad iD(p) = \pm\frac{1}{p^2+m^2} \;\;\rightarrow\;\; \pm\frac{p^2+m^2}{(p^2+m^2)^2+\epsilon^4} \simeq 0\,. \tag{4.39}$$

Here, the "$\simeq$" indicates how each type of propagator behaves on shell i.e. how it appears as an external state and how it may be replaced via the cutting rules when it represents an internal line in a diagram.

The general idea behind the fakeon solution to the ghost problem is thus clear; if ghost modes are quantized as fakeons, they do not appear as asymptotic states and do not contribute to (spoil) the unitarity sum whether the ghost is stable or not. It is important to stress that one does not due away with the standard prescription entirely after adopting the fakeon prescription since there must of course still exist some kind of asymptotic states. Rather, when writing down a quantum theory based on some classical action, one has the choice to quantize each DOF as either a standard particle or a fakeon. It is also fully consistent to quantize a normal particle as a fakeon (this is not reserved strictly for ghosts), which expands the options for model-building in this hybrid quantization framework.

Anselmi and his co-authors explicitly demonstrate both unitarity and renormalizability in quadratic gravity under the fakeon prescription, however, there are important theoretical side-effects that come from including fakeons in a quantum theory. Besides the expected Lee-Wick-style violation of microcausality that goes roughly like $\Delta t = \mathcal{O}(1/m_\Phi)$ where m_Φ is the fakeon (Φ) mass, there is an unavoidable non-analyticity introduced into the calculation of loop integrals that contain fakeon propagators. In standard QFT, the $i\epsilon$ prescription employed in the propagator (4.38) infinitesimally shifts the poles to the complex plane so that they lie at $p^0 = E - i\epsilon$ and $p^0 = -E + i\epsilon$, which allows one to express the real integral over p^0 as a complex contour integral that may be Wick rotated (analytically continued) to the imaginary axis where the resulting Euclidean integral is easier to solve. Crucially, this analytic continuation is only possible when the rotated contour does not cross over a pole. In fakeon QFT, one runs into problems implementing this procedure since the propagator (4.39) effectively doubles the poles so that they lie at $p^0 = E \mp i\epsilon$ and $p^0 = -E \pm i\epsilon$. The usual method of Wick rotation is thus no longer

[3] In a talk given by Anselmi in 2019 [238], he states that this theory was in fact born in an attempt to show an inconsistency in Lee and Wick's model.

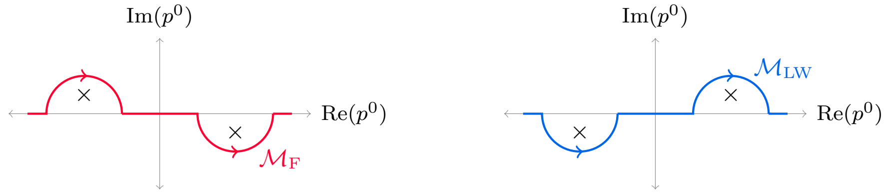


Figure 4.1: Comparison of the standard Feynman (left) and Lee-Wick (right) pole structures with the associated forward contours that enter into the fakeon prescription, labeled by the resulting matrix elements $\mathcal{M}_i$.

valid since it becomes impossible to go to Euclidean space without crossing over a pole. The author establishes a complicated non-analytic continuation that may be employed to consistently get around this issue (see [106] for details), however, they also point out a very simple method that achieves the same result. This is known as "average continuation" and involves simply taking the average of the results obtained from the Feynman and Lee-Wick contours as

$$\mathcal{M}_{\mathrm{fakeon}} = \frac{1}{2}\big(\mathcal{M}_{\mathrm{F}} + \mathcal{M}_{\mathrm{LW}}\big)\,, \tag{4.40}$$

where $\mathcal{M}_{\mathrm{i}}$ represents the matrix element that is calculated after following each prescription. The situation is summarized graphically in Figure 4.1.

Quantization under the fakeon prescription also differs from standard quantization with regard to its path integral formulation. Due to the fact that fakeon propagators vanish on-shell, the prescription dictates that one must project them out of the quantum effective action. This is achieved by setting their sources to zero at the level of the generating functional (2.6),

$$Z[J_\phi, J_\Phi] \quad\to\quad Z[J_\phi, 0] \int \mathcal{D}\phi \exp\big(i(S[\phi,\Phi] + \phi\cdot J_\phi)\big)\,, \tag{4.41}$$

which allows one to define the projected quantum effective action $\tilde{\Gamma}[\phi] = \Gamma[\phi, \langle\Phi\rangle]$ where $\langle\Phi\rangle$ is a stationary point of the original quantum effective action defined by

$$\left.\frac{\delta\Gamma[\phi,\Phi]}{\delta\Phi}\right|_{\Phi=\langle\Phi\rangle} = 0\,. \tag{4.42}$$

Working with these projected functionals is required for consistency, but has the interesting implication that the classical limit of the quantum action is not given by $S[\phi,\Phi]$, but rather by $S[\phi,\langle\Phi\rangle]$. For practical calculations, especially with respect to QG when it is written in terms of a perturbed metric, the projections must be defined perturbatively and remain perturbative as long as $m_\Phi \lesssim M_{\mathrm{Pl}}$. This all leads to the conclusion that even the equations of classical mechanics contain small corrections when fakeons are present in a theory. For example, if one considers the basic Newtonian definition of force, the strictly correct description is not $F = ma$, but rather $\langle F \rangle = ma$ or $F = ma + \mathcal{O}(\alpha)$ for some small perturbation parameter α.

Whether or not one is willing to accept the introduction of all of the extra machinery and the resulting physical consequences of adopting the fakeon prescription, the theory at least has two of the most important characteristics of any physical theory – it is predictive and falsifiable. There are experimental signatures resulting from the violation of causality and projection operations that may be used to test the fakeon hypothesis, and though most of these signatures are currently out of reach (especially with regard to quantum gravity), cosmological implications of adopting the fakeon hypothesis [108] and predictions related to treating the Higgs boson as a fakeon [239] have already been derived. In the end only time will tell if the idea that some particles exist only as internal states may accurately describe Nature.

4.4.2 Generalizing the inner product

Aside from the Lee-Wick based theories that we have just reviewed, there exists another approach toward the ghost problem that broadly involves a generalization of how probability is defined in quantum mechanics through relations like (4.26). This kind of approach centers around the definition of inner product itself which is often taken for granted in the standard framework. Traditionally, the inner product between two normalized states a and a' is expressed through the relation

$$\left\langle a' \middle| a \right\rangle = \langle 0 | a' a^\dagger | 0 \rangle = g_{aa'} \,, \tag{4.43}$$

where $g_{aa'}$ is the inner product metric that is defined solely in terms of the commutation relations between the state operators, $g_{aa'} = \left[a', a^\dagger\right]$. There is however room to generalize this definition provided that the modified inner product satisfies the requirements of linearity and some notion of symmetry under conjugation. To see how this relates to the ghost problem, we need only recall some very basic definitions in quantum mechanics.

At the most fundamental level, the notion of quantum probability is defined by the Born rule. Any general state $|\psi\rangle$ may be decomposed in terms of a basis of (normalized) eigenstates $|a\rangle$ of some observable, for example the Hamiltonian, as

$$|\psi\rangle = \sum_a C_a \, |a\rangle \,, \tag{4.44}$$

and the Born rule states that the probability for finding the state $|\psi\rangle$ in the particular configuration $|a\rangle$ is given by

$$P_a = \frac{|C_a|^2}{\sum_b |C_b|^2} = \frac{\left| \langle a|\psi\rangle_V \right|^2}{\langle \psi|\psi\rangle_V} \,. \tag{4.45}$$

The second equality here expresses the Born rule in terms of a general inner product on the Hilbert space of $|\psi\rangle$ that may be defined in terms of some adjoint-defining norm operator V as

$$\langle \psi_2|\psi_1\rangle_V = \langle \psi_2|V|\psi_1\rangle \,. \tag{4.46}$$

This relation is actually perhaps best interpreted in terms of non-selfadjoint operators where the adjoint of $|\psi\rangle$ is not the usual $\langle\psi|$, but rather $\langle\psi| V$. The standard inner product is related to this definition via $V = 1$, though as we saw explicitly in Section 4.2.1, this may yield a negative value when the product is taken between ghost states, which in turn leads to negative probabilities through the definition (4.45).

The preferable situation is thus given in terms of some non-trivial norm operator that satisfies

$$\langle n|m\rangle_V = \langle n|V|m\rangle = \delta_{mn} \qquad\qquad \mathbb{1} = \sum_n |n\rangle \langle n| V \tag{4.47}$$

for all multiparticle states $|m\rangle$ and $|n\rangle$, even when they contain ghost states with negative commutation relations. If such a norm operator may be consistently defined, all probabilities come out positive and perturbative unitary may, in principle, be established. This kind of sentiment is expressed in [120, 121], and though it resolves the issue of negative probabilities at the basic level shown above, one must formally define the generalized norm in a physically consistent manner and thoroughly investigate all of the theoretical ramifications that it implies.

$\mathcal{PT}$-symmetric QFT

The most promising theory that follows this norm-redefining line of reasoning is based on $\mathcal{PT}$-symmetric quantum theory as introduced by Bender [109–114]. The basic premise behind this idea is that the standard requirement of Hermiticity for a quantum Hamiltonian may be extended to a symmetry under discrete parity-time ($\mathcal{PT}$) transformations. In this paradigm, a wide range of non-Hermitian Hamiltonians that would traditionally be considered non-viable are shown to determine a spectrum of positive real eigenstates and govern unitary time evolution, and thus become candidates to describe real physical theories. $\mathcal{PT}$ symmetry as a guiding principle also benefits from the clear physical interpretation as a symmetry under spacetime reflections, in contrast to the more abstract mathematical concept of Hermiticity.

The crucial link between $\mathcal{PT}$-symmetric quantum theory and the ghost problem in QG was found by Bender and Mannheim through their demonstration that the Pais-Uhlenbeck oscillator, the same toy quantum mechanical model of QG that we discussed in detail in Section 4.1, represents a unitary theory with positive real norms and Hamiltonian eigenstates when reinterpreted as a $\mathcal{PT}$-symmetric theory [240, 241]. The proof of this fact and its implications for quantum gravity have also since been expanded on by the authors as well as others [97, 115–119].

The basic idea behind the unitarity of the PU oscillator in this context stems from the assertion that the Hamiltonian need not be its own Hermitian conjugate, but rather that this usual relationship should be replaced with a more general anti-linear symmetry that is expressed through a similarity transformation given in terms of the norm operator V,

$$\mathcal{H}^\dagger = \mathcal{H} \ \ \rightarrow \ \ \mathcal{H}^\dagger = V\mathcal{H}V^{-1} \,. \tag{4.48}$$

One may in fact show that establishing such a symmetry is all that is necessary to guarantee that the Hamiltonian possesses strictly positive eigenvalues[4] [109]. As previously alluded to, this implies that while the eigenvalue equation takes the standard form with respect to ket vectors, $\mathcal{H}\,|a\rangle = E_a\,|a\rangle$, the bra eigenvector is not the standard Hermitian conjugate since one finds $\langle a|\,V\mathcal{H} = E_a\,\langle a|\,V$. Unitary time evolution is ensured in this way as, using the general inner product (4.46), it is straightforward to show that

$$\langle\psi_2(t)|\psi_1(t)\rangle_V = \langle\psi_2(0)|e^{i\mathcal{H}t}e^{-i\mathcal{H}t}|\psi_1(0)\rangle_V = \langle\psi_2(0)|\psi_1(0)\rangle_V \ . \tag{4.49}$$

The underlying assumption here, that the left vacuum need not necessarily be the Hermitian conjugate of the right vacuum, is what leads to the important unitarity-restoring features in perturbative $\mathcal{PT}$-QFT. Namely, one may derive a unit operator and propagators that do not carry the troublesome minus signs that are indicative of the ghost problem in standard QFT.

To see how all of this general background on $\mathcal{PT}$ quantum theory applies to the PU oscillator specifically, we follow the discussion in [242] and begin with a convenient parameterization of the classical PU Hamiltonian that is related to the Hamiltonian one would derive from our auxiliary action (4.2) after including a small mass for $\boldsymbol{z}$ and applying the appropriate field redefinitions,

$$\mathcal{H} = \frac{1}{2}p_x^2 + p_z x + \frac{1}{2}\Big((\omega_1^2+\omega_2^2)x^2 - \omega_1^2\omega_2^2 z^2\Big)\,. \tag{4.50}$$

Here, ω_1 and ω_2 are massive constants, while $x(t)$ and $z(t)$ serve as one-dimensional scalar analogs of the spin-2 DOFs in QG with the associated canonical momenta p_x and p_z. Naturally, these variables respect the canonical commutation relations $[x,p_x] = [z,p_z] = i$. One may note the presence of the Ostrogradsky instability (unbounded-ness from below) that results from the $-z^2$ term above which, as we have already seen in detail, implies the presence of a negative norm at the quantum level. We recall that this may be seen by expanding each canonical variable in terms of creation and annihilation operators, deriving the resulting Hamiltonian operator through the Heisenberg equation, and selecting the "+" vacuum for the operator, just as in Section 4.2.1.

We now come to the crux of the $\mathcal{PT}$ solution to the ghost problem – all the issues that result from the negative norm may be avoided if we assume that z (the ghost mode) lives in the complex plane. While this is not allowed in traditional quantum mechanics, since z would not be Hermitian, it is allowed in the present framework provided that z respects the less strict anti-linear $\mathcal{PT}$ symmetry. If we thus assume that z is actually imaginary, we may express our theory in terms of the real time-dependent quantity $y(t)$ via a similarity transformation given in terms of the rotation $A = e^{\pi p_z z/2}$ (recalling that $p_z = -i\partial_z$) so as to define the new variables

$$y = AzA^{-1} = -iz \qquad\qquad p_y = Ap_zA^{-1} = ip_z\,, \tag{4.51}$$

[4] In light of this fact, one may interpret the usual more strict requirement of Hermiticity as a sufficient but not necessary condition for realizing positive eigenvalues.

which still respect the required canonical relation $[y, p_y] = i$. This same rotation applied to the Hamiltonian (4.50) then yields

$$\tilde{\mathcal{H}} = A\mathcal{H}A^{-1} = \frac{1}{2}p_x^2 - ip_y x + \frac{1}{2}\Big((\omega_1^2 + \omega_2^2)x^2 + \omega_1^2\omega_2^2 y^2\Big) . \tag{4.52}$$

Noting that x and y (p_x and p_y) are $\mathcal{PT}$ odd (even), it is straightforward to confirm that this classical Hamiltonian is indeed $\mathcal{PT}$ symmetric. This guarantees the positivity of its eigenvalues, a feature that is made even more clear by noting that the Ostrogradsky instability is no longer present thanks to the replacement $-z^2 = y^2$.

Forgoing a demonstration of the complete proof for the sake of brevity, we may get a better feeling for why positivity is guaranteed by performing yet another (eigenvalue preserving) similarity transformation in terms of the operator

$$Q = \left[\frac{1}{\omega_1\omega_2}\ln\left(\frac{\omega_1 + \omega_2}{\omega_1 - \omega_2}\right)\right](p_x p_y + \omega_1^2\omega_2^2 xy) , \tag{4.53}$$

so that we arrive at the "canonical" Hamiltonian

$$e^{Q/2}\tilde{\mathcal{H}}e^{-Q/2} = \frac{1}{2}\left(p_x^2 + \frac{1}{\omega_1^2}p_y^2 + \omega_1^2 x^2 + \omega_1^2\omega_2^2 y^2\right) , \tag{4.54}$$

which is given in terms of real quantities only, bounded from below, and is free of ghosts.

The operator (4.53) is actually a very important object in $\mathcal{PT}$ quantum theory and though we do will not discuss its role further or derive it here (see [111]), it is important to point out that it corresponds to our sought-after norm operator in (4.47) through the identification $V = e^{-Q}$. Indeed it is straightforward to show that, after the introduction of creation/annihilation operators and the quantization of (4.52), we find the desired relations

$$\langle n|e^{-Q}|m\rangle = \delta_{mn} \qquad\qquad \mathbb{1} = \sum_n |n\rangle\langle n|\, e^{-Q} , \tag{4.55}$$

where $|n\rangle$ are n-particle eigenstates of $\tilde{\mathcal{H}}$ that satisfy the eigenvalue equations

$$\tilde{\mathcal{H}}\,|n\rangle = E_n\,|n\rangle \qquad\qquad \langle n|\, e^{-Q}\tilde{\mathcal{H}} = E_n\,\langle n|\, e^{-Q} . \tag{4.56}$$

Furthermore, if we embrace this paradigm in QFT, the propagator function for some Heisenberg field ϕ must be identified in terms of the appropriate ket state as

$$D_F(x - y) = -i\,\langle 0|e^{-Q}T\phi(x)\phi(y)|0\rangle , \tag{4.57}$$

which in turn (at least in principle), allows one to proceed with other aspects of QFT as usual and without the need to assume a modified $i\epsilon$ prescription or assume the ghosts are unstable, etc. The correct interpretation in the context of $\mathcal{PT}$-QFT is that there were never any ghosts in the first place, but only a misguided assumption that the original variables are real due to the requirement of Hermiticity[5].

Though the adoption of $\mathcal{PT}$ symmetry as a guiding principle clearly represents a very promising solution to the ghost problem (as well as an interesting expansion of quantum theory in general), it is certainly too early to say that it resolves all our issues. The principle drawback to this setup is that the theory is simply not yet well-developed enough. Though $\mathcal{PT}$ symmetry's role in one-dimensional single particle quantum mechanics is well-understood, only some of its simpler implications for full-blown QFT have been worked out so far (see for example [114, 243–246]). Though establishing $\mathcal{PT}$-QFT to the level of standard Hermitian QFT is quite the daunting task, it certainly seems to be one worth undertaking and is currently an area of very active research. Even beyond its application to the ghost problem in quantum gravity, interesting examples of physical $\mathcal{PT}$ systems have already appeared in the fields of condensed matter physics [247–249] and quantum optics [250–254], just to name a few examples.

4.5 Covariant operator quantization

Now that we have gained an understanding of the ghost problem and have taken a look at some of its possible resolutions that have appeared in the literature, we may proceed with a review of the formalism that we will employ to investigate the ghost problem from our own point of view. A key part of this process involves isolating the physically propagating independent DOFs, which requires one to address the inherent redundancy between physically equivalent states that are related by gauge transformations.

4.5.1 Gauge fixing and BRST symmetry

The process of isolating gauge-invariant quantities in a gauge theory may broadly be referred to as gauge fixing. For many calculations of interest, gauge fixing may be achieved by following the original work of Dirac and Bergman on constrained systems [255], however this procedure inherently comes with a loss of explicit Lorentz covariance, a fact that makes it practically impossible to carry out renormalization of the associated quantum theory. Moreover, when this simplest method of gauge fixing is applied, the original information about the theory's inherent symmetry properties is lost after a particular gauge is chosen. In certain calculations involving theories based on a simple gauge group like QED, the issue of covariance may actually be ameliorated by appealing to the Gupta-Bleuler formalism [256, 257], which incorporates covariant gauge-fixing terms into the action that lead to constraints which the gauge fields must satisfy, as dictated by the EOMs. However, choosing covariant gauge conditions alone is not generally sufficient in

[5]The obvious corollary here is that if $\mathcal{PT}$ symmetry is able to resolve the ghost problem in quantum gravity, the metric must actually be anti-Hermitian i.e. $g_{\alpha\beta} \to ig_{\alpha\beta}$ and $g^{\alpha\beta} \to -ig^{\alpha\beta}$. Interestingly, though this may seem like an impossibility at first glance, the implications of a complex metric have been worked out in some detail with no inconsistencies arising, provided of course that one stays in the $\mathcal{PT}$ framework [241].

more complex theories with non-simple gauge groups such as QCD due to complications that arise from self-interactions between the gauge fields. The solution to this particular issue was eventually put forth by Faddeev and Popov [258, 259], when they introduced *fictitious* ghost particles (not to be confused with physical Ostrogradsky ghosts) that serve to cancel unphysical contributions to asymptotic observables order by order. The end result of all the years of work that went into solving these problems in quantized gauge theories has culminated in what we now know as BRST theory. Indeed, it is now understood that to rigorously isolate the physical states within a quantum theory while maintaining explicit covariance, the most general and comprehensive approach is to establish a BRST symmetry in the theory. The BRST construction now plays a crucial role in the Standard Model, as the formal proofs of stability, renormalizability, and unitarity rely heavily on its application [260–262][6]. We will thus also employ the BRST formalism in this work, following a brief introduction to its key elements that closely follows [266].

Given some classical gauge theory, the first step towards setting up the BRST formalism is to choose a set of gauge fixing conditions $G_a = 0$, which are functions of the gauge fields ϕ_a that are present in the classical action S_{cl}. With these conditions established one may then introduce the first of a set unphysical BRST fields, the bosonic auxiliary "Nakanishi-Lautrup" (NL) fields B_a that will act as Lagrange multipliers and enforce the G_a after being integrated out. One may then in turn introduce the gauge fixing action

$$S_{\text{gf}} = \int \mathrm{d}^4x \, B^a G_a \,, \tag{4.58}$$

which is reminiscent of simpler Gupta-Bleuler-style methods of gauge-fixing.

The next step in the BRST construction is to introduce the remaining unphysical BRST fields that directly compensate for the unphysical states at each order in perturbation theory; the Faddeev-Popov (FP) ghost and anti-ghost fields, C^a and $\bar{C}_a$. As the role of these fields is to precisely cancel unphysical bosonic degrees of freedom, they are defined to carry integer spin while obeying fermionic statistics. Naturally, we must ensure that only the contributions from unphysical modes of the classical fields are canceled and that this cancellation is precise so that no spin-statistic-theorem-violating (anti)ghosts appear as asymptotic states. This feature is achieved by introducing (anti)ghosts into the action so as to establish a BRST symmetry. The associated BRST algebra is generated by the nilpotent fermionic charge $\mathcal{Q}$ and is a graded algebra where the grading is referred to as the "ghost number", which is assigned to each type of field as

$$\mathrm{gh}\big(\phi_a\big) = 0 \qquad \mathrm{gh}\big(B_a\big) = 0 \qquad \mathrm{gh}\big(C^a\big) = 1 \qquad \mathrm{gh}\big(\bar{C}_a\big) = -1 \,. \tag{4.59}$$

In order to consistently introduce the (anti)ghosts and construct the total BRST action, we simply require that the total action, as well as all observables, carry ghost number zero and that $\mathcal{Q}$ generates nilpotent ($\mathcal{Q}^2 = 0$) BRST transformations. The $\mathcal{Q}$

[6]Since its introduction, BRST theory, and in particular BRST cohomology, has been well-studied by many other theoreticians and was also expanded upon into an even more rigorous Hamiltonian-based framework known as the BFV (Batalin-Fradkin-Vilkovisky) formalism [263–265].

operator is naturally defined to act on other operators in terms of (anti)commutators, though it is related to infinitesimal BRST transformations on fields through the relation

$$[i\mathcal{Q}, X]_{\mp} = \delta X \tag{4.60}$$

where $\mp$ stands for commutator or anti-commutator as appropriate. With this, BRST transformations of fields may be expressed in a general fashion as

$$\Phi'_A = \Phi_A + \epsilon\, \delta\Phi_A\,, \tag{4.61}$$

where ϵ is a constant, anti-commuting, and anti-Hermitian parameter of the transformation, $\Phi_A = \{\phi_a, B_a, C_a, \bar{C}_a\}$, and

$$\begin{aligned} \delta\phi_a &= \sum_\xi \left(\delta^{(\xi)}\phi_a\right)\Big|_{\xi^b = C^b} \qquad\qquad & \delta B_a &= 0 \\ \delta C^a &= C^b\partial_b C^a & \delta\bar{C}_a &= iB_a\,. \end{aligned} \tag{4.62}$$

Here, $\delta^{(\xi)}\phi_a$ represents the gauge transformation of ϕ_a with respect to the local gauge transformation parameter $\xi^a(x)$. At this stage, one of the principal benefits of the BRST is already manifest; despite the fact that we have fixed the gauge by introducing (4.58) into our action, the formalism retains all the information about its original gauge symmetry through the action of $\mathcal{Q}$ on the original fields.

To finally construct the total action, which we require to be Hermitian, BRST-invariant, and carry ghost number zero, we need only consider the transformation rules (4.62). Since the classical action $S_{\rm cl}$ already satisfies these properties thanks to its gauge symmetry, we simply need to add a ghost number zero action made up of ghost and antighosts that cancels the BRST transformation of (4.58). The most straightforward way to derive this ghost action is to transform the so-called "gauge fixing fermion" $\bar{C}^a G_a$, leading to the BRST action

$$S_{\rm BRST} = -i \int \mathrm{d}^4x\, \delta\big(\bar{C}^a G_a\big)\,. \tag{4.63}$$

As a result of (4.62), transformation of the gauge fixing fermion necessarily generates the gauge fixing action (4.58) as well as the desired unique FP ghost action ($S_{\rm FP}$) that, thanks to the nilpotency of $\mathcal{Q}$, precisely cancels the BRST transformation of $S_{\rm gf}$. The total BRST action is thus finally given by

$$S_{\rm T} = S_{\rm cl} + S_{\rm BRST} = S_{\rm cl} + S_{\rm gf} + S_{\rm FP}\,, \tag{4.64}$$

where $\delta S_{\rm T} = 0$ and $\mathrm{gh}(S_{\rm T}) = 0$.

At this stage it is interesting to point out that BRST symmetry is in fact a supersymmetry in the sense that it comes with a Grassmann-odd charge that transforms Grassmann-odd objects into Grassmann-even objects, and vice-versa. Though BRST symmetry is actually distinct from the more familiar supersymmetry that is often considered in extensions to the SM (SUSY), both symmetries may coexist in the same theory and indeed often appear together in the study of supersymmetric gauge theories.

4.5.2 The LSZ formalism

Once the total BRST action corresponding to a given classical action is established, we may proceed with the actual quantization. We will employ the formalism originally laid out by Lehmann–Symanzik–Zimmerman (LSZ) [267, 268] and elaborated on by others [266, 269], which follows similar logic to a traditional second quantization in the Heisenberg picture, with the important caveat being that it will allow us to establish covariant commutation relations between our fields in contrast to the more commonly seen equal-time commutation relations. In what follows we will ignore effects such as wave function renormalization since they do not effect the essence of our results, though it is straightforward to include such phenomena in the formalism as well. The LSZ formalism dictates that all the fields in a theory, which we denote generally as $\Phi(x)$, be considered Heisenberg fields with time-independent state vectors. It also makes the assumption that the $\Phi(x)$ act as free fields that satisfy the free equations of motion in the asymptotic limit $t = x^0 \to \pm\infty$:

$$\Phi(x) \to \begin{cases} \Phi^{\text{in}}(x)\,, & x^0 \to -\infty \\ \Phi^{\text{out}}(x)\,, & x^0 \to +\infty \end{cases} . \tag{4.65}$$

In what follows we will designate asymptotic free fields in these particular limits with the superscripts "in" or "out" as above and will also write "as" when referring to a general asymptotic field. It should also be noted that the $x^0 \to \pm\infty$ limit taken here should, strictly speaking, be considered a weak limit.

Moving forward, we decompose each asymptotic field as a sum of products of oscillators and plane wave functions as

$$\Phi^{\text{as}}(x) = \sum_{\boldsymbol{p}} \Big(\hat{\Phi}^{\text{as}}(\boldsymbol{p}) f_{\boldsymbol{p}}(x) + \hat{\Phi}^{\text{as}}_g(\boldsymbol{p}) g_{\boldsymbol{p}}(x) + \hat{\Phi}^{\text{as}}_h(\boldsymbol{p}) h_{\boldsymbol{p}}(x) + \cdots + (\text{h.c.}) \Big)\,, \tag{4.66}$$

where $\boldsymbol{p}$ represents the three-dimensional spatial components of the full four-momentum p^α. Here, $f_{\boldsymbol{p}}(x)$, $g_{\boldsymbol{p}}(x)$, $h_{\boldsymbol{p}}(x)$, $\cdots$, are the plane wave functions which solve increasing powers of the Klein-Gordon equation,

$$(\Box - m^2) f_{\boldsymbol{p}}(x) = (\Box - m^2)^2 g_{\boldsymbol{p}}(x) = (\Box - m^2)^3 h_{\boldsymbol{p}}(x) = \cdots = 0\,. \tag{4.67}$$

The simple-pole function $f_{\boldsymbol{p}}(x)$ is given by

$$f_{\boldsymbol{p}}(x) = \frac{1}{\sqrt{2EV}} e^{ipx}\,, \tag{4.68}$$

where V is a finite normalization volume, $E^2 = |\boldsymbol{p}|^2 + m^2$, and $px = -E\,x^0 + \boldsymbol{p}\cdot\boldsymbol{x}$. The higher-pole functions are constructed in a similar manner and we refer the reader to Appendix A for more details, including their specific forms.

