Gauge theories and quantum gravity in a finite interval of time on a compact space manifold

Damiano Anselmi

Dipartimento di Fisica "E.Fermi", Università di Pisa, Largo B.Pontecorvo 3, 56127 Pisa, Italy and INFN, Sezione di Pisa, Largo B. Pontecorvo 3, 56127 Pisa, Italy

(Received 24 October 2023; accepted 12 December 2023; published 8 January 2024)

We study gauge theories and quantum gravity diagrammatically in a finite interval of time τ , on a compact space manifold Ω . The initial, final, and boundary conditions are formulated in gauge invariant and general covariant ways by means of purely virtual extensions of the theories, which allow us to "trivialize" the local symmetries and switch to invariant fields (the invariant metric tensor, invariant quark, and gluon fields, etc.). The evolution operator $U(t_f, t_i)$ is worked out for arbitrary initial and final states, as well as general boundary conditions on $\partial\Omega$. We show that $U(t_f, t_i)$ is well defined and diagrammatically unitary for every $\tau = t_f - t_i < \infty$. The formulation is extended to include purely virtual particles. In quantum gravity, where the cosmological constant Λ_C challenges the definition of an *S* matrix, the results allow us to prove unitarity at $\tau < \infty$. We work out the frequencies and eigenfunctions in some explicit examples, including Yang-Mills theory on the finite cylinder.

DOI: 10.1103/PhysRevD.109.025003

I. INTRODUCTION

Perturbative quantum field theory mainly focuses on the calculation of *S* matrix amplitudes, which describe scattering processes among asymptotic states, where the incoming and outgoing particles are separated by an infinite amount of time. This approximation is good for most practical purposes, especially in collider physics. However, it is just an approximation. From a theoretical point of view, it does not provide a completely satisfactory understanding. A more powerful and general approach is required, where the key issues (such as locality, renormalizability, and unitarity, among the main ones, and then symmetries, anomalies, the anomaly cancellation, etc.) are understood without making this simplification.

It is possible [1] to formulate perturbative quantum field theory diagrammatically in a finite interval of time $\tau = t_f - t_i$, and on a compact space manifold Ω , so as to move all the details about the restrictions to finite τ and compact Ω away from the internal sectors of the diagrams (apart from the discretizations of the loop momenta), and code them into external sources. The usual diagrammatic properties apply, or can be generalized with little effort. This way, the evolution operator $U(t_f, t_i)$ can be calculated perturbatively between arbitrary initial and final states, with arbitrary boundary conditions on $\partial\Omega$. Unitarity, that is to say, the equality $U^{\dagger}(t_{\rm f}, t_{\rm i})U(t_{\rm f}, t_{\rm i}) = 1$, can be studied diagrammatically by means of the spectral optical identities [2]. The theory is renormalizable whenever it is so at $\tau = \infty$, $\Omega = \mathbb{R}^{D-1}$, where *D* denotes the spacetime dimension. Purely virtual particles are introduced by removing the on-shell contributions of some physical particles, and all the ghosts, from the core diagrams, as explained in [2], and trivializing their initial and final conditions.

In this paper we consider the cases of gauge theories and gravity in detail, because certain issues that are specific to local symmetries deserve attention, when τ is finite and the space manifold Ω is compact. For example, we must specify the initial, final, and boundary conditions without breaking the local symmetries. We cannot just use the gauge potential A^a_μ and the metric tensor $g_{\mu\nu}$, for this purpose. Nor can we use the field strength $F^a_{\mu\nu}$, and the curvature tensors R, $R_{\mu\nu}$, $R_{\mu\nu\rho\sigma}$, because they are not invariant.

What comes to the rescue is the purely virtual extension of gauge theories and gravity formulated in ref.s [3,4], which is based on the introduction of extra bosonic fields, together with their anticommuting partners. The extra fields can be used to perturbatively "dress" the noninvariant fields and make them invariant: we can build invariant gauge fields A_d^{μ} , invariant quark fields ψ_d , and an invariant metric tensor $g_{\mu\nu d}$. The ordinary physical quantities, such as the *S* matrix amplitudes and the correlation functions of the usual (nonlinear) invariant composite fields (like $F_{\mu\nu}^a F^{\mu\nu a}$, $\bar{\psi}\psi$, etc.) are unaffected. In addition, new, physical correlation functions can be defined, and calculated perturbatively,

damiano.anselmi@unipi.it

Published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI. Funded by SCOAP³.

such as those of the invariant fields A_d^{μ} , ψ_d , and $g_{\mu\nu d}$. The reason why the extra fields must be purely virtual is to preserve unitarity: if they were not purely virtual, the extended theory would propagate ghosts.

These tools are also useful to provide invariant initial, final, and boundary conditions in gauge theories and gravity in a finite interval of time τ , on a compact space manifold Ω . A crucial simplification comes from the possibility of "trivializing" the local symmetries, that is to say, reduce them to simple shifts of fields. This is achieved by switching to the invariant variables ψ_d , A_d^{μ} , and $g_{\mu\nu d}$, by means of a field redefinition. Then, it is relatively straightforward to organize the action efficiently, work out the eigenfunctions and the frequencies for the expansions of the fields, and introduce coherent states [5], which are crucial to study the $U(t_{\rm f}, t_{\rm i})$ diagrammatics and make perturbative calculations without introducing unnecessary burdens [1]. The functional integral is *defined* as the integral on the coefficients of the expansions. The local symmetries are under control in all the operations we make, so $U(t_{\rm f}, t_{\rm i})$ is gauge invariant and invariant under general coordinate transformations.

We illustrate the basic properties of our formalism in Yang-Mills theory on two relatively simple space manifolds: the semi-infinite cylinder and the finite cylinder.

The coherent states are the eigenstates of the annihilation operator. In the Lagrangian approach, which we adopt here, the switch to coherent states is just a change of variables in the functional integral, combined with a wise way of setting the initial and final conditions. In quantum mechanics, we switch from coordinates q and momenta p to $z \sim q + ip$, $\overline{z} \sim q - ip$, and set the initial conditions on z, the final conditions on \overline{z} . In quantum field theory analogous operations are made on the fields. Uncovering the specifics of these operations in gauge theories and gravity is part of the problem we need to face, and its solution is given in the paper. For convenience, we keep referring to the new variables by means the Hamiltonian terminology "coherent states".¹

Purely virtual particles are a key ingredient of the whole formulation, so we discuss this concept in some detail. A theory that contains purely virtual particles is built from an extended (possibly unphysical) theory,² which is quantized as usual (that is to say, by means of the common diagrammatics, defined by the Feynman *ic* prescription), and performing a certain set of operations on it, like rearranging the diagrammatics, and making a projection on the space of states, to define the physical space. The projection defines the final, physical theory. The new diagrammatics is built by removing the on-shell contributions of all the ghosts χ_{gh} , and possibly some physical particles χ_{ph} , from the diagrams of the extended theory, at every order of the perturbative expansion. This is done in one of the following equivalent ways: (i) a certain nonanalytic Wick rotation [7,8], (ii) dropping the spectral optical identities associated with the unwanted on-shell contributions [2] from the Cutkosky-Veltman identities [9,10] (which are the diagrammatic versions of the unitarity equation $S^{\dagger}S = 1$), or (iii) replacing the standard diagrams with suitable combinations of non-time-ordered diagrams, as shown in Ref. [11].

In addition, one has to make the projection mentioned above. At $\tau = \infty$, the projection amounts to ignore the diagrams that have χ_{gh} and χ_{ph} on the external legs. When $\tau < \infty$, it amounts to choose trivial initial and final conditions for the coherent states of χ_{gh} and χ_{ph} . The final theory is unitary, provided all the ghosts of the extended theory are rendered purely virtual.

Certain aspects of the construction of theories with purely virtual particles resemble what we normally do to gauge-fix a gauge theory, where we extend the theory by including unphysical excitations, such as the Faddeev-Popov ghosts, and project the extension away at the end. The crucial difference is that, in the case of purely virtual particles, no symmetry is there to help us. This is why we need to switch to a different diagrammatics, before making the projection.

It is worth to stress that, before the projection, the extended theory is just a mathematical tool to get to the correct, final theory. It is not possible to solve the problem of ghosts by just changing the viewpoint on a theory, or focusing on different quantities (e.g., "in-in" correlation functions, instead of "in-out" ones, or different prescriptions for the propagators, such as the retarded potentials, instead of the Feynman one, and so on), or moving back and forth among negative norms, unbounded Hamiltonians, non-Hermitian Hamiltonians, negative probabilities, etc. None of these operations really changes the theory: they just change the reference frame, so to speak, within the same theory. Even the Lee-Wick idea of making "abnormal particles" decay [12] cannot solve the problem,³ because a theory with unstable ghosts is still a theory with ghosts. Necessarily, it must be abandoned at some point, in favor of a different theory, and the switch from one to the other must be a radical operation that cuts out the sick portion, like a guillotine: this is the projection we are talking about.

The main application of the idea of purely virtual particle is the formulation of a theory of quantum gravity [8], which provides testable predictions [14] in inflationary cosmology [15]. In phenomenology, purely virtual particles open new possibilities, by evading many constraints that are

¹Details on the correspondence between the operatorial approach to coherent states and the functional integral can be found in the paragraph 9-1-2 of [6].

²The extended theory is unphysical if it contains ghosts (fields with kinetic terms multiplied by the wrong signs).

³For Lee-Wick ghosts in quantum gravity, see [13].

typical of normal particles (see [16] and references therein). The diagrammatic calculations are not more difficult than those based on physical particles. It is possible to implement them in softwares like FeynCalc, FormCalc, LoopTools and Package-X [17].

Purely virtual particles can also be used as mere mathematical tools, to study uncommon aspects of common theories, as shown in [3,4] and here. In this paper, we are using them to deal with the local symmetries at finite τ and on a compact Ω , to express the initial, final, and boundary conditions in invariant ways.

In common textbooks, the diagrammatic formulation of quantum field theory focuses on the *S* matrix ($\tau = \infty$), while the $\tau < \infty$ case is mostly treated formally, from the operatorial definition $U(t_f, t_i) = e^{-iH\tau}$. Not only, but when a compact space manifold is considered, it is typically the torus, which does not pose particular difficulties. Beyond the textbook approaches, and besides our previous paper [1], we point out the results of Nomoto and Fukuda, who studied QED at finite τ in ref. [18], still on the torus. Yet, the challenges of non-Abelian Yang-Mills theories and quantum gravity at $\tau < \infty$ on an arbitrary (especially, compact) space manifold Ω require the general formalism developed here.

The results of this paper and [1] make us less dependent on the paradigms that have dominated the scene in quantum field theory since its birth. For example, we can study unitarity without being tied to the S matrix. This is important in quantum gravity, where it makes no sense to talk about the unitarity of the S matrix (if the cosmological constant Λ_C is nonvanishing), since proper definitions of asymptotic states and S matrix amplitudes are unavailable at $\Lambda_C \neq 0$. Yet, unitarity is an essential requirement for a theory to be physically acceptable. Other concerns revolve around the definition of energy and the treatment of the Hamiltonian. Here we bypass these problems. We show that the evolution operator $U(t_{\rm f}, t_{\rm i})$ of quantum gravity with purely virtual particles, defined by the functional integral, is diagrammatically unitary for arbitrary $\tau < \infty$. This means that the problems of the S matrix at $\Lambda_C \neq 0$ are not inherent to the issue of unitarity per se.