In (4.66), $\hat{\Phi}^{\text{as}}(\boldsymbol{p})$ is a quantum mechanical operator that is referred to as an oscillator. In our nomenclature, the first operator in (4.66) with no subscript represents the fundamental simple-pole oscillator associated with the Heisenberg field $\Phi(x)$. Oscillators with

g, h, etc. subscripts are referred to as double-pole, triple-pole, etc. oscillators and do not correspond to independent DOFs, rather, they are functions of simple-pole oscillators and their derivatives that are fixed by the free equations of motion. A key feature of the decomposition (4.66) is its invertability, which comes as a result of the orthogonality relations between plane wave solutions (A.6 – A.9) and allows one to write a simple-pole oscillator in terms of its original Heisenberg field as

$$\hat{\Phi}^{\mathrm{as}}(\boldsymbol{p}) = \lim_{x^0 \to \pm\infty} \int \mathrm{d}^3\boldsymbol{x}\, i \Big(f^*_{\boldsymbol{p}}(x) \overleftrightarrow{\partial}_0 + g^*_{\boldsymbol{p}}(x) \overleftrightarrow{\partial}_0 (\Box - m^2) + h^*_{\boldsymbol{p}}(x) \overleftrightarrow{\partial}_0 (\Box - m^2)^2 + \cdots \Big) \Phi(x)\,, \tag{4.69}$$

where $A \overleftrightarrow{\partial}_0 B = A\partial_0 B - B\partial_0 A$.

Oscillators should be understood as products of creation(annihilation) operators and, when $\Phi(x)$ corresponds to a field carrying space-time indices, polarization tensors. Specifically, this means that for a general asymptotic spin-1 vector oscillator $\hat{v}_\alpha(\boldsymbol{p})$ we may write the decomposition $\hat{v}_\alpha(\boldsymbol{p}) = \sum_i \hat{v}_i(\boldsymbol{p}) \underset{i}{\varepsilon}_\alpha(\boldsymbol{p})$ where the $\hat{v}_i$ are independent creation/annihilation operators and $\underset{i}{\varepsilon}_\alpha(\boldsymbol{p})$ denotes a set of orthonormal and complete polarization vectors ($i = 0, 1, 2, 3$). Naturally, a general asymptotic tensor oscillator $\hat{t}_{\alpha\beta}(\boldsymbol{p})$ may be decomposed in the analogous way as $\hat{t}_{\alpha\beta}(\boldsymbol{p}) = \sum_i \hat{t}_i(\boldsymbol{p}) \underset{i}{\varepsilon}_{\alpha\beta}(\boldsymbol{p})$.

We will be mostly concerned with the physical (gauge-invariant) components of vector and tensor fields that by definition correspond to transverse polarization tensors that satisfy

$$p^\alpha \underset{j}{\varepsilon}_\alpha = 0 \qquad\qquad p^\alpha \underset{j}{\varepsilon}_{\alpha\beta} = 0\,. \tag{4.70}$$

In this spirit, it is convenient to select the specific vector basis

$$\big(\underset{1}{\varepsilon}_\alpha\big) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad \big(\underset{2}{\varepsilon}_\alpha\big) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad \big(\underset{3}{\varepsilon}_\alpha\big) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}\,, \tag{4.71}$$

which may also be used to define the convenient tensor basis

$$\begin{aligned}
\big(\underset{+}{\varepsilon}_{\alpha\beta}\big) &= \frac{1}{\sqrt{2}} \big(\underset{1}{\varepsilon}_\alpha \underset{1}{\varepsilon}_\beta - \underset{2}{\varepsilon}_\alpha \underset{2}{\varepsilon}_\beta\big) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
\big(\underset{\times}{\varepsilon}_{\alpha\beta}\big) &= \frac{1}{\sqrt{2}} \big(\underset{1}{\varepsilon}_\alpha \underset{2}{\varepsilon}_\beta + \underset{2}{\varepsilon}_\alpha \underset{1}{\varepsilon}_\beta\big) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\
\big(\underset{1}{\varepsilon}_{\alpha\beta}\big) &= \frac{1}{\sqrt{2}} \big(\underset{1}{\varepsilon}_\alpha \underset{3}{\varepsilon}_\beta + \underset{3}{\varepsilon}_\alpha \underset{1}{\varepsilon}_\beta\big) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}
\end{aligned} \tag{4.72}$$

$$\left(\varepsilon_{2\alpha\beta}\right) = \frac{1}{\sqrt{2}}\left(\varepsilon_{2\alpha}\varepsilon_{3\beta} + \varepsilon_{3\alpha}\varepsilon_{2\beta}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\left(\varepsilon_{3\alpha\beta}\right) = \frac{1}{\sqrt{6}}\left(\varepsilon_{1\alpha}\varepsilon_{1\beta} + \varepsilon_{2\alpha}\varepsilon_{2\beta} - 2\varepsilon_{3\alpha}\varepsilon_{3\beta}\right) = \frac{1}{\sqrt{6}}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} .$$

For massless fields, this basis of polarization states corresponds to a choice of Lorentz frame with motion along the z-axis as defined by

$$p^\alpha = \left\{E, 0, 0, E\right\} , \tag{4.73}$$

where transverse vectors are identified with $j = 1, 2$ in (4.71) and transverse tensors are identified with $j = +, \times$ in (4.72). The same basis (4.71, 4.72) may also be used to describe transverse massive fields in the center of mass frame

$$p^\alpha = \left\{m, 0, 0, 0\right\} , \tag{4.74}$$

where $j = 1, 2, 3$ ($j = +, \times, 1, 2, 3$) is needed to describe all three (five) physical DOFs in a massive vector (tensor) field. Choosing one of these frames is possible without loss of generality for our purposes, as all (anti)commutators derived in either frame are also valid in general [270]. This is of course related to the fact that our polarization tensors depend only on the direction of the three-momentum and not on its magnitude i.e. $\partial_E \varepsilon_{j\,\alpha}(\boldsymbol{p}) = \partial_E \varepsilon_{j\,\alpha\beta}(\boldsymbol{p}) = 0$, which comes as a result of the orthogonality relations (4.70).

Moving forward, after each asymptotic field in a theory is decomposed in terms of oscillators and plane wave functions, and the higher-pole oscillators have been solved for in terms of simple-pole oscillators using the EOMs, we may proceed by reading off the commutation relations between each field from the propagator matrix $\Omega^{-1}_{AB}(p)$. The propagator matrix is given by the inverse of the Hessian matrix

$$\Omega^{AB}(p) = \int \mathrm{d}^4x\, \frac{\delta^2 S_{\mathrm{T}}}{\delta\Phi_A(x)\delta\Phi_B(y)}\, e^{-ip(x-y)} , \tag{4.75}$$

where each entry corresponds to the second variation of the total BRST action with respect to each combination of the fields. With the propagators in hand, the commutators between fields are then easily obtained from each entry in $\Omega^{-1}_{AB}(p)$ by making the replacements

$$\begin{aligned} &\frac{ip_\alpha}{-(p^2+m^2)} \to \partial^x_\alpha D(x-y) && \frac{ip_\alpha}{(p^2+m^2)^2} \to \partial^x_\alpha E(x-y) \\ &\frac{ip_\alpha}{-(p^2+m^2)^3} \to \partial^x_\alpha F(x-y) && \cdots , \end{aligned} \tag{4.76}$$

where the superscript refers to differentiation with respect to x, and $D(x-y)$, $E(x-y)$, $F(x-y)$, $\cdots$ are invariant delta functions associated with the power n of the pole $(p^2+m^2)^n$. The simple-pole delta function is given explicitly by

$$D(x-y) = \int \mathrm{d}^3\boldsymbol{p} \frac{1}{2E(2\pi)^3}\Big(e^{ip(x-y)} - (\mathrm{h.c.})\Big) \tag{4.77}$$

while the higher-pole delta functions are constructed from similar sums of the higher-pole plane wave functions. These delta functions are also naturally related to Feynman propagators (Green's functions), though we once again defer to Appendix A for more details and precise definitions.

At this stage, it is crucial to point out that the covariant-ness of the present setup is directly related to the fact that the definition of $D(x-y)$ above is given in terms of an integral rather than a sum over $\boldsymbol{p}$. This feature is achieved by taking the continuum limit $V \to \infty$ so that

$$\lim_{V\to\infty} \frac{1}{V}\sum_{\boldsymbol{p}} = \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3}\,, \tag{4.78}$$

which is what allows one to ensure that all (anti)commutation relations derived in a specific Lorentz frame will also be valid in any other frame. After rescaling each operator according to

$$\hat{\Phi}(\boldsymbol{p}) \to (2\pi)^{3/2} V^{-1/2}\hat{\Phi}(\boldsymbol{p})\,, \tag{4.79}$$

it is straightforward to show that, in the continuum limit (4.78), one finds that $\sqrt{E'}\hat{\Phi}'(\boldsymbol{p}) \to \sqrt{E}\hat{\Phi}(\boldsymbol{p})$. This in turn allows one to recover the Lorentz-invariant statement $E'\delta^3(\boldsymbol{p}'-\boldsymbol{q}') = E\delta^3(\boldsymbol{p}-\boldsymbol{q})$ and confirm that the rescaled operators are indeed Lorentz scalars.

Finally, we may derive the commutation relations between the simple-pole oscillators $\big[\hat{\Phi}_A(\boldsymbol{p}), \hat{\Phi}_B(\boldsymbol{q})\big]$ using the commutators between fields, the field's oscillator decompositions (4.66), and the definitions of the invariant delta function propagators. With this the full quantum theory corresponding to the original classical theory is well defined, though the task of rigorously establishing what constitutes the physical subspace of quantum states still remains.

4.5.3 The Kugo-Ojima quartet mechanism

So far we have seen how to setup the BRST total action and how to quantize the resulting theory in a covariant manner in terms of plane-wave functions and invariant delta function propagators, however, we still need to address specifically how this whole construction leads to the desired cancellation of unphysical degrees of freedom. In [271–274], Kugo and Ojima (KO) demonstrated this crucial feature of BRST-invariant actions explicitly by showing that the physical subspace $\mathcal{V}_{\mathrm{phys}} \ni |f_{\mathrm{phys}}\rangle$ of the total Fock space $\mathcal{V} \ni |f\rangle$ of such a theory, which generically contains both physical and unphysical states, is fully populated by the states which are annihilated by the BRST charge:

$$\mathcal{Q}\,|f_{\mathrm{phys}}\rangle = 0\,. \tag{4.80}$$

Though these states are all physical in the sense that they all carry a non-negative inner product (norm), we must still go a step further to single out the subspace that contains only physically propagating transverse states i.e. the space with no longitudinal or zero-norm states. This desired subspace is defined by the quotient space below and is referred to as the "BRST cohomology space[7]",

$$\mathcal{V}_{\mathrm{tr}} = \mathrm{Ker}\, \mathcal{Q}/\mathrm{Im}\, \mathcal{Q}\,, \tag{4.81}$$

where $\mathrm{Ker}\, \mathcal{Q} = \mathcal{V}_{\mathrm{phys}}$ and $\mathrm{Im}\, \mathcal{Q} = \mathcal{Q}\mathcal{V} = \mathcal{V}_0$ is the BRST co-boundary [277]. Of course, the definitions above are only a mathematical backbone that supports practical application of the "Kugo-Ojima quartet mechanism" and the precise identification of the transverse physical subspace from a given complete Fock space that it entails. The full proof of this mechanism is laid out very nicely by Nakanishi in [266], though it is worthwhile to sketch out the important parts here.

We begin with some classifications, noting that all the members of the complete space $\mathcal{V}$ must be either singlets or doublets under BRST symmetry i.e. they are annihilated by the charge, or they are transformed into another state. This fact comes from the nilpotency of $\mathcal{Q}$, which guarantees that no higher n-plet representations may exist. The two members of each doublet may also be categorized as either parent or daughter states, which we denote as $|\pi\rangle$ and $|\delta\rangle$ respectively. Their familial relationships are characterized by the relations

$$\mathcal{Q}\,|\pi_0\rangle = |\delta_1\rangle \neq 0 \qquad\qquad \mathcal{Q}\,|\pi_{-1}\rangle = |\delta_0\rangle \neq 0\,, \tag{4.82}$$

where subscripts indicate FP ghost number. With this and the transformations (4.62) in mind, it is straightforward to see that each of these operators will always correspond to the components of certain types of fields: longitudinal components of $\phi_a \to \pi_0$, $C^a \to \delta_1$, $\bar{C}_a \to \pi_{-1}$, and $B_a \to \delta_0$. An important corollary to the existence of these doublets is that, due to the fact that the ghost number of the total action is required to be zero, each doublet $\{|\pi_0\rangle\,, |\delta_1\rangle\}$ is necessarily paired with an FP-conjugate doublet $\{|\pi_{-1}\rangle\,, |\delta_0\rangle\}$. It is these pairs of doublets that constitute the titular quartets and populate the BRST co-boundary $\mathcal{V}_0$. All the remaining states in $\mathcal{V}_{\mathrm{phys}}$ are thus guaranteed to be BRST singlets that live in $\mathcal{V}_{\mathrm{tr}}$.

The crux of the KO quartet mechanism lies in the fact that matrix elements between transverse states and members of the quartets are always vanishing, while matrix elements between quartet states that are non-vanishing necessarily satisfy the relation

$$\langle\pi_{-1}|\delta_1\rangle = \langle\pi_{-1}|\, \mathcal{Q}\,|\pi_0\rangle = \langle\delta_0|\pi_0\rangle \neq 0\,, \tag{4.83}$$

which guarantees that all intermediate contributions to covariant correlation functions that arise from the non-transverse bosonic DOFs are precisely canceled by the FP ghosts. This important conclusion is reached by appealing to the inherent freedom in how one defines parent and daughter states. Without loss of generality, one may always define

[7] BRST cohomology is an interesting and well-studied subject that we will not go into further detail on here, though for the curious reader we recommend [275, 276].

the parents and daughters in such a way that the quartet states are orthogonal to the transverse states, and that the n-particle states constructed from quartet members may be written in terms of the projection operator

$$P^{(n)} = \frac{1}{n} \sum_{a,b=1}^{4} (g^{-1})_{ab} \hat{\varphi}_a^\dagger P^{(n-1)} \hat{\varphi}_b \,, \tag{4.84}$$

where n counts the number of unphysical particles, g_{ab} is the inner product metric defined by $\left[\hat{\varphi}_a(\boldsymbol{p}), \hat{\varphi}_b^\dagger(\boldsymbol{q})\right] = g_{ab}\delta^3(\boldsymbol{p}-\boldsymbol{q})$, and $\hat{\varphi}_a = \{\pi_0, \delta_0, \pi_{-1}, \delta_1\}$ are the annihilation operators for each of the quartet members. Now, since $\mathcal{V}_{\text{tr}}$ is by definition the subspace with zero unphysical particles, we may define it in terms of this projection operator as $\mathcal{V}_{\text{tr}} = P^{(0)}\mathcal{V}$. Then, taking advantage of the recursive nature of the definition above, a straightforward proof by induction implies that $\mathcal{V}_0 = \sum_{n=1}^\infty P^{(n)}\mathcal{V}_{\text{phys}} = \mathcal{Q}\mathcal{V}$ and

$$\langle f_{\text{phys}} | P^{(n)} | g_{\text{phys}} \rangle = 0 \qquad \text{for} \qquad n \geq 1 \,. \tag{4.85}$$

Therefore, despite the fact that quartet states may appear as asymptotic multi-particle states in $\mathcal{V}_{\text{phys}}$ as defined in (4.80), their inner product with any other state in $\mathcal{V}_{\text{phys}}$ is always zero. In other words, the quartet states that satisfy (4.83) do not pose a problem for establishing unitarity of the physical S-matrix on $\mathcal{V}_{\text{tr}}$. As we will see in the coming sections, it is indeed possible to confirm that the relationship (4.83) holds for all of the non-transverse states in quadratic gravity. Construction of the gauge-fixed (Heisenberg picture) quantum Hamiltonian, representations of the physical S-matrix, and all of the resulting analyses then follow using standard techniques.

4.6 Quantum quadratic gravity

4.6.1 Second-order quadratic gravity

We begin our investigations of the ghost problem in scale-invariant QG by following the work presented in [3] and considering the previously studied scale-invariant action (3.37) which, as we have already seen, generates an Einstein Hilbert term through the non-minimal $\phi^2 R$ coupling after ϕ acquires a VEV via the spontaneous breakdown of scale symmetry. Without loss of generality, we may rewrite the gravitational part of this action in the broken phase as

$$S_{\text{QG}} = \int \mathrm{d}^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2}{2} R - \frac{1}{\alpha_g^2} \left(R_{\alpha\beta}R^{\alpha\beta} - \frac{1}{3}R^2 + \beta R^2 \right) \right] , \tag{4.86}$$

where we have assumed that $M_{\text{Pl}} = M_{\text{Pl}}(v_\phi)$ has been generated dynamically and we have reparameterized the couplings κ and γ in terms of the new dimensionless couplings α_g and β (which should not be confused with the β in (3.37)) for future convenience. Here we have also used the identity

$$C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta} = 2R_{\alpha\beta}R^{\alpha\beta} - \frac{2}{3}R^2 + \mathcal{G} \tag{4.87}$$

to re-express the Weyl-squared term where $\mathcal{G}$ is the Gauß-Bonnet invariant shown in (2.35), which is a total derivative (boundary term) that may be neglected for our purposes.

Though global scale symmetry is not clearly manifest in the action (4.86), indeed, it is precisely the action describing standard non-scale-invariant QG as in Stelle's proof of renormalizability, it is important to recall that SI may be realized non-linearly if one was to reintroduce the scalar kinetic term and calculate how the NG boson transforms under scale symmetry, similarly to the toy model demonstration in Section 2.2.2.

In order to proceed with the quantization of our theory using the methods established in Section 4.5, it will be greatly beneficial to first reorganize the DOFs by rewriting the fourth-order action (4.86) in an equivalent second-order form. This is most easily achieved by introducing auxiliary fields which we include by adding the term $\sqrt{-g}\,\frac{1}{4}H^{\alpha\beta}M_{\alpha\beta,\gamma\delta}H^{\gamma\delta}$ to the action, where $H_{\alpha\beta}(x)$ is an auxiliary tensor field and the rank-four "metric" M is defined according to

$$\begin{aligned} M_{\alpha\beta,\gamma\delta} &= \delta_{\alpha\beta\gamma\delta} - g_{\alpha\beta}g_{\gamma\delta} \\ {M^{-1}}^{\alpha\beta,\gamma\delta} &= \delta^{\alpha\beta\gamma\delta} - \frac{1}{3}g^{\alpha\beta}g^{\gamma\delta} \\ M_{\alpha\beta,\mu\nu}{M^{-1}}^{\mu\nu,\gamma\delta} &= \delta^{\gamma\delta}_{\alpha\beta}\,, \end{aligned} \tag{4.88}$$

with the rank-four identity matrix $\delta_{\alpha\beta\gamma\delta}$ defined in the usual way,

$$\delta_{\alpha\beta\gamma\delta} = \frac{1}{2}\big(g_{\alpha\gamma}g_{\beta\delta} + g_{\alpha\delta}g_{\beta\gamma}\big)\,. \tag{4.89}$$

Crucially, adding this kind of term to the action does not change the physics since the EOM that follows, $H_{\alpha\beta} = 0$, may easily be used to return the original set of EOMs for the metric. The trick here comes in the fact that this statement remains true if we shift $H \to H + cM^{-1}G$ for some constant c which, paired with the identity

$$R_{\alpha\beta}R^{\alpha\beta} - \frac{1}{3}R^2 = G_{\alpha\beta}{M^{-1}}^{\alpha\beta,\gamma\delta}G_{\gamma\delta} \tag{4.90}$$

where $G_{\alpha\beta} = R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R$ is the Einstein tensor, allows us to complete a square by writing

$$-\frac{c^2}{4}GM^{-1}G + \frac{1}{4}\big(MH + cG\big)^{\mathrm{T}}M^{-1}\big(MH + cG\big) = \frac{c}{2}GH + \frac{1}{4}HMH\,. \tag{4.91}$$

Then, with $c = 2\alpha_g^{-1}$, we may eliminate the Weyl-squared term (4.87) from the original action.

The other quadratic βR^2 term may be eliminated in an analogous way, just as it was in in Section 3.2 when we exposed the scalaron. This requires the introduction of an auxiliary scalar field $\chi(x)$ which, using the relation

$$\frac{\beta}{\alpha_g^2}R^2 - \frac{1}{\beta}\left(\frac{1}{2}\chi - \frac{\beta}{\alpha_g}R\right)^2 = \frac{1}{\alpha_g}R\chi - \frac{1}{4\beta}\chi^2\,, \tag{4.92}$$

allows us to establish the complete auxiliary action

$$S_{\mathrm{QGaux}} = \int \mathrm{d}^4x\,\sqrt{-g}\bigg[\frac{M_{\mathrm{Pl}}^2}{2}R + \frac{1}{\alpha_g}\Big(G_{\alpha\beta}H^{\alpha\beta} + R\chi\Big) + \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big) - \frac{1}{4\beta}\chi^2\bigg]. \tag{4.93}$$

It is then a simple matter to confirm that this action and (4.86) are classically equivalent by integrating out the auxiliary fields $H_{\alpha\beta}$ and χ with their EOMs,

$$H_{\alpha\beta} = -\frac{1}{\alpha_g}\left(2R_{\alpha\beta} - \frac{1}{3}g_{\alpha\beta}R\right) \qquad \chi = \frac{2\beta}{\alpha_g}R\,. \tag{4.94}$$

Naturally, due to the classical equivalence at the level of the EOMs, the auxiliary action (4.93) is invariant under local diffeomorphisms just as the original action is. These (infinitesimal) transformations act on each of the fields as

$$g'_{\alpha\beta} = g_{\alpha\beta} + \alpha_g\mathcal{L}_\xi g_{\alpha\beta} \qquad H'_{\alpha\beta} = H_{\alpha\beta} + \alpha_g\mathcal{L}_\xi H_{\alpha\beta} \qquad \chi' = \chi + \alpha_g\mathcal{L}_\xi\chi\,, \tag{4.95}$$

where $\mathcal{L}_\xi$ is the Lie derivative in the direction of the arbitrary vector field $\xi^\alpha(x)$. When viewed in the language of constrained systems [278], these four symmetries imply that S_{aux} generates a set of eight first-class constraints which eliminate sixteen of the forty-two DOFs in phase space, however, it is a well established fact that QG propagates eight independent DOFs; a massless spin-2 graviton, a massive spin-2 ghost, and a massive scalar [279]. This implies the existence of an additional ten second-class constraints according to Dirac's rule, $1/2(20 + 20 + 2 - 2*8 - \mathbf{10}) = 8$, whose presence is rather inconvenient for covariant quantization.

To get around this troublesome feature, we appeal to the Stückelberg mechanism which allows us to replace the second-class constraints in our system with first-class constraints by introducing new fields that enforce new gauge symmetries (which correspond to the new first-class constraints) [280]. This mechanism may be realized in the present theory by introducing both a vector $A_\alpha(x)$ and a scalar $\pi(x)$ through the replacement

$$H_{\alpha\beta} \;\;\rightarrow\;\; H_{\alpha\beta} - \big(\nabla_\alpha A_\beta + \nabla_\beta A_\alpha\big) + \frac{2}{m}\nabla_\alpha\nabla_\beta\pi\,, \tag{4.96}$$

which, applied to the action (4.93), yields the second-order action that will serve as a basis for all of our upcoming analyses,

$$\begin{aligned} S_{\mathrm{SOQG}} = \int \mathrm{d}^4x\,\sqrt{-g}\bigg[&\frac{m^2}{\alpha_g^2}R + \frac{1}{\alpha_g}(G_{\alpha\beta}H^{\alpha\beta} + R\chi) + \frac{1}{4}(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta) \\ &- \frac{1}{4\beta}\chi^2 + \frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} + (\nabla_\beta H_\alpha{}^\beta - \nabla_\alpha H_\beta{}^\beta)\Big(A^\alpha - \frac{1}{m}\nabla^\alpha\pi\Big) \\ &- R_{\alpha\beta}\Big(A^\alpha - \frac{1}{m}\nabla^\alpha\pi\Big)\Big(A^\beta - \frac{1}{m}\nabla^\beta\pi\Big)\bigg]. \end{aligned} \tag{4.97}$$

Here, we have integrated by parts and used the contracted Bianchi identity $\nabla^\alpha G_{\alpha\beta} = 0$ to simplify and collect terms, introduced the mass scale $m = \alpha_g M_{\rm Pl}/\sqrt{2}$, and written the standard field strength $F_{\alpha\beta} = \nabla_\alpha A_\beta - \nabla_\beta A_\alpha$. An important feature of the Stückelberg mechanism is its preservation of the physical content in a theory despite the introduction of new fields and symmetries. We may confirm that this occurs here by once again integrating out the auxiliary fields with the EOMs obtained from (4.97),

$$H_{\alpha\beta} = -\frac{1}{\alpha_g}\left(2R_{\alpha\beta} - \frac{1}{3}g_{\alpha\beta}R\right) + \nabla_\alpha A_\beta + \nabla_\beta A_\alpha - \frac{2}{m}\nabla_\alpha\nabla_\beta\pi \tag{4.98}$$

$$\chi = \frac{2\beta}{\alpha_g}R\,. \tag{4.99}$$

As previously eluded to, our second order action has acquired new gauge symmetries that correspond to the new first-class constraints introduced by the Stückelberg procedure. The first of these is associated with A_α and it acts on each of the fields as

$$\begin{aligned} &g'_{\alpha\beta} = g_{\alpha\beta} && H'_{\alpha\beta} = H_{\alpha\beta} + \nabla_\alpha\zeta_\beta + \nabla_\beta\zeta_\alpha && \chi' = \chi \\ &A'_\alpha = A_\alpha + \zeta_\alpha && \pi' = \pi\,, && \end{aligned} \tag{4.100}$$

where $\zeta_\alpha(x)$ is a local parameter of the transformation. Likewise, we find a new symmetry associated with π whose transformations are given by

$$\begin{aligned} &g'_{\alpha\beta} = g_{\alpha\beta} && H'_{\alpha\beta} = H_{\alpha\beta} && \chi' = \chi \\ &A'_\alpha = A_\alpha + \nabla_\alpha\sigma && \pi' = \pi + m\sigma\,, && \end{aligned} \tag{4.101}$$

in terms of the local parameter $\sigma(x)$. Naturally, the action (4.97) has maintained its original diffeomorphism invariance as well, where the new Stückelberg fields transform in terms of Lie derivatives just as the original fields in (4.95). Finally, we may confirm that the Stückelberg mechanism has worked as intended by counting the DOFs in our new action. After the introduction of A_α and π we find twenty-six fields and nine gauge symmetries which allows us to count $1/2(20 + 20 + 2 + 8 + 2 - 2 * 18) = 8$ DOFs as expected, without any second-class constraints.

4.6.2 Quantization

Gauge-fixing

In order to address the ghost problem that presents itself in the classical second-order theory we have just established, it must first be quantized. We follow the procedure outlined in Section 4.5 by first establishing a BRST symmetry in order to gauge fix the theory. This process will be similar to the BRST treatments of GR and massive spin-2 Fierz-Pauli theory carried out in [270] and [281], though the presence of additional gauge symmetries and ghosts will naturally complicate matters in the present case.

To begin, we define a set of BRST fields for the diffeomorphism, Stückelberg vector, and Stückelberg scalar symmetries,

$$\begin{aligned} B_a &= \{b_\alpha(x), B_\alpha(x), B(x)\} \\ C^a &= \{c^\alpha(x), C^\alpha(x), C(x)\} \\ \bar{C}_a &= \{\bar{c}_\alpha(x), \bar{C}_\alpha(x), \bar{C}(x)\}\,, \end{aligned} \tag{4.102}$$

where the B_a are bosonic NL fields and the C^a and $\bar{C}_a$ are fermionic FP ghosts and anti-ghosts which, despite the over-bar notation, are independent fields and not Hermitian conjugates of one another. Our next task is to establish a BRST-invariant gauge fixing action composed of the fields above for each of our three gauge symmetries, which requires that we establish how each field behaves under a BRST transformation.