The paper is organized as follows. In Sec. II we consider a simple warm-up toy model to illustrate some of the issues we need to face when we want to find the right eigenfunctions for the expansions of the gauge fields. In Sec. III we work out the general formalism for coherent states in gauge theories. In Sec. IV we rearrange the Lagrangian in Yang-Mills theories to make it ready for the restriction to finite τ and compact Ω . In Sec. V we introduce coherent states in Yang-Mills theories at the quadratic level. In Sec. VI we include the interactions. In Secs. VII and VIII we illustrate the formalism in two relatively simple cases: Yang-Mills theory on the semi-infinite cylinder, and on the finite τ and compact Ω . In Sec. X we extend the formulation to quantum gravity with purely virtual particles, and discuss the problems that occur in the limit $\tau \to \infty$, $\Omega \to \mathbb{R}^{D-1}$, in the presence of a cosmological constant. Section XI contains the conclusions.

II. A WARM-UP TOY MODEL

The first difficulty we meet when we want to formulate gauge theories and gravity on a compact manifold Ω , is that we do not know the eigenfunctions we should use for the expansions of the fields. In a generic setting, the eigenfunctions of the Laplacian are not the right ones. In this section we study a toy model that illustrates the main issue, as well as its solution.

Specifically, we consider the simple quadratic Lagrangian

$$L = \frac{\dot{\phi}^2}{2} + \alpha \dot{\phi} \phi' - \frac{\nu^2}{2} \phi'^2$$
 (2.1)

for a scalar field ϕ on a segment $\Omega = [0, \ell]$ in a finite interval of time (t_i, t_f) , $t_f = t_i + \tau$, with Dirichlet boundary conditions $\phi = 0$ on $\partial\Omega$. The dot denotes the time derivative, while the prime denotes the space derivative.

What is not clear is how to deal with the term $\phi \phi'$. We could eliminate it by means of a redefinition of space and time, but this would complicate the investigation in another way, by mixing the boundary conditions with the initial and final conditions. Moreover, we can apply the redefinition only once (i.e., for a single field), which makes it useless in the presence of more fields with kinetic Lagrangians of the same type. It is necessary to work out a general approach that can be easily exported to the cases treated in the next sections.

We begin by working out the momentum π_{ϕ} and the Hamiltonian *H*, which are

$$\pi_{\phi} = \dot{\phi} + \alpha \phi', \qquad H(\pi_{\phi}, \phi) = \frac{1}{2}(\pi_{\phi} - \alpha \phi')^2 + \frac{\nu^2}{2} \phi'^2.$$

Note that *H* is positive definite for every real α . Then we extend the Lagrangian to

$$L'(\phi, \dot{\phi}, \pi_{\phi}, \dot{\pi}_{\phi}) = \frac{1}{2} (\pi_{\phi} \dot{\phi} - \dot{\pi}_{\phi} \phi) - H(\pi_{\phi}, \phi), \quad (2.2)$$

which is convenient because it contains both ϕ and π_{ϕ} as independent variables.

The equations of motion must be solved with the Dirichlet boundary conditions $\phi = 0$ on $\partial\Omega$. There is no boundary condition on π_{ϕ} , because, as we are going to see, the coherent states are not built with ϕ and π_{ϕ} , but with ϕ and $\dot{\phi}$. Note that $\phi = 0$ on $\partial\Omega$ implies $\dot{\phi} = 0$ on $\partial\Omega$. This way, the coherent states automatically vanish on $\partial\Omega$ as well. For these reasons, it is convenient to introduce the shifted momenta

$$\bar{\pi}_{\phi} = \pi_{\phi} - \alpha \phi', \qquad (2.3)$$

and add $\left. \bar{\pi}_{\phi} \right|_{\partial\Omega} = 0$ to the boundary conditions.

The integrated Lagrangian (2.2) can be written as

$$\mathcal{L}' = \int_0^\ell L' dx = \frac{1}{2} \int_0^\ell (\bar{\pi}_\phi \quad \phi) \begin{pmatrix} -1 & \partial_t \\ -\partial_t & \nu^2 \partial_x^2 - 2\alpha \partial_t \partial_x \end{pmatrix} \times \begin{pmatrix} \bar{\pi}_\phi \\ \phi \end{pmatrix} dx.$$
(2.4)

The boundary conditions allow us to freely integrate by parts.

The field equations can be read from (2.4). The eigenfunctions with energy ω ($\partial_t = -i\omega$) are

$$\phi_n(x) = i \sqrt{\frac{2\nu^2}{\ell(\nu^2 + \alpha^2)}} \exp\left(-\frac{i\alpha\omega_n x}{\nu^2}\right) \sin\left(\frac{n\pi x}{\ell}\right),$$

$$\bar{\pi}_{\phi_n} = -i\omega_n \phi_n, \qquad \omega_n = \frac{n\pi\nu^2}{\ell\sqrt{\nu^2 + \alpha^2}}, \qquad (2.5)$$

having normalized them as explained below. We have $\phi_n^*(x) = \phi_{-n}(x), \ \omega_{-n} = -\omega_n$.

The expansions of the fields in terms of these eigenfunctions read

$$\phi(t,x) = \sum_{n \neq 0} a_n(t)\phi_n(x), \quad \bar{\pi}_{\phi}(t,x) = -i\sum_{n \neq 0} a_n(t)\omega_n\phi_n(x),$$
$$a_{-n}(t) = a_n^*(t). \tag{2.6}$$

The functional integral is the integral on the variables a_n (or, equivalently, the coherent states, see below). It is important to stress that the expansions (2.6) *define* the space of functions on which the functional integral is calculated. In this spirit, we do not need to prove, or require, that the expansions converge.

The orthogonality relations obeyed by the eigenfunctions can be worked out as follows. From (2.4), we find

$$\begin{pmatrix} -1 & -i\omega_n \\ i\omega_n & \nu^2 \partial_x^2 + 2i\alpha\omega_n \partial_x \end{pmatrix} \begin{pmatrix} \bar{\pi}_{\phi_n} \\ \phi_n \end{pmatrix} = 0.$$

Multiplying by the row $(\bar{\pi}_{\phi_m} \phi_m)$ and integrating on Ω , we obtain

$$0 = \int_{0}^{\ell} (\bar{\pi}_{\phi_{m}} \quad \phi_{m}) \begin{pmatrix} -1 & -i\omega_{n} \\ i\omega_{n} & \nu^{2}\partial_{x}^{2} + 2i\alpha\omega_{n}\partial_{x} \end{pmatrix} \begin{pmatrix} \bar{\pi}_{\phi_{n}} \\ \phi_{n} \end{pmatrix} dx.$$
(2.7)

Transposing this expression, exchanging n with m, integrating by parts where necessary, and subtracting the result to (2.7), we find

$$0 = (\omega_n + \omega_m) \int_0^\ell (\bar{\pi}_{\phi_m} \quad \phi_m) \begin{pmatrix} 0 & -1 \\ 1 & 2\alpha\partial_x \end{pmatrix} \begin{pmatrix} \bar{\pi}_{\phi_n} \\ \phi_n \end{pmatrix} \mathrm{d}x.$$

Dividing by $\omega_n + \omega_m$, we obtain the orthogonality relations for $m \neq -n$. Choosing the normalization as in (2.5), the orthonormality relations read

$$\int_{0}^{\ell} (\bar{\pi}_{\phi_{-m}} \quad \phi_{-m}) \begin{pmatrix} 0 & 1 \\ -1 & -2\alpha\partial_{x} \end{pmatrix} \begin{pmatrix} \bar{\pi}_{\phi_{n}} \\ \phi_{n} \end{pmatrix} \mathrm{d}x = 2i\omega_{n}\delta_{mn}.$$
(2.8)

Now we work out the expansion of the integrated Lagrangian (2.4). Consider the right-hand side of the identity (2.7). Multiplying it by $a_m a_n/2$, summing on *m* and *n*, and adding the result to (2.4), we get

$$\mathcal{L}' = \frac{1}{2} \sum_{n \neq 0, m \neq 0} a_m (\dot{a}_n + i\omega_n a_n) \int_0^{\ell} (\bar{\pi}_{\phi_m} \quad \phi_m) \\ \times \begin{pmatrix} 0 & 1 \\ -1 & -2\alpha\partial_x \end{pmatrix} \begin{pmatrix} \bar{\pi}_{\phi_n} \\ \phi_n \end{pmatrix} dx.$$

Formula (2.8) ensures that all the terms with $m \neq -n$ drop out, and we remain with

$$\mathcal{L}' = \sum_{n>0} i\omega_n (a_n^* \dot{a}_n - \dot{a}_n^* a_n) - 2 \sum_{n>0} \omega_n^2 a_n^* a_n,$$

having halved the sum by using $a_{-n} = a_n^*$.

At this point, we define the coherent states $z_n = a_n$ and $\bar{z}_n = a_n^*$, and proceed as usual (see [1] for a derivation in the notation we are using here). Once we include the right endpoint corrections, to have the correct variational problem, the complete action is

$$S = -i \sum_{n>0} \omega_n (\bar{z}_{nf} z_n(t_f) + \bar{z}_n(t_i) z_{ni}) + \sum_{n>0} \int_{t_i}^{t_f} dt [i \omega_n (\bar{z}_n \dot{z}_n - \dot{\bar{z}}_n z_n) - 2\omega_n^2 \bar{z}_n z_n], \quad (2.9)$$

where $z_{ni} = z_n(t_i)$, $\bar{z}_{nf} = \bar{z}_n(t_f)$ are the initial and final conditions.

III. COHERENT STATES IN GAUGE THEORIES AND GRAVITY

A nontrivial issue is to introduce coherent states in gauge theories and gravity, and set invariant initial, final, and boundary conditions. The goal is to work in a general setting, which means without shortcuts (like choosing particular gauge-fixings), because we want to have gauge independence under control, and be able to make computations with arbitrary gauge-fixing parameters, as we normally do at $\tau = \infty$, in $\Omega = \mathbb{R}^{D-1}$.

The properties we lay out in this section are useful for both gauge theories and gravity, because they do not rely of the particular form of the local symmetry. This is possible because, by means of the formalisms of Refs. [3,4], which we review in the next sections, we can rephrase the local symmetries in a universal form, which amounts to arbitrary shifts $\delta_{\Lambda} \varphi = \Lambda$ of certain (purely virtual) extra fields φ . This is precisely the trick we need to specify invariant conditions on the fields.

We start from a Lagrangian $L(\phi, \dot{\phi})$ that depends on a certain number of fields ϕ^{I} and their first derivatives. We assume that it can be decomposed as

$$L(\phi, \dot{\phi}) = L_{\text{free}}(\phi, \dot{\phi}) + L_{\text{int}}(\phi, \dot{\phi}), \qquad (3.1)$$

where L_{free} is quadratic, and L_{int} is the part to be treated perturbatively (which may also include certain linear and quadratic terms), to which we refer as "interaction Lagrangian." For the moment, we assume that the boundary conditions on the fields ϕ^I are $\phi^I|_{\partial\Omega} = 0$. Nontrivial boundary conditions are studied at the end of this section.

We assume that no Lagrangian term contains more than two derivatives. Higher-derivative theories must be first turned into two-derivative theories (by introducing extra fields, for example). Moreover, at finite τ , on a compact space manifold Ω , we assume that terms like $\phi_1 \cdots \phi_{n-1} \partial \partial \phi_n$ have been eliminated in favor of terms like $\phi_1 \cdots \phi_{n-2} \partial \phi_{n-1} \partial \phi_n$, by adding total derivatives. In the next sections we show how to do these and other operations while preserving gauge invariance and general covariance.

Next, we assume that *L* it is "orthodoxically symmetric" with respect to certain infinitesimal transformations $\delta_{\Lambda}\phi^{I}$. By this we mean that

- (i) the functions $\delta_{\Lambda}\phi^I$ depend only on the fields ϕ^I , but not on their derivatives,
- (ii) the Lagrangian satisfies

$$0 = \delta_{\Lambda} \phi^{I} \frac{\partial L}{\partial \phi^{I}} + \delta_{\Lambda} \dot{\phi}^{I} \frac{\partial L}{\partial \dot{\phi}^{I}}, \qquad (3.2)$$

where

$$\delta_{\Lambda} \dot{\phi}^{I} = \partial_{t} (\delta_{\Lambda} \phi^{I}) = \frac{\partial (\delta_{\Lambda} \phi^{I})}{\partial \phi^{J}} \dot{\phi}^{J}.$$
(3.3)

What is important, in point (ii), is that not only the action is symmetric, but also the Lagrangian is, i.e., the right-hand side of (3.2) is exactly zero, not just a total derivative.

Next, we introduce the momenta and the Hamiltonian as usual⁴:

$$\begin{split} \pi^{I}_{\phi}(\phi, \dot{\phi}) &= \frac{\partial L}{\partial \dot{\phi}^{I}} \Rightarrow \dot{\phi}^{I} = \dot{\phi}^{I}(\pi_{\phi}, \phi) \equiv \dot{\tilde{\phi}}^{I}, \\ H(\pi_{\phi}, \phi) &= \pi^{I}_{\phi} \dot{\tilde{\phi}}^{I} - L(\phi, \dot{\tilde{\phi}}). \end{split}$$

We can work out the symmetry transformations of the momenta π_{ϕ}^{I} by means of the identities (3.2) and (3.3). We find

$$\delta_{\Lambda}\pi^{I}_{\phi} = -\frac{\partial(\delta_{\Lambda}\dot{\phi}^{J})}{\partial\dot{\phi}^{I}}\pi^{J}_{\phi} = -\frac{\partial(\delta_{\Lambda}\phi^{J})}{\partial\phi^{I}}\pi^{J}_{\phi}.$$
 (3.4)

Since $\delta_{\Lambda} \dot{\phi}^{J}$ is linear in $\dot{\phi}^{I}$, $\delta_{\Lambda} \pi_{\phi}^{I}$ depends only on ϕ and π_{ϕ} , but not on $\dot{\phi}$.

We want to prove that the equivalent, extended Lagrangian

$$L''(\phi, \dot{\phi}, \pi_{\phi}) = \pi_{\phi}^{I} \dot{\phi}^{I} - H(\pi_{\phi}, \phi) = \pi_{\phi}^{I} (\dot{\phi}^{I} - \dot{\tilde{\phi}}^{I}) + L(\phi, \dot{\tilde{\phi}})$$

is orthodoxically symmetric, the transformations being $\delta_{\Lambda}\phi^{I}$ and (3.4).

Since the transformations $\delta_{\Lambda}\phi^I$ and $\delta_{\Lambda}\pi^I_{\phi}$ do not depend on the derivatives of the fields, point (i) is satisfied. It remains to prove the equation

$$0 = \delta_{\Lambda} \phi^{I} \frac{\partial L''}{\partial \phi^{I}} + \delta_{\Lambda} \dot{\phi}^{I} \frac{\partial L''}{\partial \dot{\phi}^{I}} + \delta_{\Lambda} \pi^{I}_{\phi} \frac{\partial L''}{\partial \pi^{I}_{\phi}}.$$
 (3.5)

For this purpose, note that formula (3.2) with the replacement $\dot{\phi}^I \rightarrow \tilde{\phi}^I$ gives

$$0 = \delta_\Lambda \phi^I rac{\partial L(\phi, ilde \phi^I)}{\partial \phi^I} \Big|_{\dot{ at \phi}} + \pi^I_\phi rac{\partial (\delta_\Lambda \phi^I)}{\partial \phi^J} \dot{ at \phi}^J,$$

using (3.3). Then it is easy to check that the right-hand side of the identity (3.5) is equal to

$$(\dot{\phi}^{I}-\dot{\tilde{\phi}}^{I})\left(\delta_{\Lambda}\pi_{\phi}^{I}+\frac{\partial(\delta_{\Lambda}\phi^{J})}{\partial\phi^{I}}\pi_{\phi}^{J}
ight),$$

which vanishes by (3.4).

We need to make a further step, because the extended Lagrangian we must start from, in the coherent-state approach, is not L'', but

$$L'(\phi, \dot{\phi}, \pi_{\phi}, \dot{\pi}_{\phi}) = \frac{1}{2} (\pi_{\phi}^{I} \dot{\phi}^{I} - \dot{\pi}_{\phi}^{I} \phi^{I}) - H(\pi_{\phi}, \phi)$$
$$= L'' - \frac{1}{2} \frac{d}{dt} (\pi_{\phi}^{I} \phi^{I}).$$
(3.6)

We will also need to add certain endpoint corrections to the action, in order to have the right variational problem. This part can be ignored for the moment, because it will be easy to deal with it at the very end.

⁴In order to keep the notation simple, we adopt the following conventions for fields with fermionic statistics. Once their kinetic terms are diagonalized, we have pairs $\bar{\psi}$, ψ . The quadratic terms we write must be understood as follows: $\bar{\psi}$ is placed to the left, and ψ is placed to the right; π_{ψ} is defined as the left derivative with respect to $\bar{\psi}$, and is placed to the right; $\pi_{\bar{\psi}}$ is defined as the right derivative with respect to ψ , and is placed to the left.

It is not obvious that the total derivative L' - L'' is invariant under the transformation δ_{Λ} . Actually, in general it is not, since (3.4) gives

$$\delta_{\Lambda}(\pi_{\phi}^{I}\phi^{I}) = \pi_{\phi}^{I} \bigg(\delta_{\Lambda}\phi^{I} - \frac{\partial(\delta_{\Lambda}\phi^{I})}{\partial\phi^{J}}\phi^{J} \bigg), \qquad (3.7)$$

which vanishes only if the transformations are linear:

$$\delta_{\Lambda}\phi^{I} = \frac{\partial(\delta_{\Lambda}\phi^{I})}{\partial\phi^{J}}\phi^{J}.$$
(3.8)

Summarizing, if the symmetry is linear, the Lagrangian (3.6) is orthodoxically invariant.

It may seem that the requirement of having linear symmetry transformations is very restrictive. Actually, it is not, if we take advantage of the formalism developed in Refs. [3,4]. Indeed, it is always possible to convert Abelian and non-Abelian gauge symmetries, as well as general covariance, into a universal linear form, by introducing purely virtual fields that do not change the *S* matrix amplitudes.

It is easy to check that the momenta π_{ϕ}^{I} are not guaranteed to vanish on $\partial\Omega$. The structure of the Lagrangian ensures that $\pi_{\phi}^{I}(\phi, \dot{\phi})$ has the form

$$\pi^{I}_{\phi}(\phi,\dot{\phi}) = \mathcal{A}^{IJ}(\phi)\dot{\phi}^{J} + \mathcal{B}^{IJi}(\phi)\partial_{i}\phi^{J} + \mathcal{C}^{I}(\phi),$$

for certain functions $\mathcal{A}^{IJ}(\phi)$, $\mathcal{B}^{IJi}(\phi)$, and $\mathcal{C}^{I}(\phi)$. Thus, $\phi^{I}|_{\partial\Omega} = 0$ implies

$$\left. \pi_{\phi}^{I}(\phi, \dot{\phi}) \right|_{\partial\Omega} = \mathcal{B}^{IJi}(0)\partial_{i}\phi^{J}|_{\partial\Omega} + \mathcal{C}^{I}(0). \tag{3.9}$$

We can assume $C^{I}(0) = 0$. First, note that a nonvanishing $C^{I}(0)$ means that the Lagrangian includes a term $C^{I}(0)\dot{\phi}^{I}$. This is not going to happen in the cases of Yang-Mills theories and gravity. Besides, a term like $C^{I}(0)\dot{\phi}^{I}$ can be removed at no cost. Since we are assuming that the symmetry transformations are linear and do not involve derivatives, $C^{I}(0)\dot{\phi}^{I}$ must be gauge invariant by itself. Besides, it is a total derivative. Thus, we can always switch to an alternative Lagrangian with the same properties, but no such term. Instead, the matrix $\mathcal{B}^{IJi}(0)$ is in general nontrivial and cannot be removed, so the right-hand side of (3.9) may be nonzero.

As in (2.3), it is useful to define new "momenta"

$$\bar{\pi}^{I}_{\phi} = \pi^{I}_{\phi} - \mathcal{B}^{IJi}(0)\partial_{i}\phi^{J}, \qquad (3.10)$$

because then it makes sense to add the boundary conditions

$$\phi^I|_{\partial\Omega} = \bar{\pi}^I_{\phi}|_{\partial\Omega} = 0. \tag{3.11}$$

As we show below, these conditions turn straightforwardly into the right boundary conditions for the coherent states.

The gauge transformations of $\bar{\pi}_{\phi}^{I}$ follow from those of π_{ϕ}^{I} and ϕ^{I} . This is enough, for the moment, but in Sec. III B we prove π_{ϕ}^{I} and $\bar{\pi}_{\phi}^{I}$ transform in exactly the same way.