In line with (4.62), the original five fields in the classical theory transform as a sum of their gauge transformations (4.95), (4.100), and (4.101) after replacing the gauge parameters with the appropriate FP ghosts:

$$\begin{aligned} \delta g_{\alpha\beta} &= \frac{\alpha_g}{m}\big(\nabla_\alpha c_\beta + \nabla_\beta c_\alpha\big) \\ \delta H_{\alpha\beta} &= m\big(\nabla_\alpha C_\beta + \nabla_\beta C_\alpha\big) + \frac{\alpha_g}{m}\big(\nabla_\gamma H_{\alpha\beta} + H_{\alpha\gamma}\nabla_\beta + H_{\beta\gamma}\nabla_\alpha\big)c^\gamma \\ \delta\chi &= \frac{\alpha_g}{m}\,c^\alpha\nabla_\alpha\chi \\ \delta A_\alpha &= mC_\alpha + \nabla_\alpha C + \frac{\alpha_g}{m}\big(\nabla_\beta A_\alpha + A_\beta\nabla_\alpha\big)c^\beta \\ \delta\pi &= mC + \frac{\alpha_g}{m}\,c^\alpha\nabla_\alpha\pi\,. \end{aligned} \tag{4.103}$$

The remaining nine new BRST fields then transform as

$$\begin{array}{lll} \delta b_\alpha = 0 & \delta B_\alpha = 0 & \delta B = 0 \\ \delta c^\alpha = \dfrac{\alpha_g}{m}c^\beta\partial_\beta c^\alpha & \delta C^\alpha = \dfrac{\alpha_g}{m}\big(c^\beta\partial_\beta C^\alpha + C^\beta\partial_\beta c^\alpha\big) & \delta C = \dfrac{\alpha_g}{m}\,c^\alpha\partial_\alpha C \\ \delta\bar{c}_\alpha = ib_\alpha & \delta\bar{C}_\alpha = iB_\alpha & \delta\bar{C} = iB\,. \end{array} \tag{4.104}$$

We proceed by selecting gauge fixing conditions $G_a = \{G^{(\xi)}_\alpha, G^{(\zeta)}_\alpha, G^{(\sigma)}\}$ for each symmetry which may in turn be used to generate our desired gauge fixing and FP ghost actions through the relation (4.63). We begin with the condition

$$G^{(\xi)}_\alpha = g^{\beta\gamma}\left(\partial_\gamma\tilde{g}_{\alpha\beta} - \frac{g_1}{2}\partial_\alpha\tilde{g}_{\beta\gamma}\right) + \frac{1}{2}b_\alpha \tag{4.105}$$

to fix diffeomorphism invariance, where

$$\tilde{g}_{\alpha\beta} = \frac{m}{\alpha_g}g_{\alpha\beta} - \frac{1}{m}\big(H_{\alpha\beta} - g_{\alpha\beta}\chi - \nabla_\alpha A_\beta - \nabla_\beta A_\alpha\big) - \frac{2}{m^2}\nabla_\alpha\nabla_\beta\pi \tag{4.106}$$

is defined so as to be invariant under both Stückelberg symmetries and thus only serves to break diffeomorphisms. The Stückelberg vector symmetry may be fixed the same spirit i.e. with the diffeomorphism and scalar-symmetry-invariant condition

$$G^{(\zeta)}_\alpha = \frac{1}{m}\left(\nabla_\beta H_\alpha{}^\beta - \frac{g_2}{2}\nabla_\alpha H_\beta{}^\beta + \nabla_\alpha\chi\right) - mA_\alpha + \nabla_\alpha\pi - \frac{1}{2}B_\alpha\,. \tag{4.107}$$

This leaves only the scalar symmetry, which we fix with the condition

$$G^{(\sigma)} = \nabla_\alpha A^\alpha - \frac{g_3}{2}H_\alpha{}^\alpha - \chi - m\pi - \frac{B}{2}\,. \tag{4.108}$$

The g_i in the above conditions are arbitrary constants akin to the ξ that appears in the R_ξ gauge-fixing scheme often employed in the SM [123]. These constants may be fixed to select analogues of some of the most commonly employed gauges in QFT, as we will see shortly. With all of the above we may write the gauge-fixed total action S_T as a sum of the classical action (4.97) and the BRST actions generated by our chosen gauge conditions through the relation (4.63):

$$\begin{aligned} S_\mathrm{T} &= S_\mathrm{SOQG} - i\int \mathrm{d}^4x\,\sqrt{-g}\,\delta\Big(\bar{c}^\alpha G^{(\xi)}_\alpha + \bar{C}^\alpha G^{(\zeta)}_\alpha + \bar{C}G^{(\sigma)}\Big) \\ &= S_\mathrm{SOQG} + S_{\mathrm{gf}\xi} + S_{\mathrm{gf}\zeta} + S_{\mathrm{gf}\sigma} + S_{\mathrm{FP}\xi} + S_{\mathrm{FP}\zeta} + S_{\mathrm{FP}\sigma}\,. \end{aligned} \tag{4.109}$$

This action describes the full interacting theory in the gravitational sector, however, it is the free part of the action that is quadratic in the dynamical fields that will be of most interest for our purposes. To isolate the free action we may perturb S_T around Minkowski space by expanding the metric according to

$$g_{\alpha\beta} \;\;\to\;\; \eta_{\alpha\beta} + \alpha_g h_{\alpha\beta}\,, \tag{4.110}$$

where we have singled out the coupling α_g as a small (dimensionless) perturbation parameter. Before writing the resulting free action, it is convenient to redefine the bare graviton $h_{\alpha\beta}(x)$ in terms of the Stückelberg-invariant graviton corresponding to the metric (4.106) as

$$\tilde{h}_{\alpha\beta} = mh_{\alpha\beta} - \frac{1}{m}\big(H_{\alpha\beta} - g_{\alpha\beta}\chi - \partial_\alpha A_\beta - \partial_\beta A_\alpha\big) - \frac{2}{m^2}\partial_\alpha\partial_\beta\pi \tag{4.111}$$

in order to simplify gauge fixing terms and diagonalize the spin-2 kinetic terms. We may also define

$$\tilde{H}_{\alpha\beta} = \frac{1}{m}H_{\alpha\beta} \qquad\qquad \tilde{\chi} = \frac{\sqrt{3}}{m}\chi \qquad\qquad \tilde{\pi} = \pi + \frac{1}{m}\chi \tag{4.112}$$

to normalize the auxiliary fields and diagonalize the scalar sector in a similar manner. All together, the graviton expansion and redefinitions above lead to the free action

$$S^{(0)}_\mathrm{T} = S^{(0)}_\mathrm{SOQG} + S^{(0)}_\mathrm{gf} + S^{(0)}_\mathrm{FP}\,, \tag{4.113}$$

$$\begin{aligned}
S^{(0)}_{\text{SOQG}} = \int \mathrm{d}^4x \bigg[&\frac{1}{2}\Big(\tilde{h}^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\tilde{h}^{\gamma\delta} - \tilde{H}^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\tilde{H}^{\gamma\delta}\Big) + \frac{m^2}{4}\Big(\tilde{H}_{\alpha\beta}\tilde{H}^{\alpha\beta} - \tilde{H}_\alpha{}^\alpha\tilde{H}_\beta{}^\beta\Big) \\
&+ \frac{1}{2}\tilde{\chi}\big(\Box - m_\beta^2\big)\tilde{\chi} - \frac{1}{2}A^\alpha\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)A^\beta \\
&+ mA_\alpha\Big(\partial_\beta\tilde{H}^{\alpha\beta} - \partial^\alpha\tilde{H}_\beta{}^\beta\Big) - \tilde{\pi}\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)\tilde{H}^{\alpha\beta}\bigg] \qquad (4.114)
\end{aligned}$$

$$\begin{aligned}
S^{(0)}_{\text{gf}} = \int \mathrm{d}^4x \bigg[&b_\alpha\Big(\partial_\beta\tilde{h}^{\alpha\beta} - \frac{g_1}{2}\partial^\alpha\tilde{h}_\beta{}^\beta + \frac{1}{2}b^\alpha\Big) \\
&+ B_\alpha\Big(\partial_\beta\tilde{H}^{\alpha\beta} - \frac{g_2}{2}\partial^\alpha\tilde{H}_\beta{}^\beta + \partial^\alpha\tilde{\pi} - mA^\alpha - \frac{1}{2}B^\alpha\Big) \\
&+ B\Big(\partial_\alpha A^\alpha - \frac{g_3 m}{2}\tilde{H}_\alpha{}^\alpha - m\tilde{\pi} - \frac{1}{2}B\Big)\bigg] \qquad (4.115)
\end{aligned}$$

$$\begin{aligned}
S^{(0)}_{\text{FP}} = i\int \mathrm{d}^4x \bigg[&\bar{c}^\alpha\big(\eta_{\alpha\beta}\Box + (1-g_1)\partial_\alpha\partial_\beta\big)c^\beta \\
&+ \bar{C}^\alpha\big(\eta_{\alpha\beta}\big(\Box - m^2\big) + (1-g_2)\partial_\alpha\partial_\beta\big)C^\beta \\
&+ \bar{C}\big(\big(\Box - m^2\big)C + m(1-g_3)\partial_\alpha C^\alpha\big)\bigg], \qquad (4.116)
\end{aligned}$$

where we have integrated by parts, dropped all $\mathcal{O}(\alpha_g)$ interaction terms, and identified the canonical mass of $\tilde{\chi}$ as $m_\beta^2 = m^2/(6\beta)$.

The spin-2 kinetic terms in (4.114) are defined in terms of the flat space Lichnerowicz operator (the kinetic operator of linearized GR)

$$\mathcal{E}_{\alpha\beta\gamma\delta} = E_{\alpha\beta\gamma\delta}\big|_{g_{\alpha\beta}=\eta_{\alpha\beta}}, \qquad (4.117)$$

where the general Lichnerowicz operator[8] is defined in terms of the Hessian of the Einstein-Hilbert Lagrangian as

$$\begin{aligned}
E_{\alpha\beta\gamma\delta} &= \frac{2}{\sqrt{-g}}\left(\frac{\partial^2\big(\sqrt{-g}R\big)}{\partial g_{\alpha\beta}\partial g_{\gamma\delta}}\right) \\
&= \frac{1}{2}\Big(\big(\delta_{\alpha\beta\gamma\delta} - g_{\alpha\beta}g_{\gamma\delta}\big)\nabla_\mu\nabla^\mu + g_{\alpha\beta}\nabla_\gamma\nabla_\delta + g_{\gamma\delta}\nabla_\alpha\nabla_\beta - \mathcal{D}_{\alpha\beta\gamma\delta}\Big) \\
&\quad + C_{\alpha(\gamma}{}^{\beta}{}_{\delta)} - \frac{1}{3}\Big(\delta_{\alpha\beta\gamma\delta} - \frac{1}{4}g_{\alpha\beta}g_{\gamma\delta}\Big)R, \qquad (4.118)
\end{aligned}$$

where we have defined the totally symmetric derivative operator

$$\mathcal{D}_{\alpha\beta\gamma\delta} = \frac{1}{2}\big(g_{\alpha\gamma}\nabla_\beta\nabla_\delta + g_{\alpha\delta}\nabla_\beta\nabla_\gamma + g_{\beta\gamma}\nabla_\alpha\nabla_\delta + g_{\beta\delta}\nabla_\alpha\nabla_\gamma\big). \qquad (4.119)$$

We also note that in the current parameterization, the gauge-invariant scalar $\tilde{\chi}$ (which may be identified as the scalaron familiar from Section 3.4.1) completely decouples from

[8] We thank Taichiro Kugo for pointing out this definition.

the rest of the free theory, a feature that will lead to a practically trivial quantization compared to the other fields.

As previously mentioned, our general choice of gauge fixing conditions allows us to investigate several realizations of well-known gauges in the present theory, the first of which corresponds to something like a unitary gauge after fixing the parameters to

$$\text{unitary gauge:} \qquad g_1 = 1 \qquad\qquad g_2 = 2 \qquad\qquad g_3 = 0\,. \tag{4.120}$$

Under this particular choice of parameters, it is possible to redefine $\tilde{H}_{\alpha\beta}$ in terms of a gauge-invariant tensor field reminiscent of the Proca field parameterization in the SM by writing

$$U_{\alpha\beta} = \tilde{H}_{\alpha\beta} - \frac{1}{m}\left(\partial_\alpha A_\beta + \partial_\beta A_\alpha\right) - \frac{1}{m^2}\left(\partial_\alpha B_\beta + \partial_\beta B_\alpha - 2\partial_\alpha\partial_\beta\tilde{\pi}\right). \tag{4.121}$$

After rewriting the action in terms of this "Proca" field, one finds that the classical part (4.114) reduces to

$$\begin{aligned} S^{(0)}_{\text{SOQG}} = \int \mathrm{d}^4x \Bigg[&\frac{1}{2}\Big(\tilde{h}^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\tilde{h}^{\gamma\delta} - U^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}U^{\gamma\delta}\Big) + \frac{m^2}{4}\Big(U_{\alpha\beta}U^{\alpha\beta} - U_\alpha{}^\alpha U_\beta{}^\beta\Big) \\ &+ \frac{1}{2}\tilde{\chi}\left(\Box - m_\beta^2\right)\tilde{\chi}\Bigg], \end{aligned} \tag{4.122}$$

where the Stückelberg fields have been eaten by $\tilde{H}_{\alpha\beta}$, leaving only a standard massless graviton, a (ghostly) massive spin-2 Fierz-Pauli field, and a scalaron behind. Just as in the unitary gauge SM, this gauge choice allows us to easily see the physical DOFs that result from our theory, however, it is quite inconvenient for practical calculations. This is in part because the gauge fixing and FP ghost actions become rather complicated in this gauge, despite the fact that $U_{\alpha\beta}$ is not present in them. However, the real issue lies in the UV-divergent behavior of the $U_{\alpha\beta}$ propagator which comes out like

$$-i\,\langle 0|TU_{\alpha\beta}U_{\gamma\delta}|0\rangle \sim \frac{p_\alpha p_\beta p_\gamma p_\delta}{m^4(p^2+m^2)}\,. \tag{4.123}$$

We will investigate this kind of unitary gauge and Proca parameterization in more detail with respect to conformal gravity later on, so for now, we will move forward with the present theory by considering a different specific gauge that is better suited for our purposes. This is the Feynman-style gauge defined by the parameters

$$\text{Feynman gauge:} \qquad g_1 = 1 \qquad\qquad g_2 = 1 \qquad\qquad g_3 = 1\,, \tag{4.124}$$

which leads to a much more manageable set of propagators with improved UV behavior. The full propagator matrix $\Omega^{-1}_{AB}(p)$ in this gauge is defined as the inverse of the Hessian matrix of the free total action:

$$\Omega^{AB}(p) = i\int \mathrm{d}^4x\,\frac{\delta^2 S^{(0)}_{\text{T}}}{\delta\Phi_A(x)\delta\Phi_B(y)}\,e^{-ip(x-y)} \tag{4.125}$$

$$\Omega^{-1}_{AB}(p) = -i \langle 0 | T\Phi_A \Phi_B | 0 \rangle = \begin{pmatrix} \Omega^{-1}_{\text{boson}} & 0 \\ 0 & \begin{pmatrix} 0 & \Omega^{-1}_{\text{ghost}} \\ \Omega^{-1\,\dagger}_{\text{ghost}} & 0 \end{pmatrix} \end{pmatrix}_{AB} , \tag{4.126}$$

$$\Omega^{-1}_{\text{boson}} =$$

$$\begin{array}{c} \\ \tilde{h}_{\alpha\beta} \\ \tilde{H}_{\alpha\beta} \\ \tilde{\chi} \\ A_\alpha \\ \tilde{\pi} \\ b_\alpha \\ B_\alpha \\ B \end{array}
\begin{array}{c}
\begin{array}{cccccccc} \tilde{h}_{\gamma\delta} & \tilde{H}_{\gamma\delta} & \tilde{\chi} & A_\gamma & \tilde{\pi} & b_\gamma & B_\gamma & B \end{array} \\
\begin{pmatrix}
\frac{-F_{\alpha\beta\gamma\delta}}{p^2} & 0 & 0 & 0 & 0 & \frac{-i(\eta_{\alpha\gamma}p_\beta+\eta_{\beta\gamma}p_\alpha)}{p^2} & 0 & 0 \\
 & \frac{G_{\alpha\beta\gamma\delta}}{p^2+m^2} & 0 & 0 & \frac{\eta_{\alpha\beta}}{3(p^2+m^2)} & 0 & \frac{-i(\eta_{\alpha\gamma}p_\beta+\eta_{\beta\gamma}p_\alpha)}{p^2+m^2} & 0 \\
 & & \frac{-1}{p^2+m_\beta^2} & 0 & 0 & 0 & 0 & 0 \\
 & & & \frac{\eta_{\alpha\gamma}}{p^2+m^2} & 0 & 0 & \frac{-m\eta_{\alpha\gamma}}{p^2+m^2} & \frac{-ip_\alpha}{p^2+m^2} \\
 & & & & \frac{1}{3(p^2+m^2)} & 0 & 0 & \frac{-m}{p^2+m^2} \\
 & \text{(h.c.)} & & & & 0 & 0 & 0 \\
 & & & & & & 0 & 0 \\
 & & & & & & & 0
\end{pmatrix}
\end{array}$$

$$\text{where} \qquad F_{\alpha\beta\gamma\delta} = 2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta} \qquad G_{\alpha\beta\gamma\delta} = 2\delta_{\alpha\beta\gamma\delta} - \frac{2}{3}\eta_{\alpha\beta}\eta_{\gamma\delta} \,, \tag{4.127}$$

$$\Omega^{-1}_{\text{ghost}} = \begin{array}{c} \\ c_\alpha \\ C_\alpha \\ C \end{array} \begin{array}{c} \begin{array}{ccc} \bar{c}_\gamma & \bar{C}_\gamma & \bar{C} \end{array} \\ \begin{pmatrix} \frac{-i\eta_{\alpha\gamma}}{p^2} & 0 & 0 \\ 0 & \frac{-i\eta_{\alpha\gamma}}{p^2+m^2} & 0 \\ 0 & 0 & \frac{-i}{p^2+m^2} \end{pmatrix} \end{array} . \tag{4.128}$$

We thus see that the Feynman gauge (4.124) has indeed led to a set of easily-manageable simple-pole propagators that are all convergent in the UV. This type of behavior may be seen in the covariant quantization of more standard theories when the same kind of gauge is chosen as well, in particular with respect to Yang-Mills theory [274], General Relativity [270], and Fierz-Pauli massive gravity [281].

Asymptotic fields

As outlined in Section 4.5.2, the next step in the covariant quantization process is to establish asymptotic solutions to the EOMs in terms of plane waves and oscillators. Varying the total action (4.113) in the Feynman gauge (4.124) with respect to the graviton, auxiliary fields, and Stückelberg fields yields the EOMs

$$\begin{aligned}
&\mathcal{E}_{\alpha\beta\gamma\delta}h^{\gamma\delta} + \partial_{(\alpha}b_{\beta)} - \frac{1}{2}\eta_{\alpha\beta}\partial_\gamma b^\gamma = 0 \\
&\mathcal{E}_{\alpha\beta\gamma\delta}H^{\gamma\delta} + \frac{m^2}{2}\Big(H_{\alpha\beta} - \eta_{\alpha\beta}H_\gamma{}^\gamma\Big) - m\Big(\partial_{(\alpha}A_{\beta)} - \eta_{\alpha\beta}\partial_\gamma A^\gamma\Big) \\
&\qquad - \big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)\pi - \partial_{(\alpha}B_{\beta)} + \frac{1}{2}\eta_{\alpha\beta}\partial_\gamma B^\gamma - \frac{m}{2}\eta_{\alpha\beta}B = 0
\end{aligned} \tag{4.129}$$

$$
\begin{aligned}
&\big(\Box - m_\beta^2\big)\chi = 0\\
&\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)A^\beta - m\Big(\partial_\beta H_\alpha{}^\beta - \partial_\alpha H_\beta{}^\beta\Big) + mB_\alpha + \partial_\alpha B = 0\\
&\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)H^{\alpha\beta} + \partial_\alpha B^\alpha + mB = 0\,,
\end{aligned}
$$

while the NL boson EOMs are found to be

$$
\begin{aligned}
&\partial_\beta h_\alpha{}^\beta - \frac{1}{2}\partial_\alpha h_\beta{}^\beta + b_\alpha = 0\\
&\partial_\beta H_\alpha{}^\beta - \frac{1}{2}\partial_\alpha H_\beta{}^\beta - mA_\alpha + \partial_\alpha\pi - B_\alpha = 0\\
&H_\alpha{}^\alpha - \frac{2}{m}\big(\partial_\alpha A^\alpha - B\big) + 2\pi = 0\,,
\end{aligned}
\tag{4.130}
$$

and the FP ghost EOMs are given by

$$
\begin{aligned}
&\Box c_\alpha = 0 && \Box\bar{c}_\alpha = 0\\
&\big(\Box - m^2\big)C^\alpha = 0 && \big(\Box - m^2\big)\bar{C}_\alpha = 0\\
&\big(\Box - m^2\big)C = 0 && \big(\Box - m^2\big)\bar{C} = 0\,.
\end{aligned}
\tag{4.131}
$$

We have dropped all of the tildes in the equations above to avoid clutter, however, one should keep in mind that we will always consider the canonically normalized fields defined in (4.111) and (4.112) from here on out.

The present gauge choice not only leads to nice UV behavior in the propagators (4.126), but it also allows for an easy oscillator decomposition of each field due to the fact that every propagator behaves as a simple pole. In the asymptotic limit (4.65), these decompositions may be written in terms of simple-pole oscillators only as

$$
\begin{aligned}
&h_{\alpha\beta}(x) = \hat{h}_{\alpha\beta}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && H_{\alpha\beta}(x) = \hat{H}_{\alpha\beta}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&\chi(x) = \hat{\chi}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && A_\alpha(x) = \hat{A}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&\pi(x) = \hat{\pi}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && b_\alpha(x) = \hat{b}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&B_\alpha(x) = \hat{B}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && B(x) = \hat{B}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&c^\alpha(x) = \hat{c}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && \bar{c}^\alpha(x) = \hat{\bar{c}}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&C^\alpha(x) = \hat{C}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && \bar{C}^\alpha(x) = \hat{\bar{C}}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\\
&C(x) = \hat{C}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) && \bar{C}(x) = \hat{\bar{C}}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})
\end{aligned}
\tag{4.132}
$$

where the appropriate sums over $\boldsymbol{p}$ and asymptotic “as” designations (see equation (4.66)) are silently understood. We may also realize the asymptotic versions of our chosen gauge fixing conditions by plugging in the asymptotic solutions above into the EOMs (4.129–4.131), keeping in mind the plane-wave identities listed in Appendix A, which yields

$$
p^\beta\hat{h}_{\alpha\beta}(\boldsymbol{p}) = \frac{1}{2}p_\alpha\hat{h}_\beta{}^\beta(\boldsymbol{p}) + i\hat{b}_\alpha(\boldsymbol{p})
\tag{4.133}
$$

$$p^\beta \hat{H}_{\alpha\beta}(\boldsymbol{p}) = im\left(\frac{p_\alpha p_\beta}{m^2} - \eta_{\alpha\beta}\right)\hat{A}^\beta(\boldsymbol{p}) - 2p_\alpha\hat{\pi}(\boldsymbol{p}) - i\hat{B}_\alpha(\boldsymbol{p}) - \frac{1}{m}p_\alpha\hat{B}(\boldsymbol{p}) \tag{4.134}$$

$$\hat{H}_\alpha{}^\alpha(\boldsymbol{p}) = \frac{2}{m}\Big(ip^\alpha\hat{A}_\alpha(\boldsymbol{p}) - \hat{B}(\boldsymbol{p})\Big) - 2\hat{\pi}(\boldsymbol{p})\,. \tag{4.135}$$

Finally, with our asymptotic decompositions in hand, we may establish commutator relations between each oscillator by simply reading off the coefficient of the pole ($-p^{-2}$ and $-(p^2+m^2)^{-1}$ for massless and massive fields respectively) in each entry of (4.126). We thus find that the non-zero (anti)commutators are given by

$$\begin{aligned}
&\Big[\hat{h}_{\alpha\beta}(\boldsymbol{p}), \hat{h}^\dagger_{\gamma\delta}(\boldsymbol{q})\Big] = \big(2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta}\big)\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{H}_{\alpha\beta}(\boldsymbol{p}), \hat{H}^\dagger_{\gamma\delta}(\boldsymbol{q})\Big] = -\Big(2\delta_{\alpha\beta\gamma\delta} - \frac{2}{3}\eta_{\alpha\beta}\eta_{\gamma\delta}\Big)\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{\chi}(\boldsymbol{p}), \hat{\chi}^\dagger(\boldsymbol{q})\Big] = \delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{A}_\alpha(\boldsymbol{p}), \hat{A}^\dagger_\beta(\boldsymbol{q})\Big] = -\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{\pi}(\boldsymbol{p}), \hat{\pi}^\dagger(\boldsymbol{q})\Big] = -\frac{1}{3}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{h}_{\alpha\beta}(\boldsymbol{p}), \hat{b}^\dagger_\gamma(\boldsymbol{q})\Big] = \Big[\hat{H}_{\alpha\beta}(\boldsymbol{p}), \hat{B}^\dagger_\gamma(\boldsymbol{q})\Big] = \big(ip_\alpha\eta_{\beta\gamma} + ip_\beta\eta_{\alpha\gamma}\big)\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{H}_{\alpha\beta}(\boldsymbol{p}), \hat{\pi}^\dagger(\boldsymbol{q})\Big] = -\frac{1}{3}\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{A}_\alpha(\boldsymbol{p}), \hat{B}^\dagger_\beta(\boldsymbol{q})\Big] = m\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{A}_\alpha(\boldsymbol{p}), \hat{B}^\dagger(\boldsymbol{q})\Big] = ip_\alpha\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big[\hat{\pi}(\boldsymbol{p}), \hat{B}^\dagger(\boldsymbol{q})\Big] = m\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big\{\hat{c}_\alpha(\boldsymbol{p}), \hat{\bar{c}}^\dagger_\beta(\boldsymbol{q})\Big\} = \Big\{\hat{C}_\alpha(\boldsymbol{p}), \hat{\bar{C}}^\dagger_\beta(\boldsymbol{q})\Big\} = i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\Big\{\hat{C}(\boldsymbol{p}), \hat{\bar{C}}(\boldsymbol{q})\Big\} = i\delta^3(\boldsymbol{p}-\boldsymbol{q})\,.
\end{aligned} \tag{4.136}$$

Naturally, we are also interested in the (anti)commutator relations between asymptotic fields, though in the present theory that contains only simple-poles, these quantities may easily be read from the oscillator relations above and we will thus refrain from writing them all out explicitly here. For example, we may pass to the continuum limit (4.78) and find

$$\big[h_{\alpha\beta}(x), h_{\gamma\delta}(y)\big] = \big(2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta}\big)D(x-y) \tag{4.137}$$

in line with the discussion around (4.76), which may be compared with the first entry in (4.136). The same kind of relation then holds for all the other field commutators. With this, our theory is fully quantized and may be analyzed using all the techniques of operator QFT.

However, before proceeding, it is important to also nail down the BRST transformation properties of each fundamental oscillator by plugging the decompositions (4.132) into the transformation rules (4.103) and (4.104):

$$\begin{aligned}
&\left[\mathcal{Q}, \hat{h}_{\alpha\beta}\right] = 2p_{(\alpha}\hat{c}_{\beta)} && \left[\mathcal{Q}, \hat{H}_{\alpha\beta}\right] = 2p_{(\alpha}\hat{C}_{\beta)} \\
&\left[\mathcal{Q}, \hat{\chi}\right] = 0 && \left[\mathcal{Q}, \hat{A}_{\alpha}\right] = -im\hat{C}_{\alpha} + p_{\alpha}\hat{C} \\
&\left[\mathcal{Q}, \hat{\pi}\right] = -im\hat{C} && \left[\mathcal{Q}, \hat{B}_{a}\right] = 0 \\
&\left\{\mathcal{Q}, \hat{C}_{a}\right\} = 0 && \left\{\mathcal{Q}, \hat{\bar{C}}_{a}\right\} = \hat{B}_{a} \,.
\end{aligned} \tag{4.138}$$

Here we have used the relation (4.60) to express these transformations in terms of (anti)commutators with the BRST charge operator to aid us in the final part of our analyses – an establishment of the subspace of physical states in quadratic gravity and an investigation of unitarity.

4.6.3 Unitarity

The quartet mechanism

Unitarity may be formally established in the SM by appealing to the Kugo-Ojima quartet mechanism, as outlined in Section 4.5.3. We recall that this mechanism hinges on separating all of the states in our theory into BRST-invariant physical states and quartet states that satisfy the relation (4.83), repeated here for convenience:

$$\langle \pi_{-1} | \delta_1 \rangle = \langle \pi_{-1} | \, \mathcal{Q} \, | \pi_0 \rangle = \langle \delta_0 | \pi_0 \rangle \neq 0 \,. \tag{4.139}$$

Though application of this mechanism alone is not enough to demonstrate unitarity in QG due to the presence of physical ghosts, it is still important to identify which states are truly physical and which are unphysical remnants of the gauge freedom present in the original theory before we tackle the additional problems brought on by fourth-order derivatives in our classical action.