By assumption (3.1) and the absence of higher derivatives, the general form of the Lagrangian L' is

$$L' = L'_{\text{free}}(\phi, \dot{\phi}, \bar{\pi}_{\phi}, \dot{\bar{\pi}}_{\phi}) + L'_{\text{int}}(\bar{\pi}_{\phi}, \phi), \quad (3.12)$$

where L'_{free} is quadratic, and the interaction part L'_{int} is independent of the time derivatives. Note that the redefinitions (3.10) do not generate time derivatives in the interaction sector. The quadratic Lagrangian, integrated on Ω , has the form

$$\mathcal{L}'_{\text{free}} \equiv \int_{\Omega} L'_{\text{free}} \mathrm{d}^{D-1} \mathbf{x} \equiv \frac{1}{2} \int_{\Omega} (\bar{\pi}_{\phi} \quad \phi) \begin{pmatrix} M & K + \partial_t \\ \tilde{K} - \partial_t & N \end{pmatrix} \times \begin{pmatrix} \bar{\pi}_{\phi} \\ \phi \end{pmatrix} \mathrm{d}^{D-1} \mathbf{x}, \qquad (3.13)$$

where *M* is a constant, symmetric matrix, while $K = K_1^i \partial_i + K_2$, $\tilde{K} = -K_1^{iT} \partial_i + K_2^T (K_1^i \text{ and } K_2 \text{ being matrices, } T \text{ denoting the transpose})$, $N = N_1^{ij} \partial_i \partial_j + N_2^i \partial_i \partial_i + N_3^i \partial_i + N_4$, with N_1^{ij} , N_2^i , N_4 symmetric matrices and N_3^i antisymmetric. Observe that, by (3.11), we can freely integrate the space derivatives by parts.

A. Frequencies and eigenfunctions

The eigenfunctions $\bar{\pi}_n^I(\mathbf{x})$, $\phi_n^I(\mathbf{x})$ are the solutions of the problem

$$\begin{pmatrix} M & K_1^i \partial_i + K_2 - i\omega_n \\ i\omega_n - K_1^{iT} \partial_i + K_2^T & N_1^{ij} \partial_i \partial_j - i\omega_n N_2^i \partial_i + N_3^i \partial_i + N_4 \end{pmatrix} \times \begin{pmatrix} \bar{\pi}_n \\ \phi_n \end{pmatrix} = 0,$$
(3.14)

with the boundary conditions $\bar{\pi}_n^I|_{\partial\Omega} = \phi_n^I|_{\partial\Omega} = 0$, where *n* is some label.

We assume that the frequencies are real, because they are so in the applications we have in mind. A quick proof is as follows. The frequencies are real for $\tau = \infty$, $\Omega = \mathbb{R}^{D-1}$, in both Yang-Mills theory and gravity. Let us denote them by ω_{∞} . We can work out the frequencies ω_n and the eigenfunctions at finite τ , compact Ω , by considering linear combinations of the $\tau = \infty$, $\Omega = \mathbb{R}^{D-1}$ eigenfunctions with identical frequencies ω_{∞} , and fixing the coefficients by means of the boundary conditions. Eventually, the frequencies become discrete, to have solutions, but remain real.

In case of need, it is not difficult to generalize the formulas of this paper to complex frequencies. We just remark that they must appear in complex conjugate pairs, since the Lagrangian is assumed to be Hermitian.

Taking the complex conjugate of (3.14), we find that $\bar{\pi}_n^{I*}(\mathbf{x})$ and $\phi_n^{I*}(\mathbf{x})$ are also eigenfunctions, and their frequency is $-\omega_n$. We use n^* to label them, and write

$$\bar{\pi}_{n^*}^I(\mathbf{x}) = \bar{\pi}_n^{I*}(\mathbf{x}), \qquad \phi_{n^*}^I(\mathbf{x}) = \phi_n^{I*}(\mathbf{x}), \qquad \omega_{n^*} = -\omega_n.$$
(3.15)

If \mathcal{V} denotes the range of the label *n*, we write $\mathcal{V} = \mathcal{U} \cup \mathcal{U}^*$, by splitting each pair *n*, *n*^{*} between \mathcal{U} and \mathcal{U}^* .

The orthogonality relations can be worked out as in Sec. II: (i) we multiply (3.14) by $(\bar{\pi}_m, \phi_m)$ and integrate the product on Ω ; (ii) we transpose the result of (i), exchange *n* with *m*, and integrate by parts where necessary; finally, (iii) we subtract the results of (i) and (ii).

Normalizing the eigenfunctions appropriately, we have the orthonormality relations

$$\int_{\Omega} \mathrm{d}^{D-1} \mathbf{x} (\bar{\pi}_m \quad \phi_m) \begin{pmatrix} 0 & 1 \\ -1 & N_2^i \partial_i \end{pmatrix} \begin{pmatrix} \bar{\pi}_n \\ \phi_n \end{pmatrix} = 2i\tau_n \omega_n \delta_{m,n^*},$$
(3.16)

where $\tau_n = \pm 1 = \tau_{n^*}$. The value $\tau_n = -1$ signals the presence of ghosts (fields with kinetic terms multiplied by the wrong signs). Indeed, going through the toy model of the previous section, it is easy to check that, if we change the overall sign of the starting Lagrangian (2.1), the right-hand side of (2.8) turns out to be equal to $-2i\omega_n\delta_{mn}$.

We then expand $\bar{\pi}_n$ and ϕ_n in the basis we have just worked out:

$$\begin{pmatrix} \bar{\pi}_{\phi} \\ \phi \end{pmatrix} = \sum_{n \in \mathcal{V}} a_n \begin{pmatrix} \bar{\pi}_n \\ \phi_n \end{pmatrix}, \quad (3.17)$$

with $a_{n^*} = a_n^*$. By means of (3.16), we can invert the expansion and find the coefficients:

$$-2i\tau_m \omega_m a_m^*(t) = \int_{\Omega} \mathrm{d}^{D-1} \mathbf{x} (\,\bar{\pi}_m(\mathbf{x}) \quad \phi_m(\mathbf{x})\,) \\ \times \begin{pmatrix} 0 & 1 \\ -1 & N_2^i \partial_i \end{pmatrix} \begin{pmatrix} \bar{\pi}_\phi(t, \mathbf{x}) \\ \phi(t, \mathbf{x}) \end{pmatrix}.$$
(3.18)

We insert (3.17) into (3.13), and then subtract (3.14), multiplied by $(\bar{\pi}_m, \phi_m)a_m/2$, summed on $m, n \in \mathcal{V}$ and integrated on Ω . Then, we use (3.16), and mirror the sum on \mathcal{U}^* into a sum on \mathcal{U} . The result is the integrated free Lagrangian

$$\mathcal{L}_{\text{free}}' = \sum_{n \in \mathcal{U}} i \tau_n \omega_n (a_n^* \dot{a}_n - \dot{a}_n^* a_n) - 2 \sum_{n \in \mathcal{U}} \tau_n \omega_n^2 a_n^* a_n. \quad (3.19)$$

If the fields ϕ^I have, say, r independent components, I = 1, ..., r, the solutions of the eigenvalue problem

can be arranged into r independent, complete sets of eigenfunctions, each of which can be assigned to a specific component ϕ^I . We can split the set \mathcal{U} into a union $\bigcup_{I=1}^r \mathcal{U}^I$, where \mathcal{U}^I refers to the *I*th complete set. For convenience, we relabel the indices n so that their range is the same for each I, to be denoted by $\hat{\mathcal{U}}$.

Let $\bar{\pi}_n^{IJ}$ and ϕ_n^{IJ} denote the *I*th components of the *n*th eigenfunction of the *J*th set. Let $z_n(t) = a_n(t)$ denote the column made by $z_n^I(t) = a_n^I(t)$, I = 1, ..., r. We have, from (3.17),

$$\begin{pmatrix} \bar{\pi}_{\phi} \\ \phi \end{pmatrix} = \sum_{n \in \hat{\mathcal{U}}} \begin{pmatrix} \bar{\pi}_{n}^{*} & \bar{\pi}_{n} \\ \phi_{n}^{*} & \phi_{n} \end{pmatrix} \begin{pmatrix} \bar{z}_{n} \\ z_{n} \end{pmatrix}, \qquad (3.20)$$

where $\bar{\pi}_n$, ϕ_n , denote the block matrices made by $\bar{\pi}_n^{IJ}$ and ϕ_n^{IJ} , while $\bar{\pi}_n^*$ and ϕ_n^* are the conjugate matrices. The coefficients \bar{z}_n^I , z_n^I of the expansion are the variables we call coherent "states." The inverse formula reads, from (3.18),

$$-2i\tau_n\omega_n\begin{pmatrix}\bar{z}_n\\z_n\end{pmatrix} = \int_{\Omega} \mathrm{d}^{D-1}\mathbf{x}\begin{pmatrix}\bar{\pi}_n & \phi_n\\-\bar{\pi}_n^* & -\phi_n^*\end{pmatrix}\begin{pmatrix}0 & 1\\-1 & N_2^i\partial_i\end{pmatrix}$$
$$\times \begin{pmatrix}\bar{\pi}_{\phi}\\\phi\end{pmatrix}.$$
(3.21)

We can rearrange (3.19) as

$$\mathcal{L}_{\text{free}}^{\prime} = \sum_{I=1}^{\prime} \sum_{n \in \hat{\mathcal{U}}} \tau_{n}^{I} [i\omega_{n}^{I} (\bar{z}_{n}^{I} \dot{z}_{n}^{I} - \dot{\bar{z}}_{n}^{I} z_{n}^{I}) - 2\omega_{n}^{I2} \bar{z}_{n}^{I} z_{n}^{I}]. \quad (3.22)$$

Typically, the τ_n^I factor we see here does not depend on n, but just on I.

At this point, it is straightforward to add the interacting Lagrangian $L'_{int}(\bar{\pi}_{\phi}, \phi)$. We recall that L'_{int} does not contain time derivatives of $\bar{\pi}_{\phi}$ and ϕ , by construction, although it can contain space derivatives. Expanding the fields and the momenta in the basis (3.20) of coherent states, and integrating by parts when needed, we obtain an integrated interacting Lagrangian

$$\mathcal{L}_{\mathrm{int}}' = \int_{\Omega} L_{\mathrm{int}}' \mathrm{d}^{D-1} \mathbf{x}$$

that just depends \bar{z}_n^I , z_n^I (no time derivatives). Finally, the total action is

$$S = -i \sum_{I=1}^{r} \sum_{n \in \hat{\mathcal{U}}} \tau_n^I \omega_n^I (\bar{z}_{nf}^I z_n^I (t_f) + \bar{z}_n^I (t_i) z_{ni}^I) + \int_{t_i}^{t_f} dt (\mathcal{L}'_{\text{free}} + \mathcal{L}'_{\text{int}}), \qquad (3.23)$$

where $z_{ni}^{I} = z_{n}^{I}(t_{i})$ parametrize the initial conditions in the coherent-state approach, while $\bar{z}_{nf}^{I} = \bar{z}_{n}^{I}(t_{f})$ parametrize

the final conditions. The sums appearing in (3.23), which we call "endpoint corrections," are there to have the correct variational problem. This means that the variations $\delta \bar{z}_n^I, \delta z_n^I$, subject to the initial and final conditions $\delta \bar{z}_n^I(t_f) =$ $\delta z_n^I(t_i) = 0$, must give the \bar{z}_n^I and z_n^I equations of motion, and no further restrictions. Note that the time derivatives of \bar{z}_n^I and z_n^I appear only inside $\mathcal{L}'_{\text{free}}$. This is the reason why the partial integrations that take care of the terms proportional to $\delta \bar{z}_n^I$ and δz_n^I are compensated by endpoint corrections as simple as those of (3.23).