Beginning with the massless sector, we consider the graviton in the reference frame (4.73) and use the oscillator gauge conditions (4.133) to express four of the ten components of $\hat{h}_{\alpha\beta}$ in terms of $\hat{b}_{\alpha}$ as

$$\begin{aligned}
&\hat{h}_{01} = -\hat{h}_{13} + \frac{i}{E}\hat{b}_1 && \hat{h}_{02} = -\hat{h}_{23} + \frac{i}{E}\hat{b}_2 \\
&\hat{h}_{03} = -\frac{1}{2}\big(\hat{h}_{00} + \hat{h}_{33}\big) + \frac{i}{2E}\big(\hat{b}_0 + \hat{b}_3\big) && \hat{h}_{22} = -\hat{h}_{11} + \frac{i}{E}\big(\hat{b}_0 - \hat{b}_3\big) \,.
\end{aligned} \tag{4.140}$$

This leaves six more components to fill the roles of gauge-invariant physical states and π_0 quartet members. Using the transformations (4.138), it is straightforward to identify the physical BRST singlet states as

$$\hat{a}_{h,+} = \frac{1}{2}\Big(\hat{h}_{11} - \hat{h}_{22}\Big) \qquad\qquad \hat{a}_{h,\times} = \hat{h}_{12} \,, \tag{4.141}$$

which, being transverse singlets, commute with the BRST charge ($[\mathcal{Q}, \hat{a}_{h,j}] = 0$) and have non-vanishing commutation relations only with themselves,

$$\left[\hat{a}_{h,j}(\boldsymbol{p}), \hat{a}^{\dagger}_{h,j'}(\boldsymbol{q})\right] = \delta_{jj'}\delta^3(\boldsymbol{p}-\boldsymbol{q})\,. \tag{4.142}$$

We have named the two independent polarizations $j = \{+, \times\}$ above in order to reinforce the fact that the states (4.141) represent the familiar "plus" and "cross" polarizations of weak-field GR. This identification is reinforced by decomposing the graviton oscillator as

$$\hat{h}_{\alpha\beta}(\boldsymbol{p}) = \sum_j \left(\varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}_{h,j}(\boldsymbol{p})\right) + \cdots + (\text{h.c.})\,, \tag{4.143}$$

where $\varepsilon_{j\,\alpha\beta}$ are the transverse-traceless polarization tensors derived in Section 4.5.2. It is important to stress that no a priori assumptions were made about the polarizations of the physical modes in this theory, rather, the required spin-2 representations of the Poincaré group appear naturally after considering the behavior of the fundamental oscillators under BRST transformation.

The "$\cdots$" in (4.143) are composed of the remaining four longitudinal (unphysical) graviton states and after once again considering the transformations (4.138), it becomes clear that these states may be most conveniently parameterized in terms of the vector oscillator

$$\left(\hat{\psi}_\alpha\right) = \frac{i}{2E}\begin{pmatrix} -\hat{h}_{00} \\ 2\hat{h}_{13} \\ 2\hat{h}_{23} \\ \hat{h}_{33} \end{pmatrix} \tag{4.144}$$

where they naturally fill the π_0 role in the quartets, being that they are BRST-non-invariant. Indeed, one may derive the transformations

$$\left[\mathcal{Q}, \hat{\psi}_\alpha\right] = i\hat{c}_\alpha \qquad \left[\mathcal{Q}, \hat{b}_\alpha\right] = 0 \qquad \{\mathcal{Q}, \hat{c}_\alpha\} = 0 \qquad \left\{\mathcal{Q}, \hat{\bar{c}}_\alpha\right\} = \hat{b}_\alpha\,, \tag{4.145}$$

to confirm this role and see that the other δ_0, δ_1, and π_{-1} roles must be played by $\hat{b}_\alpha$, $\hat{c}_\alpha$, and $\hat{\bar{c}}_\alpha$ respectively. Then, after noting that these quartet participants commute with each other according to

$$\left[\hat{\psi}_\alpha(\boldsymbol{p}), \hat{b}^{\dagger}_\beta(\boldsymbol{q})\right] = -\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \qquad \left\{\hat{c}_\alpha(\boldsymbol{p}), \hat{\bar{c}}^{\dagger}_\beta(\boldsymbol{q})\right\} = i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\,, \tag{4.146}$$

we may confirm that the massless quartet mechanism functions as required through the relation

$$\langle 0|\hat{b}_\alpha(\boldsymbol{p})\hat{\psi}^{\dagger}_\beta(\boldsymbol{q})|0\rangle = -i\,\langle 0|\hat{\bar{c}}_\alpha(\boldsymbol{p})\hat{c}^{\dagger}_\beta(\boldsymbol{q})|0\rangle = -\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\,. \tag{4.147}$$

The massive quartet mechanism functions in much the same way as the massless, though here we consider the center of mass frame defined in (4.74) and find that the following five operators represent gauge-invariant singlet components of $\hat{H}_{\alpha\beta}$ after applying the gauge conditions (4.134) and (4.135):

$$\begin{aligned} \hat{a}_{H,+} &= \frac{1}{2}\Big(\hat{H}_{11} - \hat{H}_{22}\Big) & \hat{a}_{H,\times} &= \hat{H}_{12} \\ \hat{a}_{H,1} &= \hat{H}_{13} & \hat{a}_{H,2} &= \hat{H}_{23} \\ \hat{a}_{H,3} &= \frac{1}{2\sqrt{3}}\Big(\hat{H}_{11} + \hat{H}_{22} - 2\hat{H}_{33}\Big) . \end{aligned} \tag{4.148}$$

Naturally, due to the fact that these operators represent physical ghost states, they commute with the BRST charge ($[\mathcal{Q}, \hat{a}_{H,k}] = 0$) and the commutation relations among them appear with a relative minus sign as compared to (4.142),

$$\Big[\hat{a}_{H,k}(\boldsymbol{p}), \hat{a}^{\dagger}_{H,k'}(\boldsymbol{q})\Big] = -\delta_{kk'}\delta^3(\boldsymbol{p}-\boldsymbol{q}) . \tag{4.149}$$

Here we have written $k = \{+, \times, 1, 2, 3\}$ to designate the five independent transverse polarizations (see Section 4.5.2) contained in $\hat{H}_{\alpha\beta}$ as

$$\hat{H}_{\alpha\beta}(\boldsymbol{p}) = \sum_k \Big(\varepsilon_{k\,\alpha\beta}(\boldsymbol{p})\hat{a}_{H,k}(\boldsymbol{p})\Big) + \cdots + (\text{h.c.}) . \tag{4.150}$$

All of the independent components of $\hat{H}_{\alpha\beta}$ have thus been accounted for, meaning that unlike in the massless sector where some graviton components played the π_0 role, the quartets in this sector must be made up of purely auxiliary and BRST fields. The oscillator transformations (4.138) once again allow for a straightforward identification of the π_0 operators as

$$\Big(\hat{\Psi}_\alpha\Big) = -\frac{1}{m}\begin{pmatrix} \hat{A}_0 + i\hat{\pi} \\ \hat{A}_1 \\ \hat{A}_2 \\ \hat{A}_3 \end{pmatrix} \qquad \hat{\Psi} = -\frac{1}{m}\hat{\pi} , \tag{4.151}$$

while the δ_0, δ_1, and π_{-1} roles are filled by the remaining BRST fields in an analogous fashion to the massless case. One finds as expected that all of the massive quartet participants transform according to

$$\Big[\mathcal{Q}, \hat{\Psi}_\alpha\Big] = i\hat{C}_\alpha \qquad \Big[\mathcal{Q}, \hat{B}_\alpha\Big] = 0 \qquad \Big\{\mathcal{Q}, \hat{C}_\alpha\Big\} = 0 \qquad \Big\{\mathcal{Q}, \hat{\bar{C}}_\alpha\Big\} = \hat{B}_\alpha \tag{4.152}$$

$$\Big[\mathcal{Q}, \hat{\Psi}\Big] = i\hat{C} \qquad \Big[\mathcal{Q}, \hat{B}\Big] = 0 \qquad \Big\{\mathcal{Q}, \hat{C}\Big\} = 0 \qquad \Big\{\mathcal{Q}, \hat{\bar{C}}\Big\} = \hat{B} , \tag{4.153}$$

and commute with themselves following

$$\Big[\hat{\Psi}_\alpha(\boldsymbol{p}), \hat{B}^{\dagger}_{\beta}(\boldsymbol{q})\Big] = -\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \qquad \Big\{\hat{C}_\alpha(\boldsymbol{p}), \hat{\bar{C}}^{\dagger}_{\beta}(\boldsymbol{q})\Big\} = i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \tag{4.154}$$

$$\left[\hat{\Psi}(\boldsymbol{p}), \hat{B}^\dagger(\boldsymbol{q})\right] = -\delta^3(\boldsymbol{p}-\boldsymbol{q}) \qquad \left\{\hat{C}(\boldsymbol{p}), \hat{\bar{C}}^\dagger(\boldsymbol{q})\right\} = i\delta^3(\boldsymbol{p}-\boldsymbol{q})\,. \tag{4.155}$$

With this, we encounter the required realizations of the massive quartet mechanism as confirmed by the relations

$$\langle 0|\hat{B}_\alpha(\boldsymbol{p})\hat{\Psi}^\dagger_\beta(\boldsymbol{q})|0\rangle = -i\,\langle 0|\hat{\bar{C}}_\alpha(\boldsymbol{p})\hat{C}^\dagger_\beta(\boldsymbol{q})|0\rangle = -\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \tag{4.156}$$

$$\langle 0|\hat{B}(\boldsymbol{p})\hat{\Psi}^\dagger(\boldsymbol{q})|0\rangle = -i\,\langle 0|\hat{\bar{C}}(\boldsymbol{p})\hat{C}^\dagger(\boldsymbol{q})|0\rangle = -\delta^3(\boldsymbol{p}-\boldsymbol{q})\,. \tag{4.157}$$

As a final note, we address the physical scalar sector that is fully populated by $\hat{\chi}$. Due to the fact that $\chi(x)$ is gauge-invariant before even introducing any BRST fields (none of which it interacts with), there is no quartet mechanism to be realized in this sector. Furthermore, due to the relative plus sign in its only non-vanishing commutation relation

$$\left[\hat{\chi}(\boldsymbol{p}), \hat{\chi}^\dagger(\boldsymbol{q})\right] = \delta^3(\boldsymbol{p}-\boldsymbol{q})\,, \tag{4.158}$$

χ contributes only independent and unitary interactions to the overall picture. We will thus put this scalar sector aside for the remainder of this work and focus on the remaining seven physical DOFs in the spin-2 sector: the two massless healthy graviton states and the five massive ghostly states corresponding to $H_{\alpha\beta}$.

Conditional unitarity in quadratic gravity

We begin our investigations of unitarity in the physical spin-2 subspace by constructing the physical Hamiltonian operator $\mathcal{H}$. This operator is subject to the Heisenberg equation

$$[\mathcal{H}, \phi_a(x)] = -i\partial_0\phi_a(x)\,, \tag{4.159}$$

where $\phi_a(x) = \{h_{\alpha\beta}(x),\, H_{\alpha\beta}(x)\}$, and may be solved for using the decompositions (4.132) along with the relation

$$i\partial_0 f_{\boldsymbol{p}}(x) = p^0 f_{\boldsymbol{p}}(x)\,, \tag{4.160}$$

which yields

$$\mathcal{H} = \int \mathrm{d}^3\boldsymbol{p} \sum_{j,k} \left(E_h \hat{a}^\dagger_{h,j}(\boldsymbol{p})\hat{a}_{h,j}(\boldsymbol{p}) - E_H \hat{a}^\dagger_{H,k}(\boldsymbol{p})\hat{a}_{H,k}(\boldsymbol{p})\right). \tag{4.161}$$

We have expressed $\mathcal{H}$ as normal ordered with respect to the positive energy choice of vacuum as defined by

$$\hat{a}_{h,j}(\boldsymbol{p})\,|0\rangle = \hat{a}_{H,k}(\boldsymbol{p})\,|0\rangle = 0\,, \tag{4.162}$$

per the discussion in Section 4.2.1. This feature is made apparent by considering the commutation relations (4.142) and (4.149) which imply that the Hamiltonian (4.161) commutes with each of the state operators according to

$$\left[\mathcal{H}, \hat{a}^{\dagger}_{h,j}(\boldsymbol{p})\right] = E_h \hat{a}^{\dagger}_{h,j}(\boldsymbol{p}) \qquad\qquad \left[\mathcal{H}, \hat{a}^{\dagger}_{H,k}(\boldsymbol{p})\right] = E_H \hat{a}^{\dagger}_{H,k}(\boldsymbol{p})\,, \tag{4.163}$$

thus generating independent one-particle eigenstates with positive eigenvalues for each operator as desired.

Now, following the LSZ formalism as laid out by Kugo and Ojima in [270], we may make the assumption that the asymptotic "in" and "out" Fock spaces in our theory are complete,

$$\mathcal{V}^{\text{in}} = \mathcal{V}^{\text{out}} = \mathcal{V}\,, \tag{4.164}$$

and that there exists a pseudo-unitary ($S^{\dagger}S = SS^{\dagger} = \mathbb{1}$) S-matrix operator S with elements defined by

$$S_{\alpha\beta} = \langle\beta;\text{out}|\alpha;\text{in}\rangle = \langle\beta;\text{in}|S|\alpha;\text{in}\rangle\;, \tag{4.165}$$

where $|\alpha\rangle$ and $|\beta\rangle$ are arbitrary external states in the Fock space on which S is defined. Reiterating the discussion in Section 4.5.3, we may define the physical transverse subspace of $\mathcal{V}$ (the BRST cohomology space) as

$$\mathcal{V}_{\text{tr}} = \mathcal{V}_{\text{phys}}/\mathcal{V}_0 = \text{Ker}\mathcal{Q}/\text{Im}\mathcal{Q} \tag{4.166}$$

and note that $\mathcal{V}_{\text{phys}} = S\mathcal{V}_{\text{phys}} = S^{\dagger}\mathcal{V}_{\text{phys}}$ due to the fact that $\mathcal{V}_{\text{phys}}$ is invariant under time evolution thanks to $\mathcal{Q}$ being a conserved quantity.

In the usual formulation of covariantly quantized gauge theories, $\mathcal{V}$ is generally an indefinite-metric space that is restricted to the positive-semidefinite subspace $\mathcal{V}_{\text{phys}}$ through the quartet mechanism which confines all positivity-spoiling longitudinal modes and identifies the BRST co-boundary $\mathcal{V}_0$ as the zero-norm subspace of $\mathcal{V}_{\text{phys}}$. In this case, $\mathcal{V}_{\text{tr}}$ is then necessarily a positive-definite metric space, and unitarity of S on $\mathcal{V}_{\text{tr}}$ follows from the relation

$$\begin{aligned} 1 &= \langle\alpha;\text{in}|\alpha;\text{in}\rangle = \langle\alpha;\text{in}|S^{\dagger}S|\alpha;\text{in}\rangle \\ &= \sum_n \langle\alpha;\text{in}|S^{\dagger}|n;\text{in}\rangle\,\langle n;\text{in}|S|\alpha;\text{in}\rangle = \sum_n \left|\,\langle n;\text{in}|S|\alpha;\text{in}\rangle\,\right|^2, \end{aligned} \tag{4.167}$$

where $|\alpha\rangle$ is an arbitrary (normalized) external state in $\mathcal{V}_{\text{tr}}$, $|n\rangle$ represents some n-particle external state also in $\mathcal{V}_{\text{tr}}$, and the completeness relation $\mathbb{1} = \sum_n |n;\text{in}\rangle\,\langle n;\text{in}|$ has been inserted between $S^{\dagger}$ and S. With this, the general notion of the quantum probability for the state transition $\alpha \to n$ to occur may be expressed as

$$\left|\,\langle n;\text{in}|S|\alpha;\text{in}\rangle\,\right|^2 < 1\,. \tag{4.168}$$

In other words, it is sufficient to demonstrate that the relation (4.167) holds in order to establish unitarity in a given theory.

There is however an important caveat to the demonstration of unitarity through (4.167), namely, that the positive-definiteness of $\mathcal{V}_{\text{tr}}$ is not guaranteed by the quartet mechanism alone, but also relies on the value of the inner product (the commutation relations) between the arbitrary state operators α. In traditional gauge theories these inner products are always positive, however, this is not the case in the present theory where the $\hat{a}_{H,k}$ commutators (4.149) appear with a relative minus. Despite the fact that $\mathcal{V}_{\text{tr}}$ contains no longitudinal or zero-norm modes thanks to the quartet mechanism, this indicates that $\mathcal{V}_{\text{tr}}$ as a whole is in fact an indefinite space and that the first equality in (4.167) does not hold in general, similarly to the toy model of ghost decay we encountered in Section 4.2.2. We thus finally confront the true heart of the ghost problem in the present theory since we are unable to confirm the relation (4.167) and demonstrate unitarity through a sensible interpretation of probability. It is also important to recall that choosing the other negative energy vacuum does not resolve the issue since we encounter inconsistencies with the $i\epsilon$ prescription and a violation of causality before even reaching this point in the discussion.

Even though unitarity is violated on $\mathcal{V}_{\text{tr}}$ as a whole, there is still hope for quadratic gravity as a quantum theory (possible complete resolutions aside) through the notion of conditional unitarity introduced in Section 4.3. The fact that the massive spin-2 ghost is the only source of negative norm means that we may easily define a positive-definite subspace of $\mathcal{V}_{\text{tr}}$ by projecting the ghosts out kinematically. To this end, we consider $\mathcal{V}_{\text{tr}}$ in a basis spanned by the total four-momentum eigenstates $|p_T, j\rangle$ and find that the subspace[9] populated by interactions with a total four-momentum that is less than the ghost mass,

$$\mathcal{V}_{\text{tr}}^{<} = \left\{ |p_T, j\rangle \, ; \, -p_T^2 < m^2 \right\}, \tag{4.169}$$

is indeed positive-definite. $\mathcal{V}_{\text{tr}}^{<}$ contains no ghosts (by definition), which implies that all inner products in this space are positive-definite and leads to the usual demonstration of unitarity on $\mathcal{V}_{\text{tr}}^{<}$ through the relation (4.167). It is also important to point out that when viewing conditional unitarity in the context of perturbation theory, one should replace the kinematical condition in (4.169) with

$$p_T^2 + m^2 \gtrsim \mathcal{O}\big(m^2\big)\,, \tag{4.170}$$

in order to ensure that the spin-2 ghost propagator $\sim (p_T^2 + m^2 - i\epsilon)^{-1}$ is sufficiently suppressed. Furthermore, we note that the notion of meta-stability such as that discussed in [218] has no bearing on our perturbative conditional unitarity simply due to the fact that meta-stability is a non-perturbative effect that does not appear in this context.

As a final point of order, we stress the fact that considering QG in the picture of conditional unitarity does not mean that ghosts are completely absent from the theory; they are only excluded from the space of possible external (asymptotic) states and may still mediate loop interactions. Indeed, conditional unitarity may be assumed in the

[9] It should be noted that $\mathcal{V}_{\text{tr}}^{<}$ is Lorentz invariant simply due to the fact that its supspace $\mathcal{V}_{\text{tr}} = \mathcal{V}_{\text{phys}}/\mathcal{V}_0$ is Lorentz invariant [270].

model of inflation presented in Section 3.4.1 where the ghosts contribute in important ways to the quantum effective potential, despite the fact that interaction energies related to inflation need never reach values near the ghost mass.

4.7 Quantum conformal gravity

Most of our analyses up to this point have been based on globally scale-invariant quadratic gravity though, as mentioned in the Introduction, this theory's locally invariant cousin also represents a very theoretically appealing upgrade to Einstein's GR. Despite the fact that Weyl symmetry is known to be anomalous, it is nevertheless worthwhile to quantize as if there would be no anomaly since it is a purely quantum effect whose presence may only be established after quantization. The remainder of this work will thus be focused on quantum conformal gravity and another investigation of the ghost problem therein, albeit from a more academic perspective barring any workarounds of the conformal anomaly.

After establishing a classical second-order action describing CG, we will take a brief aside to look at how the theory lends itself to a description of the current universe after the spontaneous breaking of conformal symmetry. However, in an effort to avoid repeating analyses that would almost exactly mimic those carried out in the case of QG with broken scale symmetry, we will restrict ourselves to the case of unbroken conformal symmetry when tackling the ghost problem here which, as we will see, leads to an entirely new theoretical take on the issue.

4.7.1 Second-order conformal gravity

The action that describes Weyl's conformal gravity may be derived in a similar manner to the action (4.86) of globally scale-invariant quadratic gravity though, with the requirement of local conformal invariance, no βR^2 term is allowed in the action since the Ricci scalar transforms non-linearly under conformal symmetry. Neglecting this term, as well as total derivatives, grants us the fourth-order gravitational action

$$S_{\mathrm{CG}} = -\frac{1}{\alpha_g^2}\int \mathrm{d}^4x\,\sqrt{-g}\left(R_{\alpha\beta}R^{\alpha\beta} - \frac{1}{3}R^2\right), \tag{4.171}$$

which is invariant under both infinitesimal local diffeomorphisms and Weyl transformations. Despite the fact that neither the Ricci tensor or Ricci scalar transform linearly under conformal symmetry, the relative factor of $-1/3$ in (4.171) ensures that the transformations of each term cancel exactly (up to total derivatives), thus ensuring conformal invariance of the action as a whole.

Following the same line of logic used in our analysis of the globally invariant theory in Section (4.6.1), our next task is rewrite CG in a more manageable form that is second-order in derivatives and produces only first-class constraints. To this end, we employ the same auxiliary field trick as in (4.91) and consider the action

$$S_{\text{CGaux}} = \int \mathrm{d}^4x \sqrt{-g} \left[\frac{1}{\alpha_g} G_{\alpha\beta} H^{\alpha\beta} + \frac{1}{4} \left(H_{\alpha\beta} H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta \right) \right] , \tag{4.172}$$

which is classically equivalent to the fourth-order action (4.171) after integrating out the auxiliary field. We note that since the present theory contains no fourth-order βR^2 term in the original action, no auxiliary χ is required to establish equivalence here. The further rewriting of (4.172) into a first-class theory through the introduction of Stückelberg fields and symmetries also requires fewer extra components in CG than it does in QG. No scalar like $\pi(x)$ need be included, only the vector field $A_\alpha(x)$ through the replacement

$$H_{\alpha\beta} \quad \to \quad H_{\alpha\beta} - \left(\nabla_\alpha A_\beta + \nabla_\beta A_\alpha \right) , \tag{4.173}$$

which may be compared with (4.96). Then, after applying this replacement to (4.172), we arrive at an action describing second-order CG that will serve as the classical starting point for the remainder of our work:

$$\begin{aligned} S_{\text{SOCG}} = \int \mathrm{d}^4x \sqrt{-g} \bigg[& \frac{1}{\alpha_g} G_{\alpha\beta} H^{\alpha\beta} + \frac{1}{4} \left(H_{\alpha\beta} H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta \right) \\ & + \frac{1}{4} F_{\alpha\beta} F^{\alpha\beta} + A_\alpha \Big(\nabla_\beta H^{\alpha\beta} - \nabla^\alpha H_\beta{}^\beta - A_\beta R^{\alpha\beta} \Big) \bigg] . \end{aligned} \tag{4.174}$$

It is straightforward to confirm that this action is indeed physically equivalent to the original action by integrating out the auxiliary and Stückelberg fields using the $H_{\alpha\beta}$ EOM,

$$H_{\alpha\beta} = -\frac{1}{\alpha_g} \left(2R_{\alpha\beta} - \frac{1}{3} g_{\alpha\beta} R \right) + \nabla_\alpha A_\beta + \nabla_\beta A_\alpha , \tag{4.175}$$

which returns (4.171) as desired.

In addition to invariance under the infinitesimal diffeomorphisms

$$\begin{aligned} g'_{\alpha\beta} &= g_{\alpha\beta} + \alpha_g \left(\nabla_\alpha \xi_\beta + \nabla_\beta \xi_\alpha \right) \\ H'_{\alpha\beta} &= H_{\alpha\beta} + \alpha_g \left(H_{\alpha\gamma} \nabla_\beta \xi^\gamma + H_{\beta\gamma} \nabla_\alpha \xi^\gamma + \xi^\gamma \nabla_\gamma H_{\alpha\beta} \right) \\ A'_\alpha &= A_\alpha + \alpha_g \left(A_\beta \nabla_\alpha \xi^\beta + \xi^\beta \nabla_\beta A_\alpha \right) , \end{aligned} \tag{4.176}$$

and infinitesimal Weyl transformations

$$\begin{aligned} g'_{\alpha\beta} &= g_{\alpha\beta} + \alpha_g \, \omega g_{\alpha\beta} \\ H'_{\alpha\beta} &= H_{\alpha\beta} + 2\nabla_\beta \nabla_\alpha \omega - \alpha_g \left(A_\alpha \nabla_\beta \omega + A_\beta \nabla_\alpha \omega - g_{\alpha\beta} A_\gamma \nabla^\gamma \omega \right) \\ A'_\alpha &= A_\alpha , \end{aligned} \tag{4.177}$$

the action (4.172) has also acquired an additional gauge symmetry as part of the Stückelberg mechanism. Naturally, this new symmetry acts analogously to the vector symmetry (4.100) that we introduced in the previous study:

$$g'_{\alpha\beta} = g_{\alpha\beta} \qquad H'_{\alpha\beta} = H_{\alpha\beta} + \nabla_\alpha \zeta_\beta + \nabla_\beta \zeta_\alpha \qquad A'_\alpha = A_\alpha + \zeta_\alpha . \tag{4.178}$$

To reiterate our previous discussions, the utility of this symmetry lies in the fact that it allows us to exchange second-class constraints for first-class constraints in the Hamiltonian picture. In other words, the introduction of the vector field A_α and the associated symmetry above may be viewed as a simple change of variables in phase space. After this change of variables, our action presents twenty-four fields and nine gauge symmetries, thus implying $1/2(20+20+8-2*18)=6$ DOFs through Dirac's formula. This matches the expected six independent massless DOFs of CG: a spin-2 graviton, a spin-2 ghost, and a spin-1 vector that may appear as a standard particle or as a ghost depending on the overall sign of the action [282].

The Higgs mechanism in conformal gravity

Before following the track laid out in the last section and performing a complete covariant quantization of conformal gravity, it is a good time to take a brief aside to discuss another interesting feature of the theory at hand. We have already seen how globally scale-invariant QG can generate a standard Einstein-Hilbert term after coupling to a scalar that acquires a VEV through SSB, a feature that is crucial for making touch with the low energy physics we observe in the current universe. The same general type of behavior may naturally occur in CG as well, and since the symmetry is local in this case, we will see that the generation of the Einstein-Hilbert action and mass scales in general follows very analogously to the Higgs mechanism in the SM wherein gauge bosons acquire mass terms when the scalar coupled to them acquires a non-zero VEV.

In addition to our freshly derived second-order action for CG, we consider the familiar action below,

$$S_\phi = \int \mathrm{d}^4x\,\sqrt{-g}\left(\frac{1}{2}\partial_\alpha\phi\partial^\alpha\phi + \frac{1}{12}\phi^2 R + U(\phi)\right), \tag{4.179}$$

which describes a real dilaton $\phi(x)$ conformally coupled to gravity with some potential $U(\phi)$ that we take to be conformally invariant. This is nothing more than the scalar part of the action (3.37) that we investigated with respect to inflation, with the previously arbitrary matter-gravity coupling now set to $\beta = 1/6$. Fixing the coupling this way is the only way to ensure local invariance of the whole action under conformal transformations (as opposed to the global symmetry that is present with an arbitrary coupling), as it allows the non-linear transformation of the Ricci scalar to cancel precisely with the transformation of the scalar kinetic term. This may be seen explicitly using the Weyl transformation rules

$$g'_{\alpha\beta} = e^{\alpha_g\omega} g_{\alpha\beta} \qquad\qquad \phi' = e^{-\alpha_g\omega/2}\phi \qquad\qquad U'(\phi) = e^{-2\alpha_g\omega}U(\phi)\,. \tag{4.180}$$

The complete action of interest,

$$S_{\mathrm{SOCG}\phi} = S_{\mathrm{SOCG}} + S_\phi\,, \tag{4.181}$$

is thus locally invariant under both (4.180) and the usual diffeomorphisms as in (4.176).

We have already seen that adding such a scalar action to the action for QG may lead to the spontaneous breakdown of global scale symmetry, particularly when the spin-2 ghost contributes to the one-loop effective potential as in Section 3.4.2. There is no reason to assume the case will be any different here, so for our current purposes we may assume that this occurs and interpret (4.181) in the broken phase[10]. This is achieved by making the replacement

$$\phi \;\to\; \frac{\mu}{\alpha_g}+\varphi \tag{4.182}$$

where $\mu=\alpha_g\langle\phi\rangle$ is a dimensionful constant and $\varphi(x)$ represents fluctuations around the minimum of the original ϕ. With this, the original scalar action (4.179) becomes

$$S_\phi \overset{\text{SSB}}{\to} S_\varphi=\int \mathrm{d}^4x\,\sqrt{-g}\left[\frac{1}{2}\nabla_\alpha\varphi\nabla^\alpha\varphi+\frac{1}{12}\left(\varphi^2+\frac{2\mu}{\alpha_g}\varphi+\frac{\mu^2}{\alpha_g^2}\right)R\right] \tag{4.183}$$

and an obvious analogy to the toy model describing local SSB and the Higgs mechanism laid out in Section 2.2.2 becomes clear. Though manifest conformal symmetry appears to be lost in (4.183), it is in fact preserved at the non-linear level through the Weyl transformation

$$\varphi'=e^{-\alpha_g\omega/2}\left(\frac{\mu}{\alpha_g}+\varphi\right)-\frac{\mu}{\alpha_g}\,, \tag{4.184}$$

thus identifying φ as an NG boson of the spontaneously broken conformal symmetry.

The Einstein-Hilbert term (the last term in (4.183)) that was generated through our unspecified realization of SSB inherently implies that one of the spin-2 states in our theory must become massive [57] and we may anticipate the presence of a Higgs mechanism that rearranges our originally massless DOFs into such a massive field. To see exactly how this happens here, we once again linearize our action by writing

$$g_{\alpha\beta} \;\to\; \eta_{\alpha\beta}+\alpha_g h_{\alpha\beta} \tag{4.185}$$

as in (4.110) and find that the the quadratic (free) part of (4.181) is given by

$$\begin{aligned}S^{(0)}_{\mathrm{SOCG}\varphi}=\int \mathrm{d}^4x\,\bigg[&h^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\left(\frac{\mu^2}{24}h^{\gamma\delta}-H^{\gamma\delta}\right)+\frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta}-H_\alpha{}^\alpha H_\beta{}^\beta\Big)\\&+\frac{1}{4}F_{\alpha\beta}F^{\alpha\beta}+A_\alpha\Big(\partial_\beta H^{\alpha\beta}-\partial^\alpha H_\beta{}^\beta\Big)\\&-\frac{1}{2}\varphi\Box\varphi-\frac{\mu}{6}\varphi\Big(\eta_{\alpha\beta}\Box-\partial_\alpha\partial_\beta\Big)h^{\alpha\beta}\bigg]\,,\end{aligned} \tag{4.186}$$

recalling the definition of the flat space Lichnerowicz operator $\mathcal{E}_{\alpha\beta\gamma\delta}$ in (4.117). Varying this action with respect to $H^{\alpha\beta}$, $h^{\alpha\beta}$, A^α, and φ yields the EOMs

[10] SSB has indeed been shown to occur explicitly in the closely related model of Georgi-Glashow theory conformally coupled to gravity [283, 284]. See also the discussion in [285].

$$
\begin{aligned}
&\mathcal{E}_{\alpha\beta\gamma\delta}h^{\gamma\delta} - \frac{1}{2}\Big(H_{\alpha\beta} - \eta_{\alpha\beta}H_\gamma{}^\gamma\Big) + \frac{1}{2}\Big(\partial_\alpha A_\beta + \partial_\beta A_\alpha\Big) - \eta_{\alpha\beta}\partial_\gamma A^\gamma = 0 \\
&\mathcal{E}_{\alpha\beta\gamma\delta}\Big(H^{\gamma\delta} - m^2 h^{\gamma\delta}\Big) + \frac{m}{\sqrt{3}}\Big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\Big)\varphi = 0 \\
&\Big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\Big)A^\beta - \partial_\beta H_\alpha{}^\beta + \partial_\alpha H_\beta{}^\beta = 0 \\
&\Box\varphi + \frac{m}{\sqrt{3}}\Big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\Big)h^{\alpha\beta} = 0\,,
\end{aligned}
\tag{4.187}
$$

where the canonical mass is given by $m = \mu/(2\sqrt{3})$.

After combining these EOMs and their traces, it is straightforward to identify that the field redefinition

$$
\Psi_{\alpha\beta} = \frac{1}{m}\big(H_{\alpha\beta} - \partial_\alpha A_\beta - \partial_\beta A_\alpha\big) + \frac{2}{\sqrt{3}\,m^2}\partial_\alpha\partial_\beta\varphi
\tag{4.188}
$$

allows us to interpret our theory in terms of a massive gauge field that is reminiscent of the SM Proca field parameterization. Indeed, after combining the EOMs (4.187), we may insert this definition to arrive at the EOM

$$
\mathcal{E}_{\alpha\beta\gamma\delta}\Psi^{\gamma\delta} - \frac{m^2}{2}\big(\Psi_{\alpha\beta} - \eta_{\alpha\beta}\Psi_\gamma{}^\gamma\big) = 0\,,
\tag{4.189}
$$

which is none other than the EOM of massive spin-2 Fierz-Pauli theory [286]. Similarly to the case of massive electrodynamics, we may derive non-kinetic constraint equations from this EOM,

$$
\partial_\beta\Psi_\alpha{}^\beta = 0 \qquad\qquad \Psi_\alpha{}^\alpha = 0\,,
\tag{4.190}
$$

which imply our new massive Proca field satisfies the usual Klein-Gordon equation

$$
\big(\Box - m^2\big)\Psi_{\alpha\beta} = 0\,.
\tag{4.191}
$$

It is interesting to note that these constraints are not imposed by any gauge conditions ($\Psi_{\alpha\beta}$ is gauge-invariant), rather, they are built into the EOMs just as one sees when the same kind of analysis is applied to the broken phase SM.

Taking this a step farther, we may also redefine the massless spin-2 DOF in terms of the Stückelberg-invariant field

$$
\psi_{\alpha\beta} = m h_{\alpha\beta} + \frac{1}{\sqrt{3}}\eta_{\alpha\beta}\varphi - \Psi_{\alpha\beta}\,,
\tag{4.192}
$$

which paired with (4.188), allows us to rewrite our broken phase action[11] as

$$
\begin{aligned}
S^{(0)}_{\mathrm{SOCG}\varphi} = \int \mathrm{d}^4x\,\bigg[&\frac{1}{2}\Big(\psi^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\psi^{\gamma\delta} - \Psi^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}\Psi^{\gamma\delta}\Big) \\
&+ \frac{m^2}{4}\Big(\Psi_{\alpha\beta}\Psi^{\alpha\beta} - \Psi_\alpha{}^\alpha\Psi_\beta{}^\beta\Big)\bigg]\,.
\end{aligned}
\tag{4.193}
$$

[11] Similar methods of rewriting linearized QG in terms of such massless and massive spin-2 modes have also been used in [107, 218, 287].

It is easy to see that the action above returns the EOM (4.189) when varied with respect to $\Psi^{\alpha\beta}$ as well as the usual EOM for massless spin-2 fields,

$$\mathcal{E}_{\alpha\beta\gamma\delta}\psi^{\gamma\delta} = 0\,, \tag{4.194}$$

when varied with respect to $\psi^{\alpha\beta}$. One may also notice the relative sign difference between the kinetic terms in (4.193), confirming the expected ghostly behavior of $\Psi^{\alpha\beta}$.

The fact that we are able to derive an EOM like (4.191) confirms that a Higgs mechanism is indeed in effect. In the SM Higgs mechanism, the gauge bosons eat one component of the complex Higgs field, however, here we see that there is in fact a kind of "double" Higgs mechanism taking place where two different NG bosons, A_α and φ, are eaten by the originally massless spin-2 field $H_{\alpha\beta}$ and completely removed from the action. The total number of DOFs is also conserved in this process as it must be; before SSB we find $2+2+2+1=7$ while after we count $2+5=7$.

At this stage we may also draw attention to the differences between the present scalar φ and the Stückelberg scalar π we encountered in the previous study. Though they may both be eaten through redefinitions of $H_{\alpha\beta}$ to illuminate its role as a massive spin-2 field, this was only possible in the previous study after choosing a particular gauge (see (4.121) and the surrounding discussion). Moreover, beside the simple fact that the present Weyl symmetry acts quite differently on fields in general compared to the Stückelberg symmetry associated with π, the present Higgs mechanism is associated with SSB and represents a fundamentally different phenomenology when compared with the symmetry in the previous theory that remains unbroken (prior to gauge-fixing).

Unitary gauge

Before proceeding with the quantization of CG in the unbroken phase, it is instructive to look at another important similarity between the present broken phase theory and SM-style gauge theory, namely, the existence of a unitary gauge. To this end we perform a Stückelberg vector transformation with the parameter $\zeta_\alpha = -A_\alpha$ so that

$$H'_{\alpha\beta} = H_{\alpha\beta} - \nabla_\alpha A_\beta - \nabla_\beta A_\alpha \qquad\qquad A'_\alpha = A_\alpha - A_\alpha = 0\,, \tag{4.195}$$

followed by a Weyl transformation with the parameter $\omega = 2\alpha_g^{-1}\ln(\alpha_g\phi/\mu)$ which corresponds to the transformation

$$\phi' = \left(\frac{\mu}{\alpha_g\phi}\right)\phi = \frac{\mu}{\alpha_g}\,. \tag{4.196}$$

Gauge fixing the second-order action (4.181) in this way yields

$$S^{(\mathrm{U})}_{\mathrm{SOCG}\varphi} = \int \mathrm{d}^4x\,\sqrt{-g}\left[\frac{m^2}{\alpha_g^2}R + \frac{1}{\alpha_g}G_{\alpha\beta}H^{\alpha\beta} + \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big)\right], \tag{4.197}$$

where we have dropped all the prime designations and identified $\mu = 2\sqrt{3}m$. We thus find that, analogously to the discussion in Section 2.2.2, the identification of the vector and scalar fields as NG bosons is reinforced since they may be removed from the action entirely with a gauge transformation.

This action still contains an off-diagonal kinetic term, however, one of the principle benefits of employing the unitary gauge is that it allows us to separate the kinetic terms for our massless and massive DOFs even without linearizing the metric as in (4.110). This may be achieved with a simple Taylor expansion by shifting the general metric according to

$$g_{\alpha\beta} \quad \rightarrow \quad g_{\alpha\beta} + aH_{\alpha\beta} \tag{4.198}$$

and taking successive functional derivatives, with a serving as an arbitrary constant that parameterizes the expansion. For the Einstein-Hilbert part of the action,

$$S_{\mathrm{EH}}[g] = \frac{m^2}{\alpha_g^2}\int \mathrm{d}^4x\,\sqrt{-g}R\,, \tag{4.199}$$

this process looks like

$$\begin{aligned} S_{\mathrm{EH}}\big[g+aH\big] &= S_{\mathrm{EH}}[g] + \int \mathrm{d}^4x\left(a\frac{\delta S_{\mathrm{EH}}[g]}{\delta g_{\alpha\beta}}H_{\alpha\beta} + \frac{a^2}{2}\frac{\delta^2 S_{\mathrm{EH}}[g]}{\delta g_{\alpha\beta}\delta g_{\gamma\delta}}H_{\alpha\beta}H_{\gamma\delta} + \mathcal{O}\big(H^3\big)\right) \\ &= \frac{m^2}{\alpha_g^2}\int \mathrm{d}^4x\,\sqrt{-g}\bigg(R - aG_{\alpha\beta}H^{\alpha\beta} + \frac{a^2}{2}H^{\alpha\beta}E_{\alpha\beta\gamma\delta}H^{\gamma\delta} + \mathcal{O}\big(H^3\big)\bigg)\,, \end{aligned} \tag{4.200}$$

where we naturally encounter the the full non-linear Lichnerowicz operator $E_{\alpha\beta\gamma\delta}$ defined in (4.118). The second-order CG part of the action,

$$S_{\mathrm{CGaux}}[g] = \int \mathrm{d}^4x\,\sqrt{-g}\left[\frac{1}{\alpha_g}G_{\alpha\beta}H^{\alpha\beta} + \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big)\right], \tag{4.201}$$

may then be expanded in the same way as

$$\begin{aligned} S_{\mathrm{CGaux}}\big[g+aH\big] &= S_{\mathrm{CGaux}}[g] + \int \mathrm{d}^4x\left(a\frac{\delta S_{\mathrm{SOCG}}[g]}{\delta g_{\alpha\beta}}H_{\alpha\beta} + \mathcal{O}\big(H^3\big)\right) \\ &= \int \mathrm{d}^4x\,\sqrt{-g}\bigg[\frac{1}{\alpha_g}\Big(G_{\alpha\beta}H^{\alpha\beta} - aH^{\alpha\beta}E_{\alpha\beta\gamma\delta}H^{\gamma\delta}\Big) \\ &\qquad\qquad + \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big) + \mathcal{O}\big(H^3\big)\bigg]\,. \end{aligned} \tag{4.202}$$

With this it is easy to see that the particular choice of $a = \alpha_g/m^2$ cancels the off-diagonal $G_{\alpha\beta}H^{\alpha\beta}$ terms when we sum up the expanded actions:

$$\begin{aligned} S^{(\mathrm{U})}_{\mathrm{SOCG}\varphi} &= S_{\mathrm{EH}} + S_{\mathrm{CGaux}} \\ &= \int \mathrm{d}^4x\,\sqrt{-g}\bigg[\frac{m^2}{\alpha_g^2}R - \frac{1}{2m^2}H^{\alpha\beta}E_{\alpha\beta\gamma\delta}H^{\gamma\delta} \\ &\qquad\qquad + \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big) + \mathcal{O}\big(H^3\big)\bigg]\,. \end{aligned} \tag{4.203}$$

We thus arrive at a diagonalized action that is equivalent to the complete unitary gauge action (4.197) up to terms of $\mathcal{O}(H^3)$ that includes the conventional Einstein-Hilbert contribution for the metric as well as a ghost-like massive spin-2 component for $H_{\alpha\beta}$.

Our definition of this diagonal action at the non-linear level also implies that the ability to diagonalize and eliminate kinetic mixing between $h_{\alpha\beta}$ and $H_{\alpha\beta}$ is not related to the choice of any particular background metric. We may confirm this assertion by expanding around a general background $\bar{g}_{\alpha\beta}$ with the replacement

$$g_{\alpha\beta} \quad \to \quad \bar{g}_{\alpha\beta} + \alpha_g h_{\alpha\beta} \,, \tag{4.204}$$

which paired with the normalizations $h_{\alpha\beta} = m\psi_{\alpha\beta}$ and $H_{\alpha\beta} = m^{-1}\Psi_{\alpha\beta}$, yields

$$\begin{aligned} S^{(\mathrm{U})}_{\mathrm{SOCG}\varphi} = \int \mathrm{d}^4x \,\sqrt{-\bar{g}}\bigg[&\frac{m^2}{\alpha_g^2}\bar{R} - \frac{m}{\alpha_g}\bar{G}_{\alpha\beta}\psi^{\alpha\beta} + \frac{1}{2}\Big(\psi^{\alpha\beta}\bar{E}_{\alpha\beta\gamma\delta}\psi^{\gamma\delta} - \Psi^{\alpha\beta}\bar{E}_{\alpha\beta\gamma\delta}\Psi^{\gamma\delta}\Big) \\ &+ \frac{m^2}{4}\Big(\Psi_{\alpha\beta}\Psi^{\alpha\beta} - \Psi_{\alpha}{}^{\alpha}\Psi_{\beta}{}^{\beta}\Big) + \mathcal{O}(\alpha_g)\bigg] \,. \end{aligned} \tag{4.205}$$

Here, quantities with over-bars are evaluated in terms of the background metric and it is easy to see that we find exact agreement with (4.193) when this background is Minkowski ($\bar{g}_{\alpha\beta} = \eta_{\alpha\beta}$). It is also interesting to note that there is a shortcut to deriving this action based on simply assuming that the bare metric perturbation depends on two independent spin-2 fields i.e. by writing

$$g_{\alpha\beta} \quad \to \quad \bar{g}_{\alpha\beta} + \frac{\alpha_g}{m}\big(\psi_{\alpha\beta} + \Psi_{\alpha\beta}\big) \,. \tag{4.206}$$

Applying this expansion to non-linear unitary gauge action (4.197) after setting $H_{\alpha\beta} = m^{-1}\Psi_{\alpha\beta}$ immediately grants (4.205) without the need to Taylor expand.

The ability to disentangle the kinetic mixing and separate our massless and massive spin-two fields, both at the quadratic and nonlinear levels, implies the possibility to define a conventional “Einstein” metric for theories of quadratic gravity. This Einstein metric corresponds exclusively to the two standard massless graviton degrees of freedom, unlike the original metric found in the fourth-order formulation of the theory which carries additional hidden degrees of freedom. This Einstein metric approach not only makes the theory’s physical content more clear through its expression in terms of diagonalized fields, but it also allows for a more straightforward analysis of unitarity.

It is essential to note that adopting this unitary picture for quadratic gravity is only feasible in the presence of the explicit mass scale that appears after SSB. However, as we touched on in the previous analysis, there are drawbacks to portraying quadratic gravity in this manner, as it characterizes a system where the ghostly massive spin-two field is coupled with the (non-renormalizable) Einstein-Hilbert action. Consequently, manifest power-counting renormalizability is lost, as the propagators do not behave in the desired $\sim 1/p^4$ manner at high momenta. It is however important to note that this does not mean that the theory as a whole is fundamentally non-renormalizable, indeed explicit full renormalizability was proven by Stelle [57]. To reconcile these facts, one need only consider that even though ψ and Ψ enter only linearly through the expansion (4.206), the separation of spin-2 modes can be performed at the non-linear level. This implies that Ψ may be considered a type of Pauli-Villars regulator, which further implies that the original Weyl-squared term also takes on the role of a UV regulator [288].

4.7.2 Quantization

In contrast to the unitary gauge scenario just presented, the original h–h propagator does indeed exhibit $1/p^4$ behavior in the UV prior to any diagonalization or choice of gauge. Thus, in an effort to avoid repeating previous analyses and to get a more complete picture of quantum quadratic gravity and the ghost problem, we will proceed by following the work in [4] and covariantly quantize conformal gravity in the original off-diagonal parameterization, without the addition of any external fields (ϕ) and the resulting SSB, where the full renormalizability of the theory is more readily apparent.

Gauge-fixing

The remainder of our analyses will be based on the second-order action (4.174), restated here for convenience:

$$S_{\text{SOCG}} = \int \mathrm{d}^4x\,\sqrt{-g}\Big[-\frac{1}{\alpha_g}G_{\alpha\beta}H^{\alpha\beta} - \frac{1}{4}\left(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\right) \\ - \frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} - A_\alpha\left(\nabla_\beta H^{\alpha\beta} - \nabla^\alpha H_\beta{}^\beta - A_\beta R^{\alpha\beta}\right)\Big]. \tag{4.207}$$

It should be noted that, following [4], there is an overall minus sign introduced in this action which has the effect of forcing A_α to be a standard vector field as opposed to a ghost. This parameterization has been chosen to simplify our eventual analyses of the ghost problem by relegating it to the massless spin-2 sector only, as we have already investigated the issue in the more physical broken phase (where A_α is a ghost) and the goal now is to look at the renormalizable theory in as transparent, albeit more academic, a fashion as possible.

We begin as before by introducing a gauge-fixing BRST symmetry which requires a new set of fields for each gauge symmetry of (4.207),

$$\begin{aligned} B_a &= \left\{b_\alpha(x), B_\alpha(x), B(x)\right\} \\ C^a &= \left\{c^\alpha(x), C^\alpha(x), C(x)\right\} \\ \bar{C}_a &= \left\{\bar{c}_\alpha(x), \bar{C}_\alpha(x), \bar{C}(x)\right\}, \end{aligned} \tag{4.208}$$

where the lower-case and upper-case vectors once again correspond to diffeomorphisms and Stückelberg vector symmetries. The difference in the present case is that the upper-case scalar fields above now correspond to the Weyl symmetry of our original action as opposed to the Stückelberg scalar symmetry that was present in SOQG. As we will see shortly, C and $\bar{C}$ both propagate in either case, a feature that has also been observed in the theory of a conformally coupled scalar with no Weyl-squared term [289], but should be contrasted with the discussion in [290].

Moving forward, we recall the gauge transformations (4.176–4.178) and find that BRST symmetry acts on each of the original fields as

$$\begin{aligned} \delta g_{\alpha\beta} &= \alpha_g\big(\nabla_\alpha c_\beta + \nabla_\beta c_\alpha + g_{\alpha\beta}C\big) \\ \delta H_{\alpha\beta} &= \nabla_\alpha C_\beta + \nabla_\beta C_\alpha + 2\nabla_\beta\nabla_\alpha C + \alpha_g\Big(\big(\nabla_\gamma H_{\alpha\beta} + H_{\alpha\gamma}\nabla_\beta + H_{\beta\gamma}\nabla_\alpha\big)c^\gamma \\ &\qquad - \big(A_\alpha\nabla_\beta + A_\beta\nabla_\alpha - g_{\alpha\beta}A_\gamma\nabla^\gamma\big)C\Big) \\ \delta A_\alpha &= C_\alpha + \alpha_g\big(\nabla_\beta A_\alpha + A_\beta\nabla_\alpha\big)c^\beta\,, \end{aligned} \tag{4.209}$$

while the new BRST fields transform according to

$$\begin{aligned} &\delta b_\alpha = 0 && \delta B_\alpha = 0 && \delta B = 0 \\ &\delta c^\alpha = \alpha_g\, c^\beta\partial_\beta c^\alpha && \delta C^\alpha = \alpha_g\big(c^\beta\partial_\beta C^\alpha + C^\beta\partial_\beta c^\alpha + C^\alpha C\big) && \delta C = \alpha_g\, c^\alpha\partial_\alpha C \\ &\delta\bar{c}_\alpha = ib_\alpha && \delta\bar{C}_\alpha = iB_\alpha && \delta\bar{C} = iB\,. \end{aligned} \tag{4.210}$$

Our next task is to write down convenient gauge-fixing conditions, though in the absence of explicit mass scales, our choices are somewhat limited when compared to the conditions we employed in Section 4.6.2. To fix diffeomorphism invariance, we select the condition

$$G^{(\xi)}_\alpha = \frac{1}{\alpha_g}g^{\beta\gamma}\Big(\partial_\gamma g_{\alpha\beta} - \frac{1}{2}\partial_\alpha g_{\beta\gamma}\Big)\,, \tag{4.211}$$

which is nothing more than the de Donder condition $\partial_\beta(\sqrt{-g}g^{\alpha\beta}) = 0$ that is often employed when studying weak field gravity. The Stückelberg symmetry is then fixed by the analogous condition

$$G^{(\zeta)}_\alpha = \nabla_\beta H^{\alpha\beta} - \frac{1}{2}\nabla^\alpha H_\beta{}^\beta\,, \tag{4.212}$$

while we select the Feynman-esque (with respect to A_α) condition

$$G^{(\omega)} = \frac{1}{2}\big(H_\alpha{}^\alpha - 2\nabla_\alpha A^\alpha + B\big) \tag{4.213}$$

to fix the conformal symmetry. Then, following the recipe laid out in Section 4.5, we may generate the appropriate BRST actions for our theory using (4.63) which leaves us with the the total action

$$S_{\rm T} = S_{\rm SOCG} + S_{{\rm gf}\xi} + S_{{\rm gf}\zeta} + S_{{\rm gf}\omega} + S_{{\rm FP}\xi} + S_{{\rm FP}\zeta} + S_{{\rm FP}\omega}\,. \tag{4.214}$$

We note that it is of course also possible to introduce more general conditions than those chosen above in order to consider different gauges, however, in line with our current goal of analyzing CG in the renormalizable picture, we have selected the particular options that lead to the best possible behavior in the UV.

Our next task is to isolate the free part of the non-linear total action so that we may derive the propagators for each field in our theory. This is achieved by linearizing the metric around Minkowski space with the replacement (4.110) so that the total action may be written as

$$S_{\mathrm{T}}\Big|_{g_{\alpha\beta}\to\eta_{\alpha\beta}+\alpha_g h_{\alpha\beta}} = S_{\mathrm{T}}^{(0)} + S_{\mathrm{T}}^{(\mathrm{int})}\,, \tag{4.215}$$

where $S_{\mathrm{T}}^{(\mathrm{int})} = \mathcal{O}(\alpha_g)$ may be ignored for our purposes, and $S_{\mathrm{T}}^{(0)}$ is given explicitly by

$$S_{\mathrm{T}}^{(0)} = S_{\mathrm{SOCG}}^{(0)} + S_{\mathrm{gf}}^{(0)} + S_{\mathrm{FP}}^{(0)}\,, \tag{4.216}$$

$$\begin{aligned} S_{\mathrm{SOCG}}^{(0)} = \int \mathrm{d}^4x\,\Big[&H^{\alpha\beta}\mathcal{E}_{\alpha\beta\gamma\delta}h^{\gamma\delta} - \frac{1}{4}\Big(H_{\alpha\beta}H^{\alpha\beta} - H_\alpha{}^\alpha H_\beta{}^\beta\Big) \\ &+ \frac{1}{2}A^\alpha\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)A^\beta - A_\alpha\Big(\partial_\beta H^{\alpha\beta} - \partial^\alpha H_\beta{}^\beta\Big)\Big] \end{aligned} \tag{4.217}$$

$$\begin{aligned} S_{\mathrm{gf}}^{(0)} = \int \mathrm{d}^4x\,\Big[&b_\alpha\Big(\partial_\beta h^{\alpha\beta} - \frac{1}{2}\partial^\alpha h_\beta{}^\beta\Big) + B_\alpha\Big(\partial_\beta H^{\alpha\beta} - \frac{1}{2}\partial^\alpha H_\beta{}^\beta\Big) \\ &+ \frac{1}{2}B\big(H_\alpha{}^\alpha - 2\partial_\alpha A^\alpha + B\big)\Big] \end{aligned} \tag{4.218}$$

$$S_{\mathrm{FP}}^{(0)} = i\int \mathrm{d}^4x\,\Big[\bar{c}^\alpha\big(\Box c_\alpha - \partial_\alpha C\big) + \bar{C}^\alpha\big(\Box C_\alpha + \Box\partial_\alpha C\big) + \bar{C}\Box C\Big]\,. \tag{4.219}$$

Naturally, BRST invariance is preserved under linearization of the metric so that (4.216) is invariant under the expanded transformation rules (4.209, 4.210) at zeroth order in α_g:

$$\begin{array}{lll} \delta h_{\alpha\beta} = 2\partial_{(\alpha}c_{\beta)} + \eta_{\alpha\beta}C & \delta H_{\alpha\beta} = 2\partial_{(\alpha}C_{\beta)} + 2\partial_\alpha\partial_\beta C & \delta A_\alpha = C_\alpha \\ \delta b_\alpha = 0 & \delta B_\alpha = 0 & \delta B = 0 \\ \delta c^\alpha = 0 & \delta C^\alpha = 0 & \delta C = 0 \\ \delta\bar{c}_\alpha = ib_\alpha & \delta\bar{C}_\alpha = iB_\alpha & \delta\bar{C} = iB\,. \end{array} \tag{4.220}$$

Finally, the propagator matrix $\Omega^{-1}_{AB}(p)$ may be derived in the usual way, as the inverse of the Fourier transform of the Hessian matrix $\Omega^{AB}(p)$:

$$\Omega^{AB}(p) = i\int \mathrm{d}^4x\,\frac{\delta^2 S_{\mathrm{T}}^{(0)}}{\delta\Phi_A(x)\delta\Phi_B(y)}\,e^{-ip(x-y)} \tag{4.221}$$

$$\Omega^{-1}_{AB}(p) = -i\,\langle 0|\,T\Phi_A\Phi_B\,|0\rangle = \begin{pmatrix} \Omega^{-1}_{\mathrm{boson}} & 0 \\ 0 & \begin{pmatrix} 0 & \Omega^{-1}_{\mathrm{ghost}} \\ \Omega^{-1\,\dagger}_{\mathrm{ghost}} & 0 \end{pmatrix} \end{pmatrix}_{AB}\,, \tag{4.222}$$

$$\Omega_{\text{boson}}^{-1} =$$

$$\begin{array}{c|cccccc}
 & h_{\gamma\delta} & H_{\gamma\delta} & A_\gamma & b_\gamma & B_\gamma & B \\
\hline
h_{\mu\nu} & -\frac{F_{\mu\nu\gamma\delta}}{p^4} & \frac{F_{\mu\nu\gamma\delta}}{p^2} & 0 & -\frac{i(\eta_{\nu\gamma}p_\mu+\eta_{\mu\gamma}p_\nu)}{p^2} & 0 & -\frac{\eta_{\mu\nu}}{p^2}+\frac{2p_\mu p_\nu}{p^4} \\
H_{\mu\nu} & & 0 & 0 & 0 & -\frac{i(\eta_{\nu\gamma}p_\mu+\eta_{\mu\gamma}p_\nu)}{p^2} & 0 \\
A_\mu & & & -\frac{\eta_{\mu\gamma}}{p^2} & 0 & -\frac{\eta_{\mu\gamma}}{p^2} & \frac{ip_\mu}{p^2} \\
b_\mu & & & & 0 & 0 & 0 \\
B_\mu & & \text{(h.c.)} & & & 0 & 0 \\
B & & & & & & 0
\end{array}$$

where

$$F_{\mu\nu\gamma\delta} = \eta_{\mu\nu}\eta_{\gamma\delta} - 2\delta_{\mu\nu\gamma\delta} + \frac{\eta_{\mu\gamma}p_\nu p_\delta + \eta_{\mu\delta}p_\nu p_\gamma + \eta_{\nu\gamma}p_\mu p_\delta + \eta_{\nu\delta}p_\mu p_\gamma}{p^2}\,, \tag{4.223}$$

$$\Omega_{\text{ghost}}^{-1} = \begin{array}{c|ccc}
 & \bar{c}_\gamma & \bar{C}_\gamma & \bar{C} \\
\hline
c_\mu & -\frac{i\eta_{\mu\gamma}}{p^2} & 0 & -\frac{p_\mu}{p^4} \\
C_\mu & 0 & -\frac{i\eta_{\mu\gamma}}{p^2} & -\frac{p_\mu}{p^2} \\
C & 0 & 0 & -\frac{i}{p^2}
\end{array}\,. \tag{4.224}$$