B. Gauge transformations of coherent states

Now we study the gauge transformations of the coherent states, and the conditions to have gauge invariant amplitudes. As usual, the parameters Λ of the gauge transformations are written as $\Lambda = \theta C$, where θ is a constant, anticommuting parameter and *C* are the Faddeev-Popov ghosts. The fields ϕ^I include *C* and the other fields that are necessary to gauge-fix the theory, which are the antighosts \overline{C} and certain Lagrange multipliers *B* for the gauge-fixing (see below).

Since we are assuming the linearity conditions (3.8), we can write the gauge transformations as $\delta \phi^I = \theta \Sigma^{IJ} \phi^J$, for some constants Σ^{IJ} . By means of linear field redefinitions, we can always split the set of fields ϕ^I into three subsets ϕ^{I_+} , ϕ^{I_-} and ϕ^{I_0} , where: (i) the fields ϕ^{I_+} transform into other fields; (ii) the fields ϕ^{I_-} parametrize the transformations of other fields; and (iii) the fields ϕ^{I_0} are invariant and cannot be obtained from the transformations of other fields:

$$\delta \phi^{I_{+}} = \theta \phi^{I_{-}}, \qquad \delta \phi^{I_{-}} = 0, \qquad \delta \phi^{I_{0}} = 0.$$
 (3.24)

The transformation law can be written as

$$\delta = \delta \phi^{I_+} \frac{\delta_l}{\delta \phi^{I_+}} = \theta \Delta, \qquad \Delta \equiv \phi^{I_-} \frac{\delta_l}{\delta \phi^{I_+}},$$

where δ_l denotes the left functional derivative.

The operator Δ has a standard "descent" structure. A well-known theorem (see appendix A for a direct proof) says that the most general solution of the problem $\delta X = 0$, where X is a local function, is

$$X = X_0 + \Delta Y, \tag{3.25}$$

where X_0 is a $\phi^{I_{\pm}}$ independent local function, and *Y* is a local function.

Consider the invariant quadratic terms that we can build with the fields $\phi^{I_{\pm}}$. At some point, we may need to diagonalize them. It is easy to see that we cannot build enough invariant terms, unless the diagonalization organizes the field $\phi^{I_{\pm}}$ in "pairs of pairs." Consider a single pair $\phi^{I_{\pm}}$, and observe that $\phi^{I_{+}}$ and $\phi^{I_{-}}$ have opposite statistics. By (3.25), the quadratic terms in question must be contained in ΔY . However, the expressions $\Delta(\phi^{I_{+}}\phi^{I_{+}})$, $\Delta(\phi^{I_+}\phi^{I_-})$ and $\Delta(\phi^{I_-}\phi^{I_-})$ generate just one independent quadratic term, while we need two. This means that for each pair $\phi^{I_{\pm}}$ there must be another pair $\phi^{I_{\pm}'}$, out of which the required invariants can be built.

We can organize the fields $\phi^{I_{\pm}}$, $\phi^{I_{\pm}'}$ into doublets. Using a notation that is ready for the applications to Yang-Mills theories and gravity (adapting the meaning of the index *a*), we write the doublets as

$$\phi_{+}^{a} = \begin{pmatrix} \phi^{a} \\ \bar{C}^{a} \end{pmatrix}, \qquad \phi_{-}^{a} = \begin{pmatrix} B^{a} \\ C^{a} \end{pmatrix}, \qquad (3.26)$$

where ϕ^a and B^a have bosonic statistics, while \bar{C}^a and C^a have fermionic statistics. In all the applications that we have in mind, this is the structure we need.

We can write the transformation law as

$$\delta \phi^a_+ = \theta \sigma_1 \phi^a_-, \quad \delta = \theta \Delta, \quad \Delta = \phi^{aT}_- \sigma_1 \frac{\delta_l}{\delta \phi^a_+}, \quad (3.27)$$

where σ_1 is the first Pauli matrix and the superscript "*T*" means "transpose."

The ϕ^a_+ expansions (3.20),

$$\phi_{+}^{a} = \sum_{J=1}^{\prime} \sum_{n \in \hat{\mathcal{U}}} (\phi_{+n}^{aJ} z_{n}^{J} + \phi_{+n}^{aJ*} \bar{z}_{n}^{J}),$$

must turn into the ϕ_{-}^{a} expansions under (3.27):

$$\begin{split} \delta\phi^a_+ &= \sum_{J=1}^r \sum_{n \in \hat{\mathcal{U}}} (\phi^{aJ}_{+n} \delta z^J_n + \phi^{aJ*}_{+n} \delta \bar{z}^J_n) = \theta \sigma_1 \phi^a_- \\ &= \theta \sum_{J=1}^r \sum_{n \in \hat{\mathcal{U}}} (\sigma_1 \phi^{aJ}_{-n} z^J_n + \sigma_1 \phi^{aJ*}_{-n} \bar{z}^J_n). \end{split}$$

Since the Eq. (3.14) are invariant under the symmetry, the eigenfunctions appearing in the ϕ_{-}^{a} expansions must match eigenfunctions appearing in the ϕ_{+}^{a} expansions. That is to say, we must have $\phi_{+n}^{aJ_{+}} = \sigma_{1}\phi_{-n}^{aJ_{-}}$ for some pairings of indices J_{+} , J_{-} . Then, the transformations of the coherent states read $\delta z_{n}^{J_{+}} = \theta z_{n}^{J_{-}}$, $\delta z_{n}^{J_{-}} = 0$. Moreover, the z_{n}^{J} with such indices must also be organized in doublets, for the reasons explained above. Finally, the $\phi^{I_{0}}$ expansions identify the invariant coherent states $z_{n}^{J_{0}}$. We illustrate these facts in Sec. V, formulas (5.12) and (5.13).

Summarizing, we can split the set of coherent states z_n^I into three subsets w_n^{α} , u_n^{α} and v_n^{α} (with indices α , *a* spanning appropriate ranges). Both u_n^{α} and v_n^{α} are doublets, with bosonic first components and fermionic second components. Their gauge transformations are

$$\delta w_n^a = \delta \bar{w}_n^a = 0, \qquad \delta u_n^a = \theta \sigma_1 v_n^a, \delta \bar{u}_n^a = \theta \sigma_1 \bar{v}_n^a, \qquad \delta v_n^a = \delta \bar{v}_n^a = 0.$$
(3.28)

We can obtain results that agree with the ones just found by repeating the analysis for the "momenta" $\bar{\pi}_{\phi}^{I}$. The redefinition (3.10) is due to the presence of the terms $\sim \dot{\phi}^I \partial_i \phi^J$ in the Lagrangian. Since the symmetry is orthodox and linear, the sum of these terms must be gauge invariant by itself. Taking into account the conventions we adopted for the fields $\bar{\psi}$, ψ with fermionic statistics, we can write such a sum as

$$\dot{\phi}^I \tilde{\mathcal{B}}^{IJi}(0) \partial_i \phi^J,$$

where $\tilde{\mathcal{B}}^{IJi} = \mathcal{B}^{IJi}$ if the indices *I*, *J* refer to bosonic fields, or *I* refers to $\bar{\psi}$, while $\tilde{\mathcal{B}}^{IJi} = -\mathcal{B}^{IJi}$ if *I* refers to ψ . This way, the redefinitions match (3.10) precisely. Writing the transformations $\delta_{\Lambda}\phi^{I} = \theta \Sigma^{IJ} \phi^{J}$, as above, gauge invariance gives the condition

$$\Sigma^{KI}\tilde{\mathcal{B}}^{KJi}(0) + (-1)^{\epsilon_I}\tilde{\mathcal{B}}^{IKi}(0)\Sigma^{KJ} = 0,$$

where ϵ_I is the statistics of ϕ^I . Analyzing all the situations one by one, we can easily see that this condition is equivalent to

$$\Sigma^{KI}\mathcal{B}^{KJi}(0) + \mathcal{B}^{IKi}(0)\Sigma^{KJ} = 0,$$

which also gives the implication

$$\delta_{\Lambda} \pi^{I}_{\phi} = -\Sigma^{JI} \pi^{J}_{\phi} \quad \Rightarrow \quad \delta_{\Lambda} \bar{\pi}^{I}_{\phi} = -\Sigma^{JI} \bar{\pi}^{J}_{\phi}, \quad (3.29)$$

from (3.4). Thus, the old and new momenta π_{ϕ}^{I} and $\bar{\pi}_{\phi}^{I}$ transform the same way.

The $\bar{\pi}_{\phi}^{I}$ expansions and their transformations can be studied as we did for the fields ϕ^{I} . Matching the eigenfunctions, we find agreement with (3.28). Alternatively, we can study the expansions of ϕ^{I} and $\bar{\pi}_{\phi}^{I}$ at the same time by working directly on (3.20).

Since the Lagrangian (3.6) in gauge invariant under the transformations $\delta_{\Lambda}\phi^I$ and (3.4), and we are assuming the linearity conditions (3.8), the Lagrangian (3.12) is invariant under $\delta_{\Lambda}\phi^I$ and (3.29). The integrated Lagrangian $\mathcal{L}'_{\text{free}} + \mathcal{L}'_{\text{int}}$ of formula (3.23) is invariant under (3.28), once it is written in the variables w_n^a , u_n^a and v_n^a and their conjugates.

The action (3.23) is gauge invariant if the endpoint corrections are invariant, which occurs if they do not contain u_n^a and \bar{u}_n^a . In addition, we require that they do not contain gauge trivial modes, which are v_n^a and \bar{v}_n^a (which can be obtained as transformations of u_n^a and \bar{u}_n^a).

Thus, the physical amplitudes are those that have

$$\bar{u}_{nf}^{a} = \bar{v}_{nf}^{a} = u_{ni}^{a} = v_{ni}^{a} = 0,$$
 (3.30)

in which case the endpoint corrections, which read

$$-i\sum_{\alpha}\sum_{n\in\hat{\mathcal{U}}}\tau_{n}^{\alpha}\omega_{n}^{\alpha}(\bar{w}_{nf}^{\alpha}w_{n}^{\alpha}(t_{f})+\bar{w}_{n}^{\alpha}(t_{i})w_{ni}^{\alpha}),$$

are manifestly gauge invariant.

The restrictions (3.30) on the endpoint corrections are analogous to the restrictions we commonly apply to the *S* matrix amplitudes: we do not consider scattering processes involving Faddeev-Popov ghosts, or the temporal and longitudinal components of the gauge fields, among the incoming and outgoing states. Yet, sometimes it may be useful to relax these requirements, and consider diagrams with all sorts of external legs, including the ones just mentioned, to study renormalization, for example, or the gauge independence of the physical quantities, or the diagrammatic versions of the unitarity equations.