Asymptotic fields

With the propagators in hand, the quantization process proceeds as in the last study by establishing asymptotic solutions to our EOMs under the LSZ formalism. The EOMs obtained from (4.216) after varying with respect to the original three bosonic fields in our theory are given by

$$\begin{aligned}
&\mathcal{E}_{\alpha\beta\gamma\delta}h^{\gamma\delta} - \frac{1}{2}\Big(H_{\alpha\beta} + \partial_\alpha\big(A_\beta - B_\beta\big) + \partial_\beta\big(A_\alpha - B_\alpha\big) \\
&\qquad\qquad - \eta_{\alpha\beta}\big(H_\gamma{}^\gamma - 2\partial_\gamma\big(A^\gamma - B^\gamma\big) + B\big)\Big) = 0 \\
&\mathcal{E}_{\alpha\beta\gamma\delta}H^{\gamma\delta} - \frac{1}{2}\Big(\partial_\alpha\, b_\beta + \partial_\beta\, b_\alpha - \eta_{\alpha\beta}\partial_\gamma\, b^\gamma\Big) = 0 \\
&\big(\eta_{\alpha\beta}\Box - \partial_\alpha\partial_\beta\big)A^\beta - \partial^\beta H_{\alpha\beta} + \partial_\alpha H_\beta{}^\beta + \partial_\alpha B = 0\,,
\end{aligned} \tag{4.225}$$

though instead of trying to solve them directly, it is easier to first combine with the NL EOMs i.e. the gauge-fixing conditions

$$\begin{aligned}
&\partial^\beta h_{\alpha\beta} - \frac{1}{2}\partial_\alpha h_\beta{}^\beta = 0 \\
&\partial^\beta H_{\alpha\beta} - \frac{1}{2}\partial_\alpha H_\beta{}^\beta = 0 \\
&\partial_\alpha A^\alpha - \frac{1}{2}H_\alpha{}^\alpha - B = 0\,,
\end{aligned} \tag{4.226}$$

so as to arrive at the simpler set of equations below where the d'Alembertian of each field is isolated:

$$\begin{aligned} &\Box h_{\alpha\beta} - H_{\alpha\beta} + \partial_\alpha\big(A_\beta - B_\beta\big) + \partial_\beta\big(A_\alpha - B_\alpha\big) = 0 \\ &\Box H_{\alpha\beta} - \partial_\alpha b_\beta - \partial_\beta b_\alpha = 0 \\ &\Box A_\alpha = 0\,. \end{aligned} \tag{4.227}$$

Our desired asymptotic solutions to (4.225) are given in terms of oscillator decompositions of each field after taking the asymptotic limit (4.65) as in (4.66). The simplest of these is given by

$$A_\alpha(x) = \hat{A}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})\,, \tag{4.228}$$

which contains a simple-pole only, where there is an implicit sum over $\boldsymbol{p}$ and $A_\alpha(x)$ is regarded as an asymptotic Heisenberg field, though we have dropped the notation describing these features to avoid clutter. When we next solve for the spin-2 decompositions, we encounter the first major deviation from the previous diagonalized broken phase quantization. Due to the fact that their propagators have poles that converge faster than p^{-2}, we must introduce higher order oscillators to fully solve the EOMs. By looking at the p^{-2n} nature of their propagators ($n =$ number of poles required) we may predict that their decompositions take the forms

$$h_{\alpha\beta}(x) = \hat{h}_{\alpha\beta}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \hat{h}_{g\alpha\beta}(\boldsymbol{p})g_{\boldsymbol{p}}(x) + \hat{h}_{h\alpha\beta}(\boldsymbol{p})h_{\boldsymbol{p}}(x) + (\text{h.c.}) \tag{4.229}$$

$$H_{\alpha\beta}(x) = \hat{H}_{\alpha\beta}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \hat{H}_{g\alpha\beta}(\boldsymbol{p})g_{\boldsymbol{p}}(x) + (\text{h.c.})\,. \tag{4.230}$$

Then, after inserting these decompositions into the simplified EOMs (4.227), the complete decompositions are found to be given in terms of

$$\hat{h}_{g\alpha\beta}(\boldsymbol{p}) = \hat{H}_{\alpha\beta}(\boldsymbol{p}) - ip_\alpha\big(\hat{A}_\beta(\boldsymbol{p}) - \hat{B}_\beta(\boldsymbol{p})\big) - ip_\beta\big(\hat{A}_\alpha(\boldsymbol{p}) - \hat{B}_\alpha(\boldsymbol{p})\big) \tag{4.231}$$

$$\hat{h}_{h\alpha\beta}(\boldsymbol{p}) = ip_\alpha\hat{b}_\beta(\boldsymbol{p}) + ip_\beta\hat{b}_\alpha(\boldsymbol{p}) \tag{4.232}$$

$$\hat{H}_{g\alpha\beta}(\boldsymbol{p}) = ip_\alpha\hat{b}_\beta(\boldsymbol{p}) + ip_\beta\hat{b}_\alpha(\boldsymbol{p})\,. \tag{4.233}$$

Applying the same kind of pole-structure-based ansätze to the NL fields we find

$$b_\alpha(x) = \hat{b}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) \tag{4.234}$$

$$B_\alpha(x) = \hat{B}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) \tag{4.235}$$

$$B(x) = \hat{B}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \hat{B}_g(\boldsymbol{p})g_{\boldsymbol{p}}(x) + (\text{h.c.})\,, \tag{4.236}$$

where the double pole oscillator $\hat{B}_g(\boldsymbol{p})$ must be solved for using the complete set of bosonic EOMs (4.225) and (4.226), yielding

$$\hat{B}_g(\boldsymbol{p}) = -ip_\alpha\hat{b}^\alpha(\boldsymbol{p})\,. \tag{4.237}$$

This same full set of equations also determines how our chosen gauge conditions manifest in terms of fixing the longitudinal parts of $\hat{h}_{\alpha\beta}$, $\hat{H}_{\alpha\beta}$, and $\hat{A}_\alpha$ to

$$\begin{aligned}
p^\beta \hat{h}_{\alpha\beta}(\boldsymbol{p}) = \frac{1}{2}\bigg[& p_\alpha \hat{h}_\beta{}^\beta(\boldsymbol{p}) - \frac{1}{E}\eta_{0\beta}\hat{H}_\alpha{}^\beta(\boldsymbol{p}) - i\hat{A}^\beta(\boldsymbol{p})\left(\eta_{\alpha\beta} - \frac{1}{E}\eta_{0\beta}p_\alpha\right) \\
& - \frac{i}{4E^2}\hat{b}^\beta(\boldsymbol{p})\left(\eta_{\alpha\beta} + \frac{1}{E}\big(\eta_{0\alpha}p_\beta - \eta_{0\beta}p_\alpha\big)\right) \\
& + i\hat{B}^\beta(\boldsymbol{p})\left(\eta_{\alpha\beta} + \frac{1}{E}\big(\eta_{0\alpha}p_\beta - \eta_{0\beta}p_\alpha\big)\right) - \frac{1}{E}\eta_{0\alpha}\hat{B}(\boldsymbol{p})\bigg]
\end{aligned} \tag{4.238}$$

$$p^\beta \hat{H}_{\alpha\beta}(\boldsymbol{p}) = \frac{1}{2}\left[p_\alpha \hat{H}_\beta{}^\beta(\boldsymbol{p}) + i\hat{b}^\beta(\boldsymbol{p})\left(\eta_{\alpha\beta} + \frac{1}{E}\big(\eta_{0\alpha}p_\beta - \eta_{0\beta}p_\alpha\big)\right)\right] \tag{4.239}$$

$$p^\alpha \hat{A}_\alpha(\boldsymbol{p}) = -\frac{i}{2}\hat{H}_\alpha{}^\alpha(\boldsymbol{p}) - i\hat{B}_f(\boldsymbol{p}), \tag{4.240}$$

where the rather odd factors of $\eta_{0\alpha}$ arise from the relations

$$\partial_\alpha g_{\boldsymbol{p}}(x) = ip_\alpha g_{\boldsymbol{p}}(x) + \frac{i}{2E}\eta_{0\alpha}f_{\boldsymbol{p}}(x) \tag{4.241}$$

$$\partial_\alpha h_{\boldsymbol{p}}(x) = ip_\alpha h_{\boldsymbol{p}}(x) + \frac{i}{2E}\eta_{0\alpha}g_{\boldsymbol{p}}(x) - \frac{i}{8E^3}\eta_{0\alpha}f_{\boldsymbol{p}}(x). \tag{4.242}$$

In the ghost sector, the EOMs are given by

$$\begin{aligned}
&\Box c^\alpha - \partial^\alpha C = 0 && \Box \bar{c}_\alpha = 0 \\
&\Box C^\alpha + \Box\partial^\alpha C = 0 && \Box \bar{C}_\alpha = 0 \\
&\Box C = 0 && \Box \bar{C} + \partial_\alpha \bar{c}^\alpha - \Box\partial_\alpha \bar{C}^\alpha = 0,
\end{aligned} \tag{4.243}$$

which, due to the lack of gauge symmetry in this sector[12], leads to the straightforward oscillator decompositions

$$\begin{aligned}
c^\alpha(x) &= \hat{c}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \hat{c}_g^\alpha(\boldsymbol{p})g_{\boldsymbol{p}}(x) + (\text{h.c.}) \\
C^\alpha(x) &= \hat{C}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) \\
C(x) &= \hat{C}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.})
\end{aligned} \tag{4.244}$$

$$\begin{aligned}
\bar{c}_\alpha(x) &= \hat{\bar{c}}_\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) \\
\bar{C}_\alpha(x) &= \hat{\bar{C}}^\alpha(\boldsymbol{p})f_{\boldsymbol{p}}(x) + (\text{h.c.}) \\
\bar{C}(x) &= \hat{\bar{C}}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \hat{\bar{C}}_g(\boldsymbol{p})g_{\boldsymbol{p}}(x) + (\text{h.c.}),
\end{aligned} \tag{4.245}$$

where the two double-pole oscillators are fixed by

$$\hat{c}_g^\alpha(\boldsymbol{p}) = ip^\alpha \hat{C}(\boldsymbol{p}) \qquad\qquad \hat{\bar{C}}_g(\boldsymbol{p}) = -ip_\alpha \hat{\bar{c}}^\alpha(\boldsymbol{p}). \tag{4.246}$$

[12]It is in fact possible to have extra gauge symmetries appear in the ghost sector, in which case additional "ghosts for ghosts" must be added into the BRST construction (see [291] for an example of this kind of theory). Our second-order first-class parameterization of CG, as well as our chosen gauge conditions, allows us to avoid this complication here.

Due to the presence of non-zero higher pole oscillators in some of our decompositions, the (anti)commutators between each of our Heisenberg fields are not as trivial to derive as they were in the broken phase study (see the discussion around (4.137)). Here, they must determined from the propagator matrix (4.222) using the replacements (4.76), restated here for convenience:

$$\frac{ip_\alpha}{-p^2} \to \partial^x_\alpha D(x-y) \qquad \frac{ip_\alpha}{(-p^2)^2} \to \partial^x_\alpha E(x-y) \qquad \frac{ip_\alpha}{(-p^2)^3} \to \partial^x_\alpha F(x-y)\,. \tag{4.247}$$

One should recall the role of $D(x-y)$, $E(x-y)$, and $F(x-y)$ as invariant delta functions corresponding to the first, second, and third powers of the d'Alembertian, which appear after passing to the continuum limit (4.78) (see Appendix A). With these considerations, we find the non-zero bosonic field propagators

$$\begin{aligned}
[h_{\alpha\beta}(x), h_{\gamma\delta}(y)] &= \big(2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta}\big)E(x-y) - \mathcal{D}^x_{\alpha\beta\gamma\delta}F(x-y)\\
[h_{\alpha\beta}(x), H_{\gamma\delta}(y)] &= \big(2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta}\big)D(x-y) - \mathcal{D}^x_{\alpha\beta\gamma\delta}E(x-y)\\
[h_{\alpha\beta}(x), b_\gamma(y)] &= \big(\eta_{\alpha\gamma}\partial^x_\beta + \eta_{\beta\gamma}\partial^x_\alpha\big)D(x-y)\\
[h_{\alpha\beta}(x), B(y)] &= \eta_{\alpha\beta}D(x-y) + 2\partial^x_\alpha\partial^x_\beta E(x-y)\\
[H_{\alpha\beta}(x), B_\gamma(y)] &= \big(\eta_{\alpha\gamma}\partial^x_\beta + \eta_{\beta\gamma}\partial^x_\alpha\big)D(x-y)\\
[A_\alpha(x), A_\beta(y)] &= \eta_{\alpha\beta}D(x-y)\\
[A_\alpha(x), B_\beta(y)] &= \eta_{\alpha\beta}D(x-y)\\
[A_\alpha(x), B(y)] &= -\partial^x_\alpha D(x-y)\,,
\end{aligned} \tag{4.248}$$

where $\mathcal{D}_{\alpha\beta\gamma\delta}$ is the differential operator defined in (4.119). The non-zero anti-commutators in the ghost sector then follow in a similar fashion:

$$\begin{aligned}
&\{c_\alpha(x), \bar{c}_\beta(y)\} = i\eta_{\alpha\beta}D(x-y) &&\big\{c_\alpha(x), \bar{C}(y)\big\} = i\partial^x_\alpha E(x-y)\\
&\big\{C_\alpha(x), \bar{C}_\beta(y)\big\} = i\eta_{\alpha\beta}D(x-y) &&\big\{C_\alpha(x), \bar{C}(y)\big\} = -i\partial^x_\alpha D(x-y)\\
&\big\{C(x), \bar{C}(y)\big\} = iD(x-y)\,.
\end{aligned} \tag{4.249}$$

We are also interested in the non-zero (anti)commutators between simple-pole oscillators which may be derived by simply reading off the coefficients of $-p^{-2}$ in the associated propagators (4.222):

$$\begin{aligned}
\Big[\hat{h}_{\alpha\beta}(\boldsymbol{p}), \hat{H}^\dagger_{\gamma\delta}(\boldsymbol{q})\Big] &= \big(2\delta_{\alpha\beta\gamma\delta} - \eta_{\alpha\beta}\eta_{\gamma\delta}\big)\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
\Big[\hat{h}_{\alpha\beta}(\boldsymbol{p}), \hat{b}^\dagger_\gamma(\boldsymbol{q})\Big] &= \big(ip_\alpha\eta_{\beta\gamma} + ip_\beta\eta_{\alpha\gamma}\big)\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
\Big[\hat{h}_{\alpha\beta}(\boldsymbol{p}), \hat{B}^\dagger(\boldsymbol{q})\Big] &= \eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})
\end{aligned}$$

$$\begin{aligned}
\left[\hat{H}_{\alpha\beta}(\boldsymbol{p}), \hat{B}^\dagger_\gamma(\boldsymbol{q})\right] &= \left(ip_\alpha\eta_{\beta\gamma} + ip_\beta\eta_{\alpha\gamma}\right)\delta^3(\boldsymbol{p}-\boldsymbol{q}) \\
\left[\hat{A}_\alpha(\boldsymbol{p}), \hat{A}^\dagger_\beta(\boldsymbol{q})\right] &= \eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \\
\left[\hat{A}_\alpha(\boldsymbol{p}), \hat{B}^\dagger_\beta(\boldsymbol{q})\right] &= \eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \\
\left[\hat{A}_\alpha(\boldsymbol{p}), \hat{B}^\dagger(\boldsymbol{q})\right] &= -ip_\alpha\delta^3(\boldsymbol{p}-\boldsymbol{q})
\end{aligned} \tag{4.250}$$

$$\begin{aligned}
&\left\{\hat{c}_\alpha(\boldsymbol{p}), \hat{\bar{c}}^\dagger_\beta(\boldsymbol{q})\right\} = i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) &\qquad &\left\{\hat{C}_\alpha(\boldsymbol{p}), \hat{\bar{C}}^\dagger_\beta(\boldsymbol{q})\right\} = i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \\
&\left\{\hat{C}_\alpha(\boldsymbol{p}), \hat{\bar{C}}^\dagger(\boldsymbol{q})\right\} = p_\alpha\delta^3(\boldsymbol{p}-\boldsymbol{q}) &\qquad &\left\{\hat{C}(\boldsymbol{p}), \hat{\bar{C}}^\dagger(\boldsymbol{q})\right\} = i\delta^3(\boldsymbol{p}-\boldsymbol{q})\,.
\end{aligned} \tag{4.251}$$

Naturally, these relations may be shown to be consistent with the field commutators (4.248) and (4.249) after decomposing them in terms of oscillators. The BRST transformation properties of each simple-pole oscillator may now also be obtained after decomposing the field transformations (4.220) and employing the relations above, which yields

$$\begin{aligned}
\left[\mathcal{Q}, \hat{h}_{\alpha\beta}\right] &= p_\alpha\hat{c}_\beta + p_\beta\hat{c}_\alpha - i\eta_{\alpha\beta}\hat{C} \\
\left[\mathcal{Q}, \hat{H}_{\alpha\beta}\right] &= p_\alpha\hat{C}_\beta + p_\beta\hat{C}_\alpha + 2ip_\alpha p_\beta\hat{C} \\
\left[\mathcal{Q}, \hat{A}_\alpha\right] &= -i\hat{C}_\alpha
\end{aligned} \tag{4.252}$$

$$\begin{aligned}
&\left[\mathcal{Q}, \hat{b}_\alpha\right] = 0 &\qquad &\left[\mathcal{Q}, \hat{B}_\alpha\right] = 0 &\qquad &\left[\mathcal{Q}, \hat{B}\right] = 0 \\
&\{\mathcal{Q}, \hat{c}^\alpha\} = 0 &\qquad &\left\{\mathcal{Q}, \hat{C}^\alpha\right\} = 0 &\qquad &\left\{\mathcal{Q}, \hat{C}\right\} = 0 \\
&\{\mathcal{Q}, \hat{\bar{c}}_\alpha\} = \hat{b}_\alpha &\qquad &\left\{\mathcal{Q}, \hat{\bar{C}}_\alpha\right\} = \hat{B}_\alpha &\qquad &\left\{\mathcal{Q}, \hat{\bar{C}}\right\} = \hat{B}\,,
\end{aligned} \tag{4.253}$$

where we have used the relation (4.60) to express these relations in the more convenient commutator form. Finally, with all of the relations above, we have fully established our desired quantization of SOCG whose total Fock space is spanned by the creation operators in each of the simple-pole oscillators.

4.7.3 Unitarity

The quartet mechanism

We proceed with an analysis of unitarity in the quantum system defined by the (anti)commutator relations (4.250) and (4.251), which begins with a classification of our total space of quantum states in terms of physical transverse states and states that belong to KO quartets. Since all of the fields in the present theory are massless, we may simplify the upcoming calculations by selecting the particular Lorentz frame (4.73), recalling the crucial fact that all (anti)commutators derived in this frame are also valid in general.

Then, after eliminating twenty four components of $\hat{h}_{\alpha\beta}$, $\hat{H}_{\alpha\beta}$, and $\hat{A}_\alpha$ using the oscillator gauge conditions (4.238–4.240), we may identify the six operators

$$\hat{a}_{h,+} = \frac{1}{2}\big(\hat{h}_{11} - \hat{h}_{22}\big) \qquad \hat{a}_{h,\times} = \hat{h}_{12} \tag{4.254}$$

$$\hat{a}_{H,+} = \frac{1}{2}\big(\hat{H}_{11} - \hat{H}_{22}\big) \qquad \hat{a}_{H,\times} = \hat{H}_{12} \tag{4.255}$$

$$\hat{a}_{A,1} = \hat{A}_1 + \frac{i}{E}\hat{H}_{13} \qquad \hat{a}_{A,2} = \hat{A}_2 + \frac{i}{E}\hat{H}_{23}\,, \tag{4.256}$$

which are BRST singlets ($[\mathcal{Q}, \hat{a}_{h,j}] = [\mathcal{Q}, \hat{a}_{H,j}] = [\mathcal{Q}, \hat{a}_{A,k}] = 0$), as the annihilation operators corresponding to our expected six physical DOFs. Naturally, there is some freedom in how one defines these operators in terms of the original oscillator components, however, the choices above are by far the most illuminating since they allow us to decompose the simple-pole oscillators in terms of the transverse polarization tensors $\varepsilon_{j\,\alpha\beta}$ and $\varepsilon_{k\,\alpha}$ where $j = \{+, \times\}$ and $k = \{1, 2\}$ (see Section 4.5.2):

$$\hat{h}_{\alpha\beta}(\boldsymbol{p}) = \sum_j \varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}_{h,j}(\boldsymbol{p}) + \cdots + (\text{h.c.}) \tag{4.257}$$

$$\hat{H}_{\alpha\beta}(\boldsymbol{p}) = \sum_j \varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}_{H,j}(\boldsymbol{p}) + \cdots + (\text{h.c.}) \tag{4.258}$$

$$\hat{A}_{\alpha}(\boldsymbol{p}) = \sum_k \varepsilon_{k\,\alpha}(\boldsymbol{p})\hat{a}_{A,k}(\boldsymbol{p}) + \cdots + (\text{h.c.})\,. \tag{4.259}$$

With this, identification of $\hat{a}_{h,j}$, $\hat{a}_{H,j}$, and $\hat{a}_{A,k}$ as the annihilation operators of physical massless spin-2 and spin-1 fields is obvious.

The remaining annihilation operators (which appear in the "$\cdots$" above) must now be redefined in terms of KO quartet participants in order to ensure that they do not threaten unitary and represent only (unphysical) longitudinal quantum states. This may be achieved by defining the nine BRST-non-trivial operators

$$\big(\hat{\psi}_\alpha\big) = \begin{pmatrix} -\frac{i\hat{h}_{00}}{2E} + \frac{i\hat{H}_{33}}{4E^3} + \frac{\hat{A}_3}{2E^2} \\ -\frac{i\hat{h}_{01}}{E} \\ -\frac{i\hat{h}_{02}}{E} \\ \frac{i\hat{h}_{33}}{2E} + \frac{i\hat{H}_{33}}{4E^3} + \frac{\hat{A}_3}{2E^2} \end{pmatrix} \qquad \big(\hat{\Psi}_\alpha\big) = \begin{pmatrix} -\hat{A}_0 \\ -\frac{i\hat{H}_{01}}{E} \\ -\frac{i\hat{H}_{02}}{E} \\ -\hat{A}_3 \end{pmatrix} \qquad \hat{\Psi} = \frac{\hat{H}_{00}}{2E^2} + \frac{i\hat{A}_0}{E}\,, \tag{4.260}$$

in addition to the modified NL and anti-ghost annihilation operators

$$\hat{\mathcal{B}} = \hat{B} - iE\big(\hat{B}_0 + \hat{B}_3\big) \qquad \hat{\bar{\mathcal{C}}} = \hat{\bar{C}} - iE\big(\hat{\bar{C}}_0 + \hat{\bar{C}}_3\big)\,. \tag{4.261}$$

These particular parameterizations have been chosen because they lead to the simple BRST transformations

$$\begin{aligned}
&\left[\mathcal{Q},\hat{\psi}_\alpha\right]=i\hat{c}_\alpha && \left[\mathcal{Q},\hat{\Psi}_\alpha\right]=i\hat{C}_\alpha && \left[\mathcal{Q},\hat{\Psi}\right]=i\hat{\mathcal{C}}\\
&\left[\mathcal{Q},\hat{b}_\alpha\right]=0 && \left[\mathcal{Q},\hat{B}_\alpha\right]=0 && \left[\mathcal{Q},\hat{\mathcal{B}}\right]=0\\
&\{\mathcal{Q},\hat{c}_\alpha\}=0 && \left\{\mathcal{Q},\hat{C}_\alpha\right\}=0 && \left\{\mathcal{Q},\hat{\mathcal{C}}\right\}=0\\
&\{\mathcal{Q},\hat{\bar{c}}_\alpha\}=\hat{b}_\alpha && \left\{\mathcal{Q},\hat{\bar{C}}_\alpha\right\}=\hat{B}_\alpha && \left\{\mathcal{Q},\hat{\bar{\mathcal{C}}}\right\}=\hat{\mathcal{B}}\,,
\end{aligned} \tag{4.262}$$

which may be derived from the oscillator transformations (4.252) and (4.253). It is important to note that the map between the original oscillators and the new operators as defined in (4.254–4.256), (4.260), and (4.261) is invertible, meaning that all original components have been accounted for. This guarantees that we may express the complete Fock space in terms of this new basis of states.

We may now consider the (anti)commutation relations between the operators in our new quartet basis. Using the relations (4.250) and (4.251), the physical subspace is found to be characterized by

$$\left[\hat{a}_{h,j}(\boldsymbol{p}),\hat{a}^\dagger_{H,j'}(\boldsymbol{q})\right]=\delta_{jj'}\delta^3(\boldsymbol{p}-\boldsymbol{q}) \qquad \left[\hat{a}_{A,j}(\boldsymbol{p}),\hat{a}^\dagger_{A,j'}(\boldsymbol{q})\right]=\delta_{jj'}\delta^3(\boldsymbol{p}-\boldsymbol{q})\,, \tag{4.263}$$

while in the quartet subspace we find

$$\begin{aligned}
&\left[\hat{\psi}_\alpha(\boldsymbol{p}),\hat{b}^\dagger_\beta(\boldsymbol{q})\right]=-\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) && \left[\hat{\Psi}_\alpha(\boldsymbol{p}),\hat{B}^\dagger_\beta(\boldsymbol{q})\right]=-\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\left[\hat{\Psi}(\boldsymbol{p}),\hat{\mathcal{B}}^\dagger(\boldsymbol{q})\right]=-\delta^3(\boldsymbol{p}-\boldsymbol{q}) && \left\{\hat{c}_\alpha(\boldsymbol{p}),\hat{\bar{c}}^\dagger_\beta(\boldsymbol{q})\right\}=i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q})\\
&\left\{\hat{C}_\alpha(\boldsymbol{p}),\hat{\bar{C}}^\dagger_\beta(\boldsymbol{q})\right\}=i\eta_{\alpha\beta}\delta^3(\boldsymbol{p}-\boldsymbol{q}) && \left\{\hat{\mathcal{C}}(\boldsymbol{p}),\hat{\bar{\mathcal{C}}}^\dagger(\boldsymbol{q})\right\}=i\delta^3(\boldsymbol{p}-\boldsymbol{q})\,.
\end{aligned} \tag{4.264}$$

Every (anti)commutation relation not shown above is vanishing, with the exception of some commutators between $\hat{\psi}_\alpha$, $\hat{\Psi}_\alpha$, and $\hat{\Psi}$, however as previously mentioned, these kind of relations between π_0 states are irrelevant in the context of the KO quartet mechanism [266].

In fact, with the transformation properties (4.262) and the (anti)commutation relations (4.263) and (4.264), we have everything we need to classify each non-transverse state in our quantum theory in terms of the parent and daughter relationships

$$\{\,|\pi_0\rangle\,\}=\left\{\hat{\psi}^\dagger_\alpha\,|0\rangle\,,\hat{\Psi}^\dagger_\alpha\,|0\rangle\,,\hat{\Psi}^\dagger\,|0\rangle\right\} \tag{4.265}$$

$$\{\,|\delta_1\rangle\,\}=\{\,\mathcal{Q}\,|\pi_0\rangle\,\}=\left\{i\hat{c}^\dagger_\alpha\,|0\rangle\,,i\hat{C}^\dagger_\alpha\,|0\rangle\,,i\hat{\mathcal{C}}^\dagger f\,|0\rangle\right\} \tag{4.266}$$

$$\{\,|\pi_{-1}\rangle\,\}=\left\{-\,\hat{\bar{c}}^\dagger_\alpha\,|0\rangle\,,-\hat{\bar{C}}^\dagger_\alpha\,|0\rangle\,,-\hat{\bar{\mathcal{C}}}^\dagger\,|0\rangle\right\} \tag{4.267}$$

$$\{\,|\delta_0\rangle\,\}=\{\,\mathcal{Q}\,|\pi_{-1}\rangle\,\}=\left\{-\,\hat{b}^\dagger_\alpha\,|0\rangle\,,-\hat{B}^\dagger_\alpha\,|0\rangle\,,-\hat{\mathcal{B}}^\dagger\,|0\rangle\right\}, \tag{4.268}$$

which as outlined in Section 4.5.3, fully characterizes the quartet mechanism through the relation (4.83) and guarantees that none of the states above will threaten the unitarity of our quantum theory. However, just as we saw in the last study, this does not necessarily mean we are safe from unitarity violation arising from the transverse physical subspace.

Analysis of the physical subspace

We begin our analyses of unitarity in the physical subspace of CG by once again appealing to the formalism established by Kugo, Ojima, and Nakanishi [266, 269] and recall that their proof of unitarity in Yang-Mills theories rests on the assumption that there exists an S-matrix on the physical Fock space $\mathcal{V}_{\mathrm{tr}}$ that is pseudo-unitary, leaves the vacuum invariant, and commutes with the gauge-fixed Hamiltonian and BRST charge operators:

$$SS^\dagger = S^\dagger S = \mathbb{1} \tag{4.269}$$

$$S\left|0\right\rangle = S^\dagger\left|0\right\rangle = \left|0\right\rangle \tag{4.270}$$

$$[\mathcal{H}, S] = [\mathcal{Q}, S] = 0\,. \tag{4.271}$$

Though we may make these assumptions in the present case as well, there is another key component to the proof of unitarity – the physical Fock space comes equipped with a positive-definite inner product,

$$\langle f|f\rangle > 0 \quad \forall \quad |f\rangle \in \mathcal{V}_{\mathrm{tr}}\,, \quad |f\rangle \neq 0\,. \tag{4.272}$$

We have already seen that this last feature is not found in the broken phase calculation carried out in the last section and the case is no different here. Specifically, we are referring to the spin-2 commutation relations in (4.263) which are off-diagonal in nature and thus represent an indefinite inner product, despite the lack of a relative minus sign. It should be noted that the presence of an indefinite inner product does not *necessarily* mean that the associated theory lacks unitarity, rather that the issue becomes subtle and must be treated rigorously. The subject of indefinite metric QFT has been studied in the past (Nakanishi's work [292] is particularly useful for what follows), though it is certainly not yet understood to the level of standard positive-definite QFT. The task of establishing a complete solution to the ghost problem in this context is thus a truly monumental task and beyond the scope of this work. We will instead content ourselves by making an important step in the right direction through a new view on where unitarity breaks down in CG, which is possible thanks to the novel covariant quantization of the theory that we performed in the previous sections.

Before proceeding with this goal in mind, we note the simplifying fact that a distinct portion of our physical subspace is in fact easily shown to be unitary based on the requirements above. This is of course the subspace of spin-1 states corresponding to $\hat{a}_{A,k}$ which possesses the positive-definite inner product

$$\langle 0|\hat{a}_{A,k}(\boldsymbol{p})\hat{a}^\dagger_{A,k'}(\boldsymbol{q})|0\rangle = \delta_{kk'}\delta^3(\boldsymbol{p}-\boldsymbol{q})\,, \tag{4.273}$$

and since there are no non-vanishing commutators between $\hat{a}_{A,k}$ and $\hat{a}_{h,j}$ or $\hat{a}_{H,j}$, we will set these states aside for the rest of our analyses.

The gauge-fixed Hamiltonian $\mathcal{H}$ corresponding the subspace of $\mathcal{V}_{\mathrm{tr}}$ spanned only by $\hat{a}_{h,j}$ and $\hat{a}_{H,j}$ may be derived by solving the Heisenberg equation

$$[\mathcal{H}, \phi_a(x)] = -i\partial_0\phi_a(x)\,, \tag{4.274}$$

where $\phi_a(x) = \{h_{\alpha\beta}(x), H_{\alpha\beta}(x)\}$. After decomposing each field in terms of its oscillators and dropping all quartet members, the right side of this equation may be evaluated with the relations

$$i\partial_0 f_{\boldsymbol{p}}(x) = E f_{\boldsymbol{p}}(x) \qquad\qquad i\partial_0 g_{\boldsymbol{p}}(x) = E g_{\boldsymbol{p}}(x) + \frac{1}{2E} f_{\boldsymbol{p}}(x)\,. \tag{4.275}$$

Then, after assuming a logical ansatz for the form of $\mathcal{H}$ and evaluating the commutation relations on the left side of the Heisenberg equation, we arrive at the definition

$$\mathcal{H} = \int \mathrm{d}^3\boldsymbol{p} \sum_j \left[E\Big(\hat{a}^\dagger_{h,j}(\boldsymbol{p})\hat{a}_{H,j}(\boldsymbol{p}) + \hat{a}^\dagger_{H,j}(\boldsymbol{p})\hat{a}_{h,j}(\boldsymbol{p})\Big) + \frac{1}{2E}\Big(\hat{a}^\dagger_{H,j}(\boldsymbol{p})\hat{a}_{H,j}(\boldsymbol{p})\Big)\right] \tag{4.276}$$

which is normal-ordered with respect to the (+) vacuum as defined by

$$\hat{a}_{h,j}(\boldsymbol{p})\,|0\rangle = \hat{a}_{H,j}(\boldsymbol{p})\,|0\rangle = 0\,, \tag{4.277}$$

and commutes with the spin-2 operators according to

$$\Big[\mathcal{H}, \hat{a}^\dagger_{h,j}(\boldsymbol{p})\Big] = E\hat{a}^\dagger_{h,j}(\boldsymbol{p}) + \frac{1}{2E}\hat{a}_{H,j}(\boldsymbol{p}) \qquad\qquad \Big[\mathcal{H}, \hat{a}^\dagger_{H,j}(\boldsymbol{p})\Big] = E\hat{a}^\dagger_{H,j}(\boldsymbol{p})\,. \tag{4.278}$$

We are interested in the one-particle eigenstates of $\mathcal{H}$, which we denote as $|\boldsymbol{p}, j\rangle$, that may be solved for using an ansatz consisting of a linear combination of creation operators acting on the vacuum,

$$|\boldsymbol{p}, j\rangle = \left(c_h \hat{a}^\dagger_{h,j}(\boldsymbol{p}) + c_H \hat{a}^\dagger_{H,j}(\boldsymbol{p})\right)|0\rangle\ , \tag{4.279}$$

where c_h and c_H are arbitrary constants that are determined by acting on the ansatz state with the Hamiltonian (4.276). This yields the eigenvalue equation

$$\mathcal{H}\,|\boldsymbol{p}, j\rangle = E\left(c_h \hat{a}^\dagger_{h,j}(\boldsymbol{p}) + \left(c_H + \frac{c_h}{2E^2}\right)\hat{a}^\dagger_{H,j}(\boldsymbol{p})\right)|0\rangle = \lambda_E\,|\boldsymbol{p}, j\rangle\ , \tag{4.280}$$

which fixes $c_h = 0$ and $c_H = 1$ after normalizing the eigenvalue to $\lambda_E = E$. This implies the existence of just a single one-particle energy eigenstate, making the generalization to n-particle eigenstates straightforward:

$$|\boldsymbol{p}_n, j_n\rangle_H = \frac{1}{\sqrt{n!}}\hat{a}^\dagger_{H,j_1}(\boldsymbol{p}_1)\cdots\hat{a}^\dagger_{H,j_n}(\boldsymbol{p}_n)\,|0\rangle \tag{4.281}$$

$$\mathcal{H}\,|\boldsymbol{p}_n, j_n\rangle_H = \sum_{i=1}^{n}\big(E_i\big)\,|\boldsymbol{p}_n, j_n\rangle_H\ . \tag{4.282}$$

The fact that there is no one-particle eigenstate associated with $\hat{a}^\dagger_{h,j}$ comes as a result of the action of the last term in the Hamiltonian (4.276), which effectively converts $\hat{a}^\dagger_{h,j}$ to $\hat{a}^\dagger_{H,j}$. However, as it turns out, the one-particle state corresponding to $\hat{a}^\dagger_{H,j}$ is only one part of the complete set of eigenstates.

There is actually a unique way to construct a particular multi-particle eigenstate[13] containing both spin-2 operators that satisfies an eigenvalue equation analogous to (4.280). To derive the precise form of this state, let us consider some general state containing at least one $\hat{a}^\dagger_{h,j}$,

$$\cdots \hat{a}^\dagger_{h,j}(\boldsymbol{p}) \cdots |0\rangle \ , \tag{4.283}$$

where the $\cdots$ represent an arbitrary number of $\hat{a}^\dagger_{h,j}$ and at least one $\hat{a}^\dagger_{H,j}$ operator. Acting on (4.283) with $\mathcal{H}$, one finds that the last term in $\mathcal{H}$ converts $\hat{a}^\dagger_{h,j}(\boldsymbol{p})$ to $(4E_{\boldsymbol{p}})^{-1}\hat{a}^\dagger_{H,j}(\boldsymbol{p})$, which should somehow be canceled if the eigenvalue equation is to be satisfied. This turns out to be possible if we separate an $\hat{a}^\dagger_{H,j}(\boldsymbol{q})$ from $\cdots$ in (4.283) so that it becomes

$$\cdots E_{\boldsymbol{p}} \hat{a}^\dagger_{h,j}(\boldsymbol{p}) \hat{a}^\dagger_{H,j}(\boldsymbol{q}) \cdots |0\rangle \ . \tag{4.284}$$

The factor of $\hat{a}^\dagger_{h,j}(\boldsymbol{p})$ may then be canceled by the analogous conversion that comes from the negative counterpart of this state,

$$(-1) \cdots E_{\boldsymbol{q}} \hat{a}^\dagger_{h,j}(\boldsymbol{q}) \hat{a}^\dagger_{H,j}(\boldsymbol{p}) \cdots |0\rangle \ . \tag{4.285}$$

All together, one finds that the (normalized) linear combination of $\hat{a}^\dagger_{h,j}$ and $\hat{a}^\dagger_{H,j}$ given by

$$\hat{a}^\dagger_{hH,j}(\boldsymbol{p},\boldsymbol{q}) = \frac{1}{2}\left(\sqrt{E_{\boldsymbol{p}}/E_{\boldsymbol{q}}}\,\hat{a}^\dagger_{h,j}(\boldsymbol{p})\hat{a}^\dagger_{H,j}(\boldsymbol{q}) - \sqrt{E_{\boldsymbol{q}}/E_{\boldsymbol{p}}}\,\hat{a}^\dagger_{h,j}(\boldsymbol{q})\hat{a}^\dagger_{H,j}(\boldsymbol{p})\right) \tag{4.286}$$

is a unique eigenstate with eigenvalue $(E_{\boldsymbol{p}} + E_{\boldsymbol{q}})$.

We may calculate the norm of this new state with the commutation relations (4.263),

$$\langle 0|\, \hat{a}_{hH,j}(\boldsymbol{p},\boldsymbol{q})\hat{a}^\dagger_{hH,j'}(\boldsymbol{p}',\boldsymbol{q}')\,|0\rangle = \delta_{jj'} D(\boldsymbol{p},\boldsymbol{q};\boldsymbol{p}',\boldsymbol{q}')\,, \tag{4.287}$$

where we have defined the shorthand

$$D(\boldsymbol{p},\boldsymbol{q};\boldsymbol{p}',\boldsymbol{q}') = \frac{1}{2}\big(\delta^3(\boldsymbol{p}-\boldsymbol{q}')\delta^3(\boldsymbol{q}-\boldsymbol{p}') - \delta^3(\boldsymbol{p}-\boldsymbol{p}')\delta^3(\boldsymbol{q}-\boldsymbol{q}')\big)\,. \tag{4.288}$$

Finally with all of the above, we may express the most general m,n-particle eigenstate of our Hamiltonian as

$$\begin{aligned} &|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n\rangle_H = \\ &\qquad \frac{1}{\sqrt{m!\,n!}}\hat{a}^\dagger_{hH,j_1}(\boldsymbol{p}_1,\boldsymbol{q}_1)\cdots\hat{a}^\dagger_{hH,j_m}(\boldsymbol{p}_m,\boldsymbol{q}_m)\hat{a}^\dagger_{H,l_1}(\boldsymbol{k}_1)\cdots\hat{a}^\dagger_{H,l_n}(\boldsymbol{k}_n)\,|0\rangle \ , \end{aligned} \tag{4.289}$$

where the corresponding eigenvalues are given by $\sum_{i=1}^m (E_{\boldsymbol{p}_i} + E_{\boldsymbol{q}_i}) + \sum_{j=1}^n E_{\boldsymbol{k}_j}$. The complete set of all these states forms a basis on the space of $\mathcal{H}$ eigenstates which we denote as $\mathcal{V}_{\mathcal{H}}$.

[13] We thank Taichiro Kugo for pointing out the existence of this additional eigenstate.

The existence of the rather odd multi-particle operator $\hat{a}_{hH,j}$ is obviously related to the off-diagonal nature of the spin-2 inner product, a feature that has another interesting consequence. Since the commutator between $\hat{a}_{H,j}$ and $\hat{a}^{\dagger}_{H,j}$ vanishes, so does the scalar product between the n-particle state and its dual, ${}_{H}\langle \boldsymbol{p}_n, j_n|$. In fact, the only general non-vanishing scalar product that we may construct on our spin-2 subspace is between the n, m-particle eigenstate (4.289) and its "off-diagonal dual" that is given by the the bra version of (4.289) with $H \leftrightarrow h$,

$$\begin{aligned} &{}_{h}\langle \boldsymbol{p}'_m, \boldsymbol{q}'_m, j'_m; \boldsymbol{k}'_n, l'_n| = \\ &\qquad \frac{1}{(m!\, n!)^{1/2}} \langle 0|\, \hat{a}_{hH,j'_1}(\boldsymbol{p}'_1, \boldsymbol{q}'_1) \cdots \hat{a}_{hH,j'_m}(\boldsymbol{p}'_m, \boldsymbol{q}'_m) \hat{a}_{h,l'_1}(\boldsymbol{k}'_1) \cdots \hat{a}_{h,l'_n}(\boldsymbol{k}'_n)\,. \end{aligned} \tag{4.290}$$

It is easy to see that the subspaces spanned by (4.289) and (4.290) are isomorphic, thus implying that the only non-vanishing scalar product involving general eigenstates is given by

$$\begin{aligned} &{}_{h}\langle \boldsymbol{p}'_m, \boldsymbol{q}'_m, j'_m; \boldsymbol{k}'_n, l'_n | \boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n\rangle_H = \\ &\qquad \frac{1}{m!\, n!}\Big[\big(\delta_{j'_1 j_1} \cdots \delta_{j'_m j_m} D(\boldsymbol{p}'_1, \boldsymbol{q}'_1; \boldsymbol{p}_1, \boldsymbol{q}_1) \cdots D(\boldsymbol{p}'_m, \boldsymbol{q}'_m; \boldsymbol{p}_m, \boldsymbol{q}_m) + \text{permutations}\big) \\ &\qquad\qquad \times \big(\delta_{l'_1 l_1} \cdots \delta_{l'_n l_n} \delta^3(\boldsymbol{k}'_1 - \boldsymbol{k}_1) \cdots \delta^3(\boldsymbol{k}'_n - \boldsymbol{k}_n) + \text{permutations}\big)\Big]\,. \end{aligned} \tag{4.291}$$

With this we may finally construct the all-important unit operator on the space of the $\mathcal{H}$ eigenstates,

$$\mathbb{1} = \sum_{m,n} \sum_{j_m, l_n} \int \mathrm{d}^3\boldsymbol{p}_m \mathrm{d}^3\boldsymbol{q}_m \mathrm{d}^3\boldsymbol{k}_n (-1)^m\, |\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n\rangle_H\, {}_h\langle \boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n|\,, \tag{4.292}$$

where it is understood that the $m, n = 0$ term gives the vacuum contribution. We note that the factor of $(-1)^m$ above appears as a result of the multi-particle eigenstate (4.286), whose existence follows from the indefinite inner-product on the space of spin-2 states.

Failure of the probability interpretation

After constructing the Hamiltonian operator, deriving the associated eigensystem, and establishing a unit operator, we are finally in a position to take a deeper look at unitarity through its definition in terms of the S-matrix. We begin by recalling the crucial assumption of asymptotic completeness that underlies the LSZ formalism,

$$\mathcal{V}^{\text{in}} \simeq \mathcal{V}^{\text{out}} \simeq \mathcal{V} \qquad \text{and} \qquad S\mathcal{V} = S^{\dagger}\mathcal{V} = \mathcal{V}\,, \tag{4.293}$$

and note that it must also apply to $\mathcal{V}_{\mathcal{H}} \subset \mathcal{V}_{\text{tr}}$ as the only subspace of spin-2 energy eigenstates. This feature, paired with the pseudo-unitarity of S and the facts that $\mathcal{V}^{\text{in}}_{\mathcal{H}}$ and $\mathcal{V}^{\text{out}}_{\mathcal{H}}$ are Hamiltonian-invariant subspaces, allows us to write

$$S\mathcal{V}^{\text{in(out)}}_{\mathcal{H}} = \mathcal{V}^{\text{in(out)}}_{\mathcal{H}}\,, \tag{4.294}$$

given that the Hamiltonian commutes with S. We point out all of these features because together they imply that the unitarity of S on $\mathcal{V}_{\mathcal{H}}^{\text{in}}$ may be expressed in terms of either of the general statements

$$S^{\dagger}\mathcal{V}_{\mathcal{H}}^{\text{in}} = \mathcal{V}_{\mathcal{H}}^{\text{in}} \quad \Leftrightarrow \quad S^{\dagger}\mathbb{1}S = S\mathbb{1}S^{\dagger} = \mathbb{1}\,. \tag{4.295}$$

Our goal now will be to explicitly check if this last statement will allow us to define a sensible notion of quantum probability in the usual way. To this end we recall the unit operator defined in (4.292) and consider the state

$$\begin{aligned}&|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}\rangle_H = \mathbb{1}^{\text{out}}\,|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}\rangle_H = \\ &\quad \sum_{m',n'}\sum_{j'_{m'},l'_{n'}}\int \mathrm{d}^3\boldsymbol{p}'_{m'}\mathrm{d}^3\boldsymbol{q}'_{m'}\mathrm{d}^3\boldsymbol{k}'_{n'}\,(-1)^{m'}\,\big|\boldsymbol{p}'_{m'}, \boldsymbol{q}'_{m'}, j'_{m'}; \boldsymbol{k}'_{n'}, l'_{n'}; \text{out}\big\rangle_H\, S_{\alpha\beta}\,,\end{aligned} \tag{4.296}$$

where we have restored the suppressed "in" and "out" designations ($\hat{a}_{h,j} \to \hat{a}^{\text{in}}_{h,j}$, etc.) which identify $\mathbb{1}^{\text{out}}$ as the unit operator written purely in terms of "out" states. Here we also see the appearance of the explicit S-matrix element

$$S_{\alpha\beta} = {}_h\langle\beta; \text{out}|\alpha; \text{in}\rangle_H\;, \tag{4.297}$$

which represents the transition amplitude between states labeled by

$$\alpha = \big(\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n\big) \qquad\qquad \beta = \big(\boldsymbol{p}'_{m'}, \boldsymbol{q}'_{m'}, j'_{m'}; \boldsymbol{k}'_{n'}, l'_{n'}\big)\,. \tag{4.298}$$

With all of these considerations, the usual consistent interpretation of probability may be expressed by

$$1 = {}_h\langle\alpha; \text{in}|\alpha; \text{in}\rangle_H \stackrel{?}{=} {}_h\langle\alpha; \text{in}|S^{\dagger}\mathbb{1}S|\alpha; \text{in}\rangle_H\;, \tag{4.299}$$

where we have used the relation (4.295). This is the same type of expression as (4.167) that was used to confirm unitarity violation in the broken phase theory, though here the first equality is actually satisfied as a result of the inner product (4.291). Here we are interested in the last equality which would establish unitarity and is thus under scrutiny. With the definition of the unit operator in (4.292), this last equality may be written explicitly as

$$\begin{aligned}1 \stackrel{?}{=} \sum_{m,n}\sum_{j_m,l_n}\int \mathrm{d}^3\boldsymbol{p}_m\mathrm{d}^3\boldsymbol{q}_m\mathrm{d}^3\boldsymbol{k}_n\Big((-1)^m\,{}_h\langle\alpha; \text{in}|S^{\dagger}\,|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}\rangle_H \\ \times\,{}_h\langle\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}|S\,|\alpha; \text{in}\rangle_H\Big)\,,\end{aligned} \tag{4.300}$$

and we encounter an integrand that is clearly not positive-definite for general n and m as a result of the troublesome factor of $(-1)^m$. This feature then implies that

$${}_h\langle\alpha; \text{in}|S^{\dagger}\,|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}\rangle_H \neq {}_H\langle\alpha; \text{in}|S^{\dagger}\,|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \text{in}\rangle_h\;, \tag{4.301}$$

which in turn means that unitarity is violated, as the integrand of (4.300) may not be interpreted as the probability for some initial state α to transition to a final $(2m+n)$-particle state as would be required.

We thus arrive at a new interpretation of the ghost problem in the context of indefinite metric QFT. It should come as no surprise that, despite the fact that the inner product (4.291) is non-negative, its off-diagonal and thus indefinite nature leads to a conclusion that is similar to that of the broken theory of Section 4.6, where the metric on spin-2 states is diagonal, but still indefinite. In the present case, we see the ghost problem arise through a different route – the off-diagonal indefinite metric structure implies the presence of the multi-particle Hamiltonian eigenstate (4.286) whose existence generates the factor of $(-1)^m$ that appears in the unit operator (4.292), and ultimately leads to a violation of perturbative unitarity through a failure to confirm (4.300). While this outcome was anticipated, to the best of our knowledge, this marks the first time that unitarity violation has been established in Weyl's conformal gravity within the framework of the covariant operator formalism and we anticipate that this new view on the ghost problem in quantum gravity will lead to new avenues of theoretical research and, hopefully, a satisfying resolution.

Chapter 5

Conclusion

5.1 Summary

In this thesis we have constructed physical theories under the guiding principle of scale invariance that may help to resolve some of the most pressing issues in high energy physics, and have also investigated the new exciting challenges that these theories present. The Higgs sector hints strongly towards fundamental scale invariance due to the simple fact that it possesses the only SI-violating term in the SM. The presence of this term raises theoretical issues regarding the stability of the measured value of the Higgs mass under radiative corrections when one considers extensions to the SM, however, these issues may be resolved if the Higgs mass is not a fundamental constant but is instead generated dynamically by quantum effects. The most straightforward renormalizable extension of Einstein's General Relativity is also naturally scale-invariant with the exception of a single term in its action that might be generated in the same fashion, while further clues pointing towards SI come from cosmology through the approximately scale-invariant primordial fluctuations measured in the CMB. Motivated by the goal of establishing a combined theory of the particle physics and gravity that is valid up to arbitrary energies and reflects the unprecedented success of the Standard Model as described by quantum field theory, one is thus naturally drawn to the idea that our universe might be insensitive to changes in scale at the most fundamental level. Embracing this paradigm comes with added complications however, since scale-invariant gravity implies the presence of physical spin-2 ghosts that threaten unitarity and must be dealt with carefully if the theory as a whole is to be considered valid.

Following this line of reasoning, we began in Chapter 2 by constructing a model that couples the SM Higgs sector with a vanishing tree-level mass parameter $\mu_H = 0$, a BSM sector containing two additional scalars ϕ and σ as well as a family of sterile right-handed neutrinos N, and a Jordan frame gravitational sector composed of the squared Weyl tensor and Ricci scalar. Besides the usual quartic scalar self-interactions, this model contains portal couplings between each of the scalars, portals between the BSM scalars and the sterile neutrinos, a mixed Higgs-sterile-SM neutrino portal, and non-minimal couplings between each scalar field and the Ricci scalar. All of these terms are consistent with the SM gauge symmetry, diffeomorphism invariance, and global SI thanks to the lack of massive constants. However, after including radiative corrections from the scalar sector we found that the one-loop effective potential possesses a non-zero minimum in the ϕ direction. The presence of the finite VEV v_ϕ in the quantum effective action gives a mass to each field that ϕ couples to and thus implies that SI is spontaneously broken in line with the Coleman(Gildener)-Weinberg mechanism [11, 151]. While the induced mass of σ is so large that we were able to safely integrate it out of the action, the non-zero VEV implies other important physical ramifications; it gives rise to the Planck scale $M_{\rm Pl} \sim \beta_\phi^{1/2} v_\phi$ and thus to an Einstein-Hilbert term, and it generates a mass $m_N = y_\phi v_\phi$ for the sterile neutrinos. We also assumed a small but technically natural Yukawa coupling $y_\phi \approx 10^{-11}$ that implies $m_N \approx 10^7$ GeV, which then allowed for a scale-invariant realization of the "neutrino option" wherein light masses are generated for the SM neutrinos and EW SSB is triggered. This in turn generates a Higgs mass and all of the other SM masses in line with the standard prescription and implies a deep connection between all of the widely separated energy scales that we observe in Nature. It should be noted that some degree of fine-tuning was required for the Higgs portal $\lambda_{H\phi}$ to achieve the correct Higgs mass in this model, however, it was argued that this value is at least safe from quantum corrections.

Chapter 3 of this work was dedicated to the study of how inflation can be incorporated into scale-invariant theories of matter and gravity. Starting from the same quantum effective action that was derived in the Jordan frame in the previous chapter, we transformed our theory to the Einstein frame in order to separate contributions from the scalaron DOF hidden in the Jordan frame R^2 term. After combining the scalaron terms with the one-loop effective potential, we arrived at a two-field inflationary potential that exhibits the valley structure displayed in Figure 3.2 if the scalaron's mass is much larger than the Hubble scale during inflation. We assumed that this was indeed the case and eliminated the scalaron in favor of ϕ, which allowed us to derive an approximated one-field inflationary potential with slow-roll behavior in the ϕ direction. After deriving expressions for the standard slow-roll parameters with this potential, we generated predictions for CMB observables for a wide range of input parameters (coupling constants) and found values of the scalar spectral index in the range $0.964 \lesssim n_s \lesssim 0.975$ and a tensor-to-scalar ratio $r \lesssim 0.08$. The complete display of our results in Figure 3.3 indicates that the inflationary period predicted by our scale-invariant model is consistent with the most stringent modern observations made by the Planck and BICEP/Keck collaborations [42–44].

We took a look at another realization of scale generation and inflation in the second part of Chapter 3. In the previous model we assumed, as other analogous studies often do, that the Weyl squared coupling constant was negligibly small so that the Weyl term played no important role. This assumption is usually made to avoid the complications that arise from the massive spin-2 ghost DOFs that are unavoidably introduced by the Weyl term, however, we found that this ghost is in fact able to effectively fill the role previously played by the scalar σ, thus rendering the introduction of this field superfluous. We derived the one-loop effective potential containing contributions from ϕ and the massive ghost part of the graviton $h_{\alpha\beta}$ which, following the same kind of analyses performed in the previous chapter, allowed us to spontaneously break global SI, dynamically generate all important mass scales, and predict inflationary parameters that nicely satisfy modern constraints (see Figure 3.4). In short, it was found that removing one assumption from the original scale-invariant model allowed us to achieve analogous or even preferable predictions while simultaneously avoiding the need to include an extra field into the model by hand. However, allowing even very massive ghosts ($m_h \approx 10^{-2} M_{\text{Pl}}$) to propagate in any model has other important ramifications that must be addressed.

The inclusion of physical effects generated by spin-2 ghosts in the second part of Chapter 3 served as a bridge to Chapter 4 where we looked into these ramifications in great detail. We began by demonstrating how actions containing four derivatives acting on their fields generally exhibit a pathology known as the Ostrogradsky instability at the classical level [98]. The quantum analog of this pathology, the ghost problem, was then shown to present in terms of either negative energy eigenvalues or negative norms between ghost states depending on how one chooses to define the quantum vacuum. We argued that consistent application of the Feynman prescription requires the negative norm choice of vacuum and we saw an example of how the standard interpretation of quantum probability can break down when such negative norms are present.