We conclude this subsection by writing down the universal structure of the kinetic terms of the coherent states, inside \mathcal{L}'_{free} . The ones of the gauge invariant sector are clearly

$$\sum_{\alpha} \sum_{n \in \hat{\mathcal{U}}} \tau_n^{\alpha} i \omega_n^{\alpha} (\bar{w}_n^{\alpha} \dot{w}_n^{\alpha} - \dot{\bar{w}}_n^{\alpha} w_n^{\alpha}), \qquad (3.31)$$

by (3.22). Using the theorem (3.25), the universal kinetic terms of the gauge sector can be written in the form

$$\sum_{a} \sum_{n \in \hat{\mathcal{U}}} \tau_n^a i \omega_n^a \Delta (\bar{u}_n^{aT} \sigma_1 \dot{u}_n^a - \dot{\bar{u}}_n^{aT} \sigma_1 u_n^a)$$

=
$$\sum_{a} \sum_{n \in \hat{\mathcal{U}}} \tau_n^a i \omega_n^a (\bar{v}_n^{aT} \dot{u}_n^a - v_n^{aT} \dot{\bar{u}}_n^a + \dot{v}_n^{aT} \bar{u}_n^a - \dot{\bar{v}}_n^{aT} u_n^a),$$

(3.32)

the right-hand side being obtained using the properties (A2) of appendix A.

C. Nontrivial boundary conditions

So far, we have been working with trivial boundary conditions $\phi^{I}|_{\partial\Omega} = 0$. Now we treat the case of general Dirichlet boundary conditions

$$\phi^{I}(t, \mathbf{x})|_{\partial\Omega} = f^{I}(t, \mathbf{x}_{\partial\Omega}), \qquad (3.33)$$

where f^I are given functions, and $\mathbf{x}_{\partial\Omega}$ denotes the space variables restricted to $\partial\Omega$. We want to show that we can reduce this situation to the previous one, with few minor modifications. In particular, the eigenfunctions, the frequencies and the orthonormality relations remain the same.

First, we shift the fields ϕ^I by some functions $\phi^I_0(t, \mathbf{x})$ that coincide with $f^I(t, \mathbf{x}_{\partial\Omega})$ on $\partial\Omega$:

$$\phi^{I}(t, \mathbf{x}) = \phi^{I}_{0}(t, \mathbf{x}) + \phi^{I}(t, \mathbf{x}), \quad \phi^{I}_{0}(t, \mathbf{x}_{\partial\Omega}) = f^{I}(t, \mathbf{x}_{\partial\Omega}),$$
(3.34)

so that the shifted fields vanish on Ω :

$$\varphi^{I}(t,\mathbf{x})|_{\partial\Omega} = 0. \tag{3.35}$$

After the shift, we are free to integrate the space integrals by parts, to move the space derivatives that act on any φ^I somewhere else.

By the assumptions we have made on the structure of the Lagrangian $L(\phi, \dot{\phi})$, its expansion can be written as

$$L(\phi, \dot{\phi}) = L_0 + \varphi^I A^I(\phi_0) + \dot{\varphi}^I B^I(\phi_0) + \nabla(\varphi^I C^I(\phi_0)) + L_{\varphi}(\varphi, \dot{\varphi}) \equiv \tilde{L}_{\varphi}(\varphi, \dot{\varphi}), \qquad (3.36)$$

where L_0 is φ -independent and $L_{\varphi}(\varphi, \dot{\varphi}) = L_{\text{free}}(\varphi, \dot{\varphi}) +$ interactions, by (3.1). We can ignore the *C*-term, since it disappears once we integrate on the space manifold Ω , by (3.35). Were it just for $L_{\varphi}(\varphi, \dot{\varphi})$ (and L_0) we could apply the formulation developed so far with no modifications. We want to explain how to treat the corrections proportional to *A* and *B* (which need not be perturbative).

Let us define

$$\frac{\partial L_{\varphi}(\varphi, \dot{\varphi})}{\partial \dot{\varphi}^{I}} = \pi_{\varphi}^{I}(\varphi, \dot{\varphi}),$$

$$\frac{\partial \tilde{L}_{\varphi}(\varphi, \dot{\varphi})}{\partial \dot{\varphi}^{I}} = \tilde{\pi}_{\varphi}^{I}(\varphi, \dot{\varphi}) = \pi_{\varphi}^{I}(\varphi, \dot{\varphi}) + B^{I},$$
(3.37)

which invert to

$$\dot{\varphi}^I = F^I(\varphi, \pi_{\varphi}), \qquad \dot{\varphi}^I = \tilde{F}^I(\varphi, \tilde{\pi}_{\varphi}), \qquad (3.38)$$

for certain functions F^I and \tilde{F}^I . We have the Hamiltonians

$$\begin{aligned} H_{\varphi}(\pi_{\varphi},\varphi) &= \pi_{\varphi}^{I} F^{I}(\varphi,\pi_{\varphi}) - L_{\varphi}(\varphi,F(\varphi,\pi_{\varphi})), \\ \tilde{H}_{\varphi}(\tilde{\pi}_{\varphi},\varphi) &= \tilde{\pi}_{\varphi}^{I} \tilde{F}^{I}(\varphi,\tilde{\pi}_{\varphi}) - \tilde{L}_{\varphi}(\varphi,\tilde{F}(\varphi,\tilde{\pi}_{\varphi})), \end{aligned}$$
(3.39)

and the extended Lagrangians

$$L'_{\varphi} = \frac{1}{2} (\pi^{I}_{\varphi} \dot{\varphi}^{I} - \dot{\pi}^{I}_{\varphi} \varphi^{I}) - H_{\varphi}(\pi_{\varphi}, \varphi),$$

$$\tilde{L}'_{\varphi} = \frac{1}{2} (\tilde{\pi}^{I}_{\varphi} \dot{\varphi}^{I} - \dot{\tilde{\pi}}^{I}_{\varphi} \varphi^{I}) - \tilde{H}_{\varphi}(\tilde{\pi}_{\varphi}, \varphi).$$
(3.40)

Equating the two expressions of $\dot{\varphi}^{I}$ in (3.38) and using the last identity of (3.37), we get

$$\tilde{F}^{I}(\varphi, \tilde{\pi}_{\varphi}) = F^{I}(\varphi, \tilde{\pi}_{\varphi} - B).$$

Using (3.36), (3.40), and (3.39), it is easy to work out the difference

$$\begin{split} \Delta L'_{\varphi} &\equiv \tilde{L}'_{\varphi} - L'_{\varphi}|_{\pi_{\varphi} \to \tilde{\pi}_{\varphi}} = L_0 + \varphi^I A^I \\ &\quad + \tilde{\pi}^I_{\varphi} [F^I(\varphi, \tilde{\pi}_{\varphi}) - F^I(\varphi, \tilde{\pi}_{\varphi} - B)] \\ &\quad + B^I F^I(\varphi, \tilde{\pi}_{\varphi} - B) + L_{\varphi}(\varphi, F(\varphi, \tilde{\pi}_{\varphi} - B)) \\ &\quad - L_{\varphi}(\varphi, F(\varphi, \tilde{\pi}_{\varphi})). \end{split}$$
(3.41)

If we switch the interactions off, we have $L_{\varphi}(\varphi, \dot{\varphi}) = L_{\text{free}}(\varphi, \dot{\varphi})$, and the functions $F^{I}(\varphi, \pi_{\varphi})$ become linear. Then formula (3.41) tells us that $\Delta L'_{\varphi}$ is made of linear terms, plus interactions. In particular, the quadratic part of \tilde{L}'_{φ} coincides with the quadratic part of $L'_{\varphi}|_{\pi_{\varphi} \to \tilde{\pi}_{\varphi}}$.

At this point, we make the analogues of the shifts (3.10),

$$\bar{\tilde{\pi}}^{I}_{\varphi} = \tilde{\pi}^{I}_{\varphi} - \mathcal{B}^{IJi}(0)\partial_{i}\varphi^{J}.$$
(3.42)

They do not change the structure of $\Delta L'_{\varphi}$, because they do not involve time derivatives, and send linear terms into linear terms, interaction terms into interaction terms. As far as the quadratic part of \tilde{L}'_{φ} is concerned, it is equal to the ones of (3.12) and (3.13) with the replacements $\phi^I \rightarrow \varphi^I$, $\bar{\pi}^I_{\phi} \rightarrow \tilde{\pi}^I_{\varphi}$. Hence, if we expand the pair $\tilde{\pi}^I_{\varphi}, \varphi^I$ exactly as we expanded $\bar{\pi}^I_{\phi}, \phi^I$ before, we obtain the same quadratic part we had before, (3.19) and (3.22), plus interactions, plus linear terms (due to $\Delta L'_{\varphi}$).

Note that $\tilde{\pi}_{\varphi}^{I}$ vanishes on the boundary $\partial\Omega$ by construction, so to speak, since it is expanded in a basis of functions that vanish there. Yet, we recall that no convergence requirements are imposed on the expansion: the expansion itself must be taken as the very definition of what $\tilde{\pi}_{\varphi}^{I}|_{\partial\Omega} = 0$ truly means. The same can be said of φ and $\varphi|_{\partial\Omega} = 0$. As we have already noted, the functional integral is defined by the very same expansions.

As a result, we obtain a Lagrangian that has the same structure as before, apart from including extra terms that are linear in the coherent states (and terms that are independent of them). The endpoint corrections are unmodified, because $\Delta L'_{\varphi}$ does not contain time derivatives. The complete action has the form (3.23), plus the corrections due to $\Delta L'_{\varphi}$:

$$S = -i \sum_{I=1}^{r} \sum_{n \in \hat{\mathcal{U}}} \tau_{n}^{I} \omega_{n}^{I} (\bar{z}_{nf}^{I} z_{n}^{I} (t_{f}) + \bar{z}_{n}^{I} (t_{i}) z_{ni}^{I}) + \int_{t_{i}}^{t_{f}} dt \bigg[\mathcal{L}_{free}^{\prime} + \mathcal{L}_{int}^{\prime} + \sum_{I=1}^{r} \sum_{n \in \hat{\mathcal{U}}} (h_{n}^{I} z_{n}^{I} + h_{n}^{I*} \bar{z}_{n}^{I}) + k \bigg],$$
(3.43)

for some, possibly time-dependent, functions h_n^I and k.

As far as the local symmetries are concerned, the shift (3.34) does change the expressions of the transformations, unless the functions ϕ_0^I are gauge invariant, which they must be, because we cannot build physical quantities with unphysical boundary conditions. Referring to the splitting of ϕ^I into the three subsets ϕ^{I_+} , ϕ^{I_-} , and ϕ^{I_0} , we must require

$$\phi_0^{I_+} = \phi_0^{I_-} = 0. \tag{3.44}$$

Although we may sometimes relax the requirements (3.30) on the initial and final conditions, we are definitely

not going to relax the requirements (3.44) on the boundary conditions, because there is no reason to do so. Having specified this, we have proved that the situation of general Dirichlet boundary conditions (3.33) reduces to the one of vanishing boundary conditions, apart from some extra terms that are linear in the coherent states, which are no source of worry.

In the case of gravity, we also need to extend the results to interaction Lagrangians that contain arbitrarily many derivatives of the fields (as long as their number grows together with the power of some coupling constant), and show that we can rearrange the Lagrangian to have a final action with the form and the properties of (3.43). We deal with this aspect in appendix B.

In conclusion, we have developed the general theory of coherent states for local symmetries. It remains to use the results of [3,4] to arrange gauge invariance and general covariance in the way we need. We do this in the next sections. Once that goal is achieved, the results of this section, combined with those of [1], allow us to build the unitary evolution operator $U(t_f, t_i)$.