After gaining this understanding of what the ghost problem actually entails, we reviewed several of the most promising attempts to address it that have appeared in the literature, and investigated the precise nature in which the ghost problem appears in scale-invariant theories of quadratic gravity. This is a rather complicated task due to the presence of gauge symmetries so, in an effort to make the process more straightforward, we rewrote both globally scale-invariant QG in the spontaneously broken phase and locally scale-invariant (conformal) QG in the unbroken phase in second-order fashions that clearly exposes their propagating DOFs. This was achieved via the introduction of auxiliary and Stückelberg fields, the latter of which were introduced along with additional gauge symmetries that allowed the theories to be expressed in terms of purely first-class constraints in phase space. Rewriting QG in this way made it clear how a spin-2 analog of the Higgs mechanism can manifest when conformal gravity is coupled to an external scalar field, and allowed for a more straightforward quantization of each realization of scale-invariant QG. We employed the covariant operator formalism of Kugo, Ojima, and Nakanishi [266, 269] to rigorously establish these quantum theories through the introduction of BRST symmetry [260–262] and subsequently identified each theory's physical transverse subspace of states by appealing to the quartet mechanism [271–274]. In the broken phase theory, we encountered the expected negative commutation relation between spin-2 ghosts that leads to a violation of unitarity in the theory as a whole. However, in this case we also made the crucial observation that unitarity was in fact satisfied on a particular subspace of the complete physical Fock space and defined the notion of "conditional unitarity" that describes how quantum QG may be considered a valid effective field theory up to energies nearing the Planck scale, even in the presence of ghosts. Analysis of the unbroken quantum theory was considerably more complicated due to the inherently off-diagonal nature of its commutation relations in the spin-2 sector, as these imply the existence of multi-particle Hamiltonian eigenstates with no simple one-particle analogs. However, a breakdown of the probability interpretation was also encountered in this theory, which came from the unusual way in which the multi-particle states manifest in the unit operator.

5.2 Discussion

Before concluding it is important that we address several unexplored topics that relate to the work in this thesis as well as the the future avenues of research that it has made available. In Section 3.1 we briefly mentioned that non-Gaussian primordial fluctuations would be neglected in our analysis due to the fact that they are known to be heavily suppressed in single-field inflationary models, however, it is also expected that they manifest more strongly in both the CMB anisotropy and measurements of large-scale structure when one considers multi-field theories [180, 181]. Though the inflationary potential we derived in [1] is well-approximated as a single field potential after confining it to a valley structure under the condition (3.23), the most general theory does strictly speaking contain two scalars fields in ϕ and the scalaron S, which may lead to relevant non-Gaussianities when the valley condition is relaxed. The influence of spin-2 DOFs on the inflationary potential may also amplify the effect of non-Gaussanities as pointed out in [214], which is particularly relevant for the second study of inflation we carried out in [2]. Techniques for explicitly computing non-Gaussanities in these contexts are already known [293] and we plan to employ them in the near future. This is a particularly interesting line of work due to the fact that there are planned experimental efforts to measure cosmological non-Gaussianities, namely the LSST [294], Euclid [295], and LiteBIRD [296] projects, which would allow us to constrain our models with real world data even further than they already have been.

There are also more theoretical topics that should be addressed in the future, first among them being the role of the conformal anomaly [73–75, 155, 297] and the cosmological constant problem [298, 299]. In our globally scale-invariant theories the anomaly generates a finite zero-point energy that should in principle match and cancel very precisely with contributions from all other sectors in order to reproduce the approximately vanishing CC that we observe. We addressed this issue in our studies with the introduction of U_Λ into the effective potential which we solved for under the assumption that such cancellations would occur, but a more in-depth understanding of this process is certainly warranted. It is also important to consider these kind of issues particularly carefully with respect to conformal gravity where a non-zero conformal anomaly violates gauge symmetry and thus implies a fundamental inconsistency [76]. Proponents of conformal gravity as a fundamental theory argue that this inconsistency only arises when gravity is treated independently from matter and that the conformal anomaly vanishes identically to all orders when gravity and matter are treated on an equal footing and renormalized together, no matter the overall field content [97, 300]. The formalism established in [3, 4] puts us in a unique place to investigate this kind of idea in detail since, after establishing a covariant operator quantization as we have, the conformal anomaly in CG manifests as a BRST anomaly. In this picture, the Wess-Zumino consistency condition [301, 302] for the conformal anomaly may in principle be understood in terms of BRST cohomology [303], which should allow for regularization-scheme-independent statements to be made about the issue that may be compared with other studies of the conformal anomaly in CG [74, 121]. Even beyond the conformal anomaly, it should also be possible to make more general regularization-independent statements about the renormalizability of QG using our BRST/operator-based description [288].

We also plan to take a deeper look into the general solutions to the ghost problem introduced in Section 4.4 through the lens of our quantum QG formalism. It would be particularly interesting to investigate Donoghue and Menezes' unstable ghost solution [102–104] from an operator-based perspective, which we recall rests heavily on Veltman's assertion that unstable particles do not correspond to asymptotic states [236]. Veltman's proof is based on a super-renormalizable scalar theory, and though his work has already been extended for application to gauge theories with complex pole masses [304] (which we may also expect to appear in gravity in analogy to the Lee-Wick models [99, 100]), it is not clear whether the same prescription of avoiding cuts through unstable particles applies when those unstable particles are ghosts. To be specific, the conventional $i\epsilon$ prescription that enters into Veltman's proof assumes that the unstable particle's pole appears in the left upper-half of the complex p^2 plane, while it is known from the Lee-Wick model, fakeon prescription, and Donoghue's own work that this pole is shifted for ghosts [99, 103, 106]. We also expect that an operator-based view would allow one to more easily check that the probability interpretation is not spoiled in this unstable ghost solution like it is in the toy model of Section 4.2.2, as this kind of behavior is tricky or perhaps even impossible to see in a purely diagram-based approach.

Bender's $\mathcal{PT}$-symmetric take on the ghost problem [109–114] also lends itself quite nicely to our operator quantization of QG. Though $\mathcal{PT}$-QFT is still in its infancy, more than enough work has already been done for the idea to be appealing and the fact that we are able to derive precise expressions for the gauge-fixed Hamiltonian in QG (see (4.161) and (4.276)) means that we are in a position to make more precise statements about $\mathcal{PT}$-symmetric gravity without the need to resort to the usual toy models. Beyond the many theoretical aspects of $\mathcal{PT}$-QFT that still need to be worked out, it would also be interesting to explore phenomenological implications for the dark matter and dark energy problems that may result from adopting $\mathcal{PT}$ theory and its assertion that the spacetime metric is complex.

Appendix

A Plane waves and Green's functions

In this appendix, we provide a summary of the definitions and properties of plane wave solutions, invariant delta functions, and propagators introduced in Section 4.5.2 as part of the LSZ formalism. Our construction closely follows that presented in [266], though we have extended the formalism to include quadrupole functions since these may appear in the quantization of second-order quadratic gravity depending on what gauge choice is considered.

The plane wave solution to the Klein-Gordon equation $(\Box - m^2) f_{\boldsymbol{p}}(x) = 0$, normalized in a finite volume V, is represented by

$$f_{\boldsymbol{p}}(x) = \frac{1}{\sqrt{2EV}} e^{ipx} \,, \tag{A.1}$$

where $E^2 = |\boldsymbol{p}|^2 + m^2$ and $px = -E\, x^0 + \boldsymbol{p} \cdot \boldsymbol{x}$. The plane wave solutions for double-poles, triple-poles, and quadruple-poles, denoted as $g_{\boldsymbol{p}}(x)$, $h_{\boldsymbol{p}}(x)$, and $k_{\boldsymbol{p}}(x)$ respectively, are given by

$$g_{\boldsymbol{p}}(x) = -\frac{1}{2\sqrt{2EV}} \left(\frac{1}{2E^2} + \frac{ix^0}{E} \right) e^{ipx} \tag{A.2}$$

$$h_{\boldsymbol{p}}(x) = \frac{1}{8\sqrt{2EV}} \left(\frac{5}{4E^4} + \frac{2ix^0}{E^3} - \frac{(x^0)^2}{E^2} \right) e^{ipx} \tag{A.3}$$

$$k_{\boldsymbol{p}}(x) = -\frac{1}{32\sqrt{2EV}} \left(\frac{15}{4E^6} + \frac{11ix^0}{2E^5} - \frac{3(x^0)^2}{E^4} - \frac{2i(x^0)^3}{3E^3} \right) e^{ipx} \,. \tag{A.4}$$

These functions are related to one another via successive application of powers of the Klein-Gordon operator according to

$$\begin{aligned}
(\Box - m^2) g_{\boldsymbol{p}}(x) &= f_{\boldsymbol{p}}(x) \qquad & (\Box - m^2)^2 g_{\boldsymbol{p}}(x) &= 0 \\
(\Box - m^2) h_{\boldsymbol{p}}(x) &= g_{\boldsymbol{p}}(x) \qquad & (\Box - m^2)^3 h_{\boldsymbol{p}}(x) &= 0 \\
(\Box - m^2) k_{\boldsymbol{p}}(x) &= h_{\boldsymbol{p}}(x) \qquad & (\Box - m^2)^4 k_{\boldsymbol{p}}(x) &= 0
\end{aligned} \tag{A.5}$$

and they satisfy the orthogonality relations

$$\int \mathrm{d}^3\boldsymbol{x}\, f^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} f_{\boldsymbol{q}}(x) = -i\delta_{\boldsymbol{p},\boldsymbol{q}} \tag{A.6}$$

$$\int \mathrm{d}^3\boldsymbol{x}\left(f^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} g_{\boldsymbol{q}}(x) + g^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} f_{\boldsymbol{q}}(x)\right) = 0 \tag{A.7}$$

$$\int \mathrm{d}^3\boldsymbol{x}\left(f^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} h_{\boldsymbol{q}}(x) + h^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} f_{\boldsymbol{q}}(x) + g^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} g_{\boldsymbol{q}}(x)\right) = 0 \tag{A.8}$$

$$\begin{aligned}\int \mathrm{d}^3\boldsymbol{x}\Big(&f^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} k_{\boldsymbol{q}}(x) + k^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} f_{\boldsymbol{q}}(x)\\ &+g^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} h_{\boldsymbol{q}}(x) + h^*_{\boldsymbol{p}}(x)\overleftrightarrow{\partial_0} g_{\boldsymbol{q}}(x)\Big) = 0\,,\end{aligned} \tag{A.9}$$

where we use the shorthand $A\overleftrightarrow{\partial_0}B = A\partial_0 B - B\partial_0 A$.

The plane wave solutions $f_{\boldsymbol{p}}(x)$, $g_{\boldsymbol{p}}(x)$, and $h_{\boldsymbol{p}}(x)$ allow us to construct the associated positive frequency invariant delta functions

$$D^{(+)}(x-y) = \sum_{\boldsymbol{p}} f_{\boldsymbol{p}}(x) f^*_{\boldsymbol{p}}(y) = \sum_{\boldsymbol{p}} \frac{1}{2EV}\, e^{ip(x-y)} \tag{A.10}$$

$$\begin{aligned}E^{(+)}(x-y) &= \sum_{\boldsymbol{p}} \left(f_{\boldsymbol{p}}(x) g^*_{\boldsymbol{p}}(y) + g_{\boldsymbol{p}}(x) f^*_{\boldsymbol{p}}(y)\right)\\ &= -\sum_{\boldsymbol{p}} \frac{1}{4EV}\left(\frac{1}{E^2} + \frac{i}{E}(x^0-y^0)\right) e^{ip(x-y)}\end{aligned} \tag{A.11}$$

$$\begin{aligned}F^{(+)}(x-y) &= \sum_{\boldsymbol{p}} \left(f_{\boldsymbol{p}}(x) h^*_{\boldsymbol{p}}(y) + h_{\boldsymbol{p}}(x) f^*_{\boldsymbol{p}}(y) + g_{\boldsymbol{p}}(x) g^*_{\boldsymbol{p}}(y)\right)\\ &= \sum_{\boldsymbol{p}} \frac{1}{16EV}\left(\frac{3}{E^4} + i\frac{3}{E^3}(x^0-y^0) - \frac{(x^0-y^0)^2}{E^2}\right) e^{ip(x-y)}\end{aligned} \tag{A.12}$$

$$\begin{aligned}G^{(+)}(x-y) &= \sum_{\boldsymbol{p}} \left(f_{\boldsymbol{p}}(x) k^*_{\boldsymbol{p}}(y) + k_{\boldsymbol{p}}(x) f^*_{\boldsymbol{p}}(y) + g_{\boldsymbol{p}}(x) h^*_{\boldsymbol{p}}(y) + h_{\boldsymbol{p}}(x) g^*_{\boldsymbol{p}}(y)\right)\\ &= -\sum_{\boldsymbol{p}} \frac{1}{64EV}\Bigg(\frac{5}{E^6} + i\frac{5}{E^5}(x^0-y^0)\\ &\qquad\qquad -\frac{2(x^0-y^0)^2}{E^4} - \frac{i(x^0-y^0)^3}{3E^3}\Bigg) e^{ip(x-y)}\,,\end{aligned} \tag{A.13}$$

which also naturally represent solutions for increasing powers of the Klein-Gordon operator:

$$\begin{aligned}(\Box - m^2)D^{(+)}(x-y) &= 0\\ (\Box - m^2)E^{(+)}(x-y) &= D^{(+)}(x-y)\\ (\Box - m^2)F^{(+)}(x-y) &= E^{(+)}(x-y)\\ (\Box - m^2)G^{(+)}(x-y) &= F^{(+)}(x-y)\,.\end{aligned} \tag{A.14}$$

The invariant delta functions that arise in the commutators (4.137), (4.248), and (4.249) are constructed from these functions and their negative frequency counterparts $D^{(-)} = (D^{(+)})^*$ (and similarly for the others),

$$\begin{aligned} D &= D^{(+)} - D^{(-)} & E &= E^{(+)} - E^{(-)} \\ F &= F^{(+)} - F^{(-)} & G &= G^{(+)} - G^{(-)} . \end{aligned} \tag{A.15}$$

In the continuum limit (4.78) where $V \to \infty$, the sums over momentum are replaced with an integral over three dimensional momentum space. In this case, the invariant delta functions take the forms

$$D(x-y) = \int \mathrm{d}^3\boldsymbol{p} \frac{1}{2E(2\pi)^3} \left(e^{ip(x-y)} - (\text{h.c.}) \right) \tag{A.16}$$

$$E(x-y) = -\int \mathrm{d}^3\boldsymbol{p} \frac{1}{4E(2\pi)^3} \left[\left(\frac{1}{E^2} + i\frac{x^0 - y^0}{E} \right) e^{ip(x-y)} - (\text{h.c.}) \right] \tag{A.17}$$

$$\begin{aligned} F(x-y) = \int \mathrm{d}^3\boldsymbol{p} \frac{1}{16E(2\pi)^3} \Bigg[\Bigg(\frac{3}{E^4} &+ i\frac{3(x^0 - y^0)}{E^3} \\ &- \frac{(x^0 - y^0)^2}{E^2} \Bigg) e^{ip(x-y)} - (\text{h.c.}) \Bigg] \end{aligned} \tag{A.18}$$

$$\begin{aligned} G(x-y) = -\int \mathrm{d}^3\boldsymbol{p} \frac{1}{64E(2\pi)^3} \Bigg[\Bigg(\frac{5}{E^6} &+ i\frac{5}{E^5}(x^0 - y^0) - \frac{2(x^0 - y^0)^2}{E^4} \\ &- \frac{i(x^0 - y^0)^3}{3E^3} \Bigg) e^{ip(x-y)} - (\text{h.c.}) \Bigg] , \end{aligned} \tag{A.19}$$

which in turn satisfy

$$\begin{aligned} D(x)\big|_{x^0=0} &= 0 & & \partial_0 D(x)\big|_{x^0=0} = -i\delta(\boldsymbol{x}) \\ \partial_0^n E(x)\big|_{x^0=0} &= 0 & (n = 0, 1, 2) \qquad & \partial_0^3 E(x)\big|_{x^0=0} = i\delta(\boldsymbol{x}) \\ \partial_0^n F(x)\big|_{x^0=0} &= 0 & (n = 0, \ldots, 4) \qquad & \partial_0^5 F(x)\big|_{x^0=0} = -i\delta(\boldsymbol{x}) \\ \partial_0^n G(x)\big|_{x^0=0} &= 0 & (n = 0, \ldots, 6) \qquad & \partial_0^7 G(x)\big|_{x^0=0} = i\delta(\boldsymbol{x}) . \end{aligned} \tag{A.20}$$

One may also express Green's functions for the Klein-Gordon operator (Feynman propagators) in terms of the invariant delta functions after including Heaviside functions in the standard way,

$$D_F(x) = \theta(x^0)D^{(+)}(x) + \theta(-x^0)D^{(-)}(x) = -i \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{e^{ipx}}{p^2 + m^2 - i\epsilon} \tag{A.21}$$

$$E_F(x) = \theta(x^0)E^{(+)}(x) + \theta(-x^0)E^{(-)}(x) = i \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{e^{ipx}}{(p^2 + m^2 - i\epsilon)^2} \tag{A.22}$$

$$F_F(x) = \theta(x^0)F^{(+)}(x) + \theta(-x^0)F^{(-)}(x) = -i \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{e^{ipx}}{(p^2 + m^2 - i\epsilon)^3} \tag{A.23}$$

$$G_F(x) = \theta(x^0)G^{(+)}(x) + \theta(-x^0)G^{(-)}(x) = i \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{e^{ipx}}{(p^2 + m^2 - i\epsilon)^4} . \tag{A.24}$$

The last important piece of this covariant LSZ construction is the integro-differential operator

$$\mathcal{E}^{(\eta)} = -\frac{1}{2}\left(\nabla^2\right)^{-1}\left(x^0\partial_0 - \eta\right), \tag{A.25}$$

where η is an arbitrary dimensionless constant. This operator acts as an inverse d'Alembertian specifically when it acts on solutions to the d'Alembert equation,

$$\Box\mathcal{E}^{(\eta)} f_{\boldsymbol{p}}(x) = f_{\boldsymbol{p}}(x)\,, \tag{A.26}$$

and also functions as an inverse d'Alembertian when applied to the propagators shown above when $m = 0$. It is also important to note that, for the Feynman propagators specifically, the arbitrary constant is fixed to $\eta = 1$. In short, one may use (A.25) and the definitions above to show

$$\Box\mathcal{E}^{(\eta)} D^{(\pm)}(x) = D^{(\pm)}(x) \qquad\qquad \Box\mathcal{E}^{(1)} D_F(x) = D_F(x)\,. \tag{A.27}$$

B The LSZ reduction formula in CG

This appendix is devoted to a demonstration of one of the most beneficial features of the second-order operator-based formulation of quantum gravity that we established in the main text, namely, that it allows us to define, and eventually calculate, precise S-matrix elements. We follow the work presented in [4] and focus on the more complicated case with off-diagonal propagators that appears in conformal gravity with unbroken symmetry, though the same kind of derivations may easily be generalized to the simpler case of quadratic gravity with spontaneously broken global scale symmetry as well.

The expressions of interest may be defined by appealing to the LSZ reduction formula which expresses the matrix elements

$$S_{\alpha\beta} = {}_h\langle\beta;\text{out}|\alpha;\text{in}\rangle_H\,, \tag{B.1}$$

where α and β are arbitrary in and out eigenstates, in terms of time-ordered correlation functions [267]. To derive the reduction formula, we must first invert the oscillator decompositions of our spin-2 fields using the relation (4.69) in order to express the state operators in terms of asymptotic Heisenberg fields. Recalling (4.229) and (4.230) paired with (4.257) and (4.258), we may restate these decompositions in the convenient forms

$$h^{\text{as}}_{\alpha\beta}(x) = \sum_{\boldsymbol{p},j}\Big(\varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}^{\text{as}}_{h,j}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}^{\text{as}}_{H,j}(\boldsymbol{p})g_{\boldsymbol{p}}(x) + \cdots + (\text{h.c.})\Big) \tag{B.2}$$

$$H^{\text{as}}_{\alpha\beta}(x) = \sum_{\boldsymbol{p},j}\Big(\varepsilon_{j\,\alpha\beta}(\boldsymbol{p})\hat{a}^{\text{as}}_{H,j}(\boldsymbol{p})f_{\boldsymbol{p}}(x) + \cdots + (\text{h.c.})\Big)\,, \tag{B.3}$$

where we have relegated all unphysical quartet and (physical but currently irrelevant) $\hat{a}_{A,j}(\boldsymbol{p})$ contributions to the "$\cdots$", as they do not play a part in the H-h scattering events of interest. Using the relation $\varepsilon^*_{j\,\alpha\beta}\varepsilon_{j'}{}^{\alpha\beta} = \delta_{jj'}$ the inverses of these decompositions are then found to be given by

$$\hat{a}^{\rm as}_{h,j}(\boldsymbol{p}) = i\int \mathrm{d}^3\boldsymbol{x}\,\varepsilon_j^{*\alpha\beta}(\boldsymbol{p})\Big(f^*_{\boldsymbol{p}}(x)\overset{\leftrightarrow}{\partial_0}h^{\rm as}_{\alpha\beta}(x) + g^*_{\boldsymbol{p}}(x)\overset{\leftrightarrow}{\partial_0}\Box h^{\rm as}_{\alpha\beta}(x)\Big) \tag{B.4}$$

$$\hat{a}^{\rm as}_{H,j}(\boldsymbol{p}) = i\int \mathrm{d}^3\boldsymbol{x}\,\varepsilon_j^{*\alpha\beta}(\boldsymbol{p})f^*_{\boldsymbol{p}}(x)\overset{\leftrightarrow}{\partial_0}H^{\rm as}_{\alpha\beta}(x)\,, \tag{B.5}$$

in line with (4.69).

As we are now working with 4D spacetime-dependent fields, it is beneficial to re-express our 3D spatial integrals in 4D by recalling the presence of the inherent asymptotic limits and appealing to the fundamental theorem of calculus,

$$\left(\lim_{x^0\to\infty} - \lim_{x^0\to-\infty}\right)\int \mathrm{d}^3\boldsymbol{x}F(x) = \int_{-\infty}^{\infty}\mathrm{d}x^0\,\partial_0\int \mathrm{d}^3\boldsymbol{x}F(x) = \int \mathrm{d}^4x\,\partial_0 F(x)\,, \tag{B.6}$$

which paired with the relations

$$\partial_0^2 f_{\boldsymbol{p}} = \nabla^2 f_{\boldsymbol{p}} \qquad\qquad \partial_0^2 g_{\boldsymbol{p}} = \nabla^2 g_{\boldsymbol{p}} - f_{\boldsymbol{p}}\,, \tag{B.7}$$

allows us to write all derivatives in terms of $\Box$ and express time-ordered products of state operators in terms of time-ordered products of fields as

$$\hat{a}^{{\rm out}\,\dagger}_{H,j}(\boldsymbol{p})T(\cdots) - T(\cdots)\hat{a}^{{\rm in}\,\dagger}_{H,j}(\boldsymbol{p}) = i\int \mathrm{d}^4x\;\varepsilon_{j\,\alpha\beta}(\boldsymbol{p})f_{\boldsymbol{p}}(x)\Box T\big(H^{\alpha\beta}(x)\cdots\big) \tag{B.8}$$

$$\begin{aligned}\hat{a}^{\rm out}_{h,j}(\boldsymbol{p})T(\cdots) - T(\cdots)\hat{a}^{\rm in}_{h,j}(\boldsymbol{p}) &= -\,i\int \mathrm{d}^4x\;\varepsilon^*_{j\,\alpha\beta}(\boldsymbol{p})\Big[f^*_{\boldsymbol{p}}(x)\Box T\big(h^{\alpha\beta}(x)\cdots\big)\\ &\qquad + \big(g^*_{\boldsymbol{p}}(x)\Box - f^*_{\boldsymbol{p}}(x)\big)T\big(\Box h^{\alpha\beta}(x)\cdots\big)\Big]\\ &= -i\int \mathrm{d}^4x\;\varepsilon^*_{j\,\alpha\beta}(\boldsymbol{p})g^*_{\boldsymbol{p}}(x)\Box T\big(H^{\alpha\beta}(x)\cdots\big)\,.\end{aligned} \tag{B.9}$$

We note that the last equality above comes after assuming that $\Box$ commutes with the T product and using the graviton equation of motion

$$\Box h_{\alpha\beta}(x) = H_{\alpha\beta}(x) + \cdots\,, \tag{B.10}$$

where the "$\cdots$" represent all of the irrelevant longitudinal (unphysical) terms in the full EOM (4.225), as well as all $\mathcal{O}(\alpha_g)$ interaction terms which are also irrelevant in the present context since they contribute no poles.

All of these preparations then finally allow us to express our S-matrix, in line with Lehmann's reduction formula [267] and Weinberg's cluster decomposition principle [123], as

$$
\begin{aligned}
&{}_h\big\langle \boldsymbol{p}'_{m'}, \boldsymbol{q}'_{m'}, j'_{m'}; \boldsymbol{k}'_{n'}, l'_{n'}; \mathrm{out}\big|\boldsymbol{p}_m, \boldsymbol{q}_m, j_m; \boldsymbol{k}_n, l_n; \mathrm{in}\big\rangle_H = \\
&\quad \prod_{a=1}^{m'} \Big[-\frac{1}{2} \int \mathrm{d}^4 x'_a \mathrm{d}^4 y'_a \Big(\big(E_{\boldsymbol{p}'_a}/E_{\boldsymbol{q}'_a}\big)^{1/2} \varepsilon^{*\,\alpha'_a\beta'_a}_{j'_a}(\boldsymbol{p}'_a) \varepsilon^{*\,\gamma'_a\delta'_a}_{j'_a}(\boldsymbol{q}'_a) g^*_{\boldsymbol{p}'_a}(x'_a) f^*_{\boldsymbol{q}'_a}(y'_a) \\
&\qquad\qquad - \big(\boldsymbol{p}'_a \leftrightarrow \boldsymbol{q}'_a\big)\Big) \Box_{x'_a} \Box_{y'_a} \Big] \prod_{b=1}^{n'} \Big[-i \int \mathrm{d}^4 z'_b \, \varepsilon^{*\,\mu'_b\nu'_b}_{l'_b}(\boldsymbol{k}'_b) g^*_{\boldsymbol{k}'_b}(z'_b) \Box_{z'_b} \Big] \\
&\quad \times \prod_{c=1}^{m} \Big[-\frac{1}{2} \int \mathrm{d}^4 x_c \mathrm{d}^4 y_c \Big(\big(E_{\boldsymbol{p}_c}/E_{\boldsymbol{q}_c}\big)^{1/2} \varepsilon_{j_c}^{\alpha_c\beta_c}(\boldsymbol{p}_c) \varepsilon_{j_c}^{\gamma_c\delta_c}(\boldsymbol{q}_c) g_{\boldsymbol{p}_c}(x_c) f_{\boldsymbol{q}_c}(y_c) \\
&\qquad\qquad - \big(\boldsymbol{p}_c \leftrightarrow \boldsymbol{q}_c\big)\Big) \Box_{x_c} \Box_{y_c} \Big] \prod_{d=1}^{n} \Big[-i \int \mathrm{d}^4 z_d \, \varepsilon_{l_d}^{\mu_d\nu_d}(\boldsymbol{k}_d) f_{\boldsymbol{k}_d}(z_d) \Box_{z_d} \Big] \\
&\quad \times G_{\alpha'_1\cdots\nu_n}\big(x'_1, \cdots, z_n\big)\,,
\end{aligned} \tag{B.11}
$$

where the Green's function $G_{\alpha'_1\cdots\nu_n}\big(x'_1, \cdots, z_n\big)$ in full form is given by

$$
\begin{aligned}
&G_{\alpha'_1\cdots\nu_n}\big(x'_1, \cdots, z_n\big) = \\
&\quad \langle 0|\, T\big(H_{\alpha'_1\beta'_1}(x'_1) \cdots H_{\alpha'_{m'}\beta_{m'}}(x'_{m'}) \cdots H_{\gamma'_{m'}\delta'_{m'}}(y'_{m'}) \cdots H_{\mu'_{n'}\nu'_{n'}}(z'_{n'}) \\
&\qquad \times H_{\alpha_1\beta_1}(x_1) \cdots H_{\alpha_m\beta_m}(x_m) \cdots H_{\gamma_m\delta_m}(y_m) \cdots H_{\mu_n\nu_n}(z_n)\big)\, |0\rangle\ .
\end{aligned} \tag{B.12}
$$

We note that the formalism developed in the body of this work also allows one to actually calculate these Green's functions, and thus also the matrix elements (B.11), at any finite order in perturbation theory though such calculations are quite time-consuming and beyond the scope of this work.

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Disclaimer

This thesis is based on four papers which have been published in peer-reviewed journals and contain original research performed by the author in collaboration with others. In particular:

- The results of Chapter 2 are based on [1] in collaboration with Jisuke Kubo, Manfred Lindner, Jonas Rezacek, Philipp Saake, and Andreas Trautner
- The results of Chapter 3 are based on [1] and [2], the latter of which was conducted in collaboration with Jisuke Kubo, Jonas Rezacek, and Philipp Saake.
- The results of Chapter 4 are based on [3] and [4], both of which were completed in collaboration with Jisuke Kubo.

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