IV. GAUGE THEORIES: REARRANGING THE LAGRANGIAN

In gauge theories, we need to face a nontrivial issue: how can we specify gauge invariant initial, final, and boundary conditions? Giving the field strength $F_{\mu\nu}$ is a possibility, but only in QED, because in non-Abelian theories it is not gauge invariant. And even in QED, there remains to give gauge invariant conditions for electrons.

These problems can be solved by introducing gauge invariant fields as explained in Refs. [3,4]. The goal is achieved by means of a particular purely virtual extension of the theory. The physical particles, the *S* matrix amplitudes and the correlation functions of common (nonlinear) composite fields (such as $F^a_{\mu\nu}F^{\mu\nu a}$, $\bar{\psi}\psi$, $\bar{\psi}\gamma^{\mu}\psi$, etc.) do not change.⁵ Nevertheless, the extension provides tools to define new, physical correlation functions, such as the ones that contain insertions of gauge invariant fields, and calculate them perturbatively. As we are going to show, it also allows us to specify gauge invariant initial, final and boundary conditions at finite τ on a compact Ω .

The extension consists of a certain set of purely virtual extra fields. In gauge theories [3] we have scalar fields ϕ^a , together with their anticommuting partners \overline{H}^a and H^a , where *a* is the Lie-algebra index. In addition, it may be convenient to include certain Lagrange multipliers E^a . The extension preserves renormalizability and unitarity. Unitarity is also the reason why the extra fields must be

purely virtual: if not, the extension would propagate ghosts, and unitarity would be lost.

The crucial property, for our purposes, is that the extension allows us to switch to gauge invariant variables, and trivialize the gauge symmetry, to fulfill the conditions (3.8). The coherent states are then introduced as explained in the previous section, and the rest follows from there.

We focus on pure gauge theories, for simplicity, since there is no difficulty to add the matter fields, when needed. We separate the time and space components of the gauge fields by writing $A^{\mu} = (A^0, \mathbf{A})$. The dot on a field denotes its time derivative.

Instead of the common Lorenz gauge-fixing, given by the function $\partial_{\mu}A^{\mu a}$, we use the more general function $\xi \dot{A}^{0a} + \nabla \cdot \mathbf{A}^{a}$, where ξ is an unspecified constant, which allows us to interpolate between different gauge choices. Then, the gauge-fixed Lagrangian is

$$egin{aligned} & ilde{L}_{
m gf} = rac{1}{2} \mathbf{F}^a \cdot \mathbf{F}^a - rac{1}{4} F^{a2}_{ij} + B^a igg(\xi \partial_0 A^{0a} + \mathbf{\nabla} \cdot \mathbf{A}^a + rac{\lambda}{2} B^a igg) \ &- \xi ar{C}^a D_0 \dot{C}^a + ar{C}^a \mathbf{\nabla} \cdot \mathbf{D} C^a, \end{aligned}$$

where $D_{\mu} = (D_0, \mathbf{D})$ is the covariant derivative, and $\mathbf{F}^a = \dot{\mathbf{A}}^a + \nabla A^{0a} + gf^{abc}A^{0b}\mathbf{A}^c$ are the 0*i* components of the field strength. The so-called special gauge [19], which we use in the examples of Secs. VII and VIII, is $\xi = \lambda$. The Feynman gauge is $\xi = \lambda = 1$. Like the Feynman gauge, the special gauge allows us to simplify many formulas. In addition, it allows us to keep a gauge-fixing parameter free, which is useful to study the gauge independence of the physical quantities.

First, we rearrange \tilde{L}_{gf} , since no fields should be differentiated twice. For reasons that will become clear later, we also turn the derivatives contained in the gauge-fixing function onto *B*. We thus obtain

$$\begin{split} L_{\rm gf} &= \frac{1}{2} \mathbf{F}^a \cdot \mathbf{F}^a - \frac{1}{4} F^{a2}_{ij} - \xi \dot{B}^a A^{0a} - \mathbf{\nabla} B^a \cdot \mathbf{A}^a + \frac{\lambda}{2} B^a B^a \\ &+ \xi \dot{\bar{C}}^a D_0 C^a - (\mathbf{\nabla} \bar{C}^a) \cdot \mathbf{D} C^a. \end{split}$$

Next, we introduce extra scalar fields ϕ^a , and their anticommuting partners H^a , transforming as [3]

$$\delta_{\Lambda}\phi = \frac{ig \,\mathrm{ad}_{\phi}}{\mathrm{e}^{ig \,\mathrm{ad}_{\phi}} - 1}\Lambda \equiv R^{a}(\phi,\Lambda)T^{a},$$

$$\delta_{\Lambda}H^{a} = H^{b}\frac{\delta R^{a}(\phi,\Lambda)}{\delta\phi^{b}}.$$
 (4.1)

where $\phi = \phi^a T^a$, $\Lambda = \Lambda^a T^a$, $\Lambda^a(x)$ are the parameters of the gauge transformation, $ad_{\phi}X \equiv [\phi, X]$, and T^a are the Lie algebra generators. We also introduce gauge invariant antipartners \bar{H}^a and Lagrange multipliers E^a .

⁵In all such cases, the extension amounts to inserting "1," written in a complicated way (a new type of "1" with respect to the "1" used to gauge-fix the theory).

The gauge invariant fields $A_{\mu d} = A^a_{\mu d} T^a$ are then

$$A_{\mu d} \equiv e^{-ig \operatorname{ad}_{\phi}} A_{\mu} - \frac{1 - e^{-ig \operatorname{ad}_{\phi}}}{ig \operatorname{ad}_{\phi}} (\partial_{\mu} \phi), \quad \delta_{\Lambda} A_{\mu d} = 0, \quad (4.2)$$

where the subscript "d" stands for "dressed."

The extension is a sort of mirror of the gauge-fixing sector. However, it must be gauge invariant. In its most convenient (and manifestly power counting renormalizable) form, it is specified by a function $\tilde{\xi}\dot{A}_{d}^{0a} + \nabla \cdot \mathbf{A}_{d}^{a}$, where $\tilde{\xi}$ is a free constant. It reads

$$\begin{split} L_{\text{ext}} &= E^a \left(\tilde{\xi} \dot{A}_{\text{d}}^{0a} + \boldsymbol{\nabla} \cdot \mathbf{A}_{\text{d}}^a + \frac{\tilde{\lambda}}{2} E^a \right) - \tilde{\xi} \dot{\bar{H}}^a \frac{\delta A_{\text{d}}^{0a}}{\delta \phi^b} H^b \\ &- (\boldsymbol{\nabla} \bar{H}^a) \cdot \frac{\delta \mathbf{A}_{\text{d}}^a}{\delta \phi^b} H^b, \end{split}$$

where $\tilde{\lambda}$ is another free constant. This expression of L_{ext} is already rearranged (with respect to the expression appearing in [3]) to eliminate the double derivatives. It is easy to check that L_{ext} is invariant under the local transformations (4.1) (for details on this, see [3]).

The total action is $L_{\rm tot} = L_{\rm gf} + L_{\rm ext}$. The parameters $\tilde{\xi}$ and $\tilde{\lambda}$ are part of the large arbitrariness we have, when we want to dress the elementary fields and make them gauge invariant. They are unique, however, in a power counting renormalizable context (preserving invariance under space rotations). Physically, they may parametrize different interplays between the physical process and the external environment, or the experimental apparatus.

The extension is equal to "1" on standard gauge invariant correlation functions (where "standard" means: independent of ϕ , \bar{H} , H, and E), as well as on the S matrix amplitudes, at $\tau = \infty$, $\Omega = \mathbb{R}^3$. We can prove this fact as follows. Focus on the *E*-dependent terms

$$E^a \left(V^a + \frac{\tilde{\lambda}}{2} E^a \right), \qquad V^a \equiv \tilde{\xi} \dot{A}^{0a}_{d} + \mathbf{\nabla} \cdot \mathbf{A}^a_{d}.$$

Insert "1" in the form of the Gaussian integral with Lagrangian $-\tilde{\lambda}(Q^a - E^a)^2/2$, where Q^a are extra integration variables. We have

$$E^{a}\left(V^{a}+\frac{\tilde{\lambda}}{2}E^{a}\right)-\frac{\tilde{\lambda}}{2}(Q^{a}-E^{a})^{2}=E^{a}(V^{a}+\tilde{\lambda}Q^{a})-\frac{\tilde{\lambda}}{2}Q^{a}Q^{a}.$$
(4.3)

Next: (i) integrate on E^a , which gives a functional delta function δ ; (ii) integrate on \bar{H}^a , and H^a , which gives a functional determinant **J**; (iii) integrate on ϕ^a , which appears only in δ and **J**; this integral gives 1, because **J** is there precisely for this purpose; finally, (iv) integrate on Q^a , which also gives 1, since the only Q^a dependence that

survives the first three operations is the one contained in the last term of (4.3).

This chain of operations cannot be repeated as is when the insertions are ϕ dependent, as are those made of the invariant fields $A_{\mu d}$. Thus, the gauge invariant insertions built with ϕ provide new, physical correlation functions and amplitudes. What we want to show is that these properties also allow us to study amplitudes between arbitrary gauge invariant initial and final states, with arbitrary gauge invariant boundary conditions, in a finite interval of time τ and on a compact space manifold Ω .

One might object that the fields ϕ^a become propagating, as well as \overline{H}^a and H^a . What are these fields, physically? They might even be ghosts, on general grounds. On top of that, we do not want to change the theory. We just want to study less common features of a standard theory.

These are the reasons why the whole extension has to be purely virtual. The extra fields ϕ^a , \bar{H}^a , and H^a propagate ghosts if they are treated as ordinary fields. They do not, if they are purely virtual. If the whole extension is purely virtual, it does not inject new degrees of freedom into the theory, and can be used as a mere mathematical tool to study uncommon quantities of a common theory.

Another great advantage of the extension is that it allows us to "trivialize" the gauge symmetry, by switching to appropriate dual variables. For example, we can abandon the original gauge potential A_{μ} in favor of the gauge invariant one $A_{\mu d}$. We can also abandon the parameters Λ of the gauge transformation in favor of

$$\Lambda^a_{\rm d} \equiv R^a(\phi, \Lambda) = \delta_\Lambda \phi^a. \tag{4.4}$$

If we express the gauge symmetry this way, it becomes trivial: $\delta \phi = \Lambda_d$, $\delta A_{\mu d} = 0$. Then, we introduce new Faddeev-Popov ghosts C_d^a , by means of the identification $\Lambda_d^a = \theta C_d^a$, where θ is a constant, anticommuting parameter. Since the gauge symmetry is just an arbitrary shift of ϕ^a , its closure is trivial, so we can take $\delta C_d^a = 0$. We can define new, gauge invariant anticommuting partners H_d by means of the relations $H = R(-\phi, H_d)$.

Inverting (4.2), we can use the relations

$$A_{\mu} = e^{ig \operatorname{ad}_{\phi}} A_{\mu d} - \frac{1 - e^{ig \operatorname{ad}_{\phi}}}{ig \operatorname{ad}_{\phi}} (\partial_{\mu} \phi),$$

$$R(\phi, C) = C_{d}, \qquad H = R(-\phi, H_{d}), \qquad (4.5)$$

as a change of variables in the functional integral, to switch from the original variables A_{μ} , C, ϕ , and H to the dual variables $A_{\mu d}$, C_d , ϕ , and H_d . The switch has a trivial Jacobian determinant (if we use the dimensional regularization [20]). We do not change \bar{C} , B, \bar{H} , and E.

It is much easier to specify gauge invariant initial, final and boundary conditions by means of the dual variables. To make the notation lighter, we put a tilde on A^a_{μ} , C^a , and H^a , to emphasize that they are functions of $A^a_{\mu d}$, C^a_d , ϕ^a , and H^a_d , now, and then drop the "d" in $A^a_{\mu d}$, C^a_d , H^a_d . It will be sufficient to recall that, in the new notation, A^a_{μ} is inert under the gauge transformations ($\delta_{\Lambda}A^a_{\mu} = 0$), and so are C^a and H^a .

After the switch (4.5), the multipliers E^a remain nonderivative (differently from *B*), so we integrate them out. At the end (check [3] for details), we obtain the total action

$$L_{\text{tot}} = \frac{1}{2} \mathbf{F}^{a} \cdot \mathbf{F}^{a} - \frac{1}{4} F^{a2}_{ij} - \xi \dot{B}^{a} \tilde{A}^{0a} - \nabla B^{a} \cdot \tilde{\mathbf{A}}^{a} + \frac{\lambda}{2} (B^{a})^{2} - \frac{1}{2\tilde{\lambda}} (\tilde{\xi} \dot{A}^{0a} + \nabla \cdot \mathbf{A}^{a})^{2} + \xi \dot{\bar{C}}^{a} \frac{\delta \tilde{A}^{0a}}{\delta \phi^{b}} C^{b} + (\nabla \bar{C}^{a}) \cdot \frac{\delta \tilde{\mathbf{A}}^{a}}{\delta \phi^{b}} C^{b} + \tilde{\xi} \dot{\bar{H}}^{a} D_{0} H^{a} - (\nabla \bar{H}^{a}) \cdot \mathbf{D} H^{a}.$$

$$(4.6)$$

The trivialized local symmetry is

$$\delta \phi = \Lambda = \theta C, \ \delta \bar{C} = \theta B, \ \delta B = \delta C = \delta A_{\mu} = \delta \bar{H} = \delta H = 0.$$

(4.7)

Note that L_{tot} is invariant without adding total derivatives. Thus, we are in the conditions of Sec. III. We can define the coherent states as explained there, and from there build the unitary operator $U(t_f, t_i)$ as explained in [1].

V. GAUGE THEORIES: QUADRATIC SECTOR

In this section we explain how to introduce coherent states in the free-field limit of gauge theories, which is the key part of the problem. In the next section it will be relatively straightforward to include the interactions.

The quadratic part of the Lagrangian is practically the same as if we were working in QED. Thus, we suppress the index a and write, from (4.6),

$$L_{\text{tot}} = \frac{1}{2} (\dot{\mathbf{A}} + \nabla A_0)^2 - \frac{1}{4} F_{ij}^2 - \frac{1}{2\tilde{\lambda}} (\tilde{\xi} \dot{A}^0 + \nabla \cdot \mathbf{A})^2 - \xi \dot{B} A^0 - \nabla B \cdot \mathbf{A} - \xi \dot{B} \dot{\phi} + \nabla B \cdot \nabla \phi + \frac{\lambda}{2} B^2 + \xi \dot{\bar{C}} \dot{C} - \nabla \bar{C} \cdot \nabla C + \tilde{\xi} \dot{\bar{H}} \dot{H} - \nabla \bar{H} \cdot \nabla H + \mathcal{O}(g).$$
(5.1)

With the variables we have chosen, gauge invariance simply means invariance under the transformations $\delta_{\Lambda}\phi = \Lambda = \theta C$, $\delta_{\Lambda}\bar{C} = \theta B$, all the other fields being inert. Note that the first line of (5.1) is manifestly invariant, to the lowest order, as are the first two terms of the second line and the *H*dependent terms, while the remaining terms transform into one another. Thus, we are in the conditions of Sec. III.

The field variables are $\hat{\Phi} \equiv (\phi, B, A^0, \mathbf{A}, C, \overline{C}, H, \overline{H})$. From the moment, we ignore H and \overline{H} , and restrict to $\tilde{\Phi} \equiv (\phi, B, A^0, \mathbf{A}, C, \overline{C})$, because it is straightforward to treat H and \overline{H} along the lines of Ref. [1]. We discuss them anyway in the next section, when we include the interactions. For the time being, we also drop $\mathcal{O}(g)$.

The boundary conditions read

$$\tilde{\Phi}_{|_{\partial\Omega}} = (\phi_0, B_0, A_0^0, \mathbf{A}_0, C_0, \bar{C}_0),$$
(5.2)

where the list on the right-hand side collects given functions on $\partial\Omega$. We can turn to vanishing boundary conditions by means of shifts

$$\tilde{\Phi} \to \tilde{\Phi} + \tilde{\Phi}_0,$$
 (5.3)

where $\tilde{\Phi}_0$ are functions defined on the whole of Ω , which coincide with the right-hand side of (5.2) on $\partial\Omega$. This way, the new $\tilde{\Phi}$ vanish on $\partial\Omega$. Since the shift does not change the quadratic sector of the free Lagrangian, on which we are concentrating in the present section, we take $\tilde{\Phi}|_{\partial\Omega} = \tilde{\Phi}_0 =$ 0 for the moment, and leave the rest of the discussion to the next section. Note that $\tilde{\Phi}|_{\partial\Omega} = 0$ allows us to freely integrate the space integrals by parts.

The momenta, which are

$$\pi_{\phi} = -\xi \dot{B}, \qquad \pi_{B} = -\xi (\dot{\phi} + A^{0}), \qquad \pi_{A^{0}} = -\frac{\tilde{\xi}}{\tilde{\lambda}} (\tilde{\xi} \dot{A}^{0} + \nabla \cdot \mathbf{A}),$$

$$\pi_{A} = \dot{\mathbf{A}} + \nabla A^{0}, \qquad \pi_{\tilde{C}} = \xi \dot{\bar{C}}, \qquad \pi_{C} = \xi \dot{C}, \qquad (5.4)$$

are either gauge invariant, or transform into one another:

$$\delta_{\Lambda}\pi_{B} = -\theta\pi_{C}, \qquad \delta_{\Lambda}\pi_{\bar{C}} = -\theta\pi_{\phi}, \qquad \delta_{\Lambda}\pi_{\phi} = \delta_{\Lambda}\pi_{A_{0}} = \delta_{\Lambda}\pi_{A} = \delta_{\Lambda}\pi_{C} = 0.$$
(5.5)

The Hamiltonian is $H = H_{\text{bos}} + H_{\text{gh}}$, where

$$\begin{split} H_{\text{bos}} &= -\frac{1}{\xi} \pi_{\phi} (\pi_{B} + \xi A^{0}) - \frac{1}{2\tilde{\xi}} \pi_{A^{0}} \left(\frac{\tilde{\lambda}}{\tilde{\xi}} \pi_{A^{0}} + 2 \nabla \cdot \mathbf{A} \right) + \frac{1}{2} \pi_{A} (\pi_{A} - 2 \nabla A^{0}) \\ &+ \frac{1}{4} F_{ij}^{2} - \nabla B \cdot \nabla \phi + \nabla B \cdot \mathbf{A} - \frac{\lambda}{2} B^{2}, \qquad H_{\text{gh}} = \frac{1}{\xi} \pi_{\bar{C}} \pi_{C} + \nabla \bar{C} \cdot \nabla C, \end{split}$$

so the extended Lagrangian L' of formula (3.6) is

$$L' = L'_{\text{bos}} + L'_{\text{gh}}, \qquad L'_{\text{bos}} = \frac{1}{2} (\pi_{\Phi} \dot{\Phi} - \dot{\pi}_{\Phi} \Phi) - H_{\text{bos}}, \qquad L'_{\text{gh}} = \frac{1}{2} (\pi_{\bar{C}} \dot{C} - \dot{\pi}_{\bar{C}} C + \dot{\bar{C}} \pi_{C} - \bar{C} \dot{\pi}_{C}) - H_{\text{gh}}, \tag{5.6}$$

where $\Phi = (\phi, B, A^0, \mathbf{A})$.

As explained in the previous two sections, it is convenient to introduce the shifted momenta (3.10), or (3.42), which are

$$\bar{\pi}_{A_0} = \pi_{A_0} + \frac{\tilde{\xi}}{\tilde{\lambda}} \nabla \cdot \mathbf{A} = -\frac{\tilde{\xi}^2}{\tilde{\lambda}} \dot{A}^0, \qquad \bar{\pi}_A = \pi_A - \nabla A^0 = \dot{\mathbf{A}}, \tag{5.7}$$

while the other momenta are unchanged. Defining $\bar{\Pi} = (\pi_{\phi}, \pi_B, \bar{\pi}_{A_0}, \bar{\pi}_A)$, the general form of the Lagrangian L'_{bos} is

$$L_{\text{bos}}' = \frac{1}{2} (\bar{\Pi} \quad \Phi) \begin{pmatrix} M & K_2 + \partial_t \\ K_2^T - \partial_t & N \end{pmatrix} \begin{pmatrix} \bar{\Pi} \\ \Phi \end{pmatrix}, \qquad M = \begin{pmatrix} 0 & \frac{1}{\xi} & 0 & 0 \\ \frac{1}{\xi} & 0 & 0 & 0 \\ 0 & 0 & \frac{\tilde{\lambda}}{\xi^2} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

where K_2 is a constant matrix and K_2^T is its transpose, while $N = N_1^{ij} \partial_i \partial_j + N_2^i \partial_i \partial_t + N_3^i \partial_i + N_4$, where N_1^{ij} , N_2^i , N_3^i and N_4 are other constant matrices. We do not specify them here (and, besides, most of their entries are just zero, as in *M*), since they can be read directly from (5.6). It is sufficient to note that N_1^{ij} , N_2^i , and N_4 are symmetric, while N_3^i are antisymmetric.

Ultimately, we are in the situation described in general terms in Sec. III A. We have eigenfunctions $\overline{\Pi}_n$, Φ_n , with (real) frequencies ω_n , where *n* is some label ranging in some set \mathcal{V} . The complex conjugate eigenfunctions are those with some "conjugate" label n^* , i.e.,

$$\bar{\Pi}_n^*(\mathbf{x}) = \bar{\Pi}_{n^*}(\mathbf{x}), \qquad \Phi_n^*(\mathbf{x}) = \Phi_{n^*}(\mathbf{x}), \qquad \omega_{n^*} = -\omega_n.$$

We then expand $\overline{\Pi}$ and Φ in such a basis:

$$\begin{pmatrix} \bar{\Pi} \\ \Phi \end{pmatrix} = \sum_{n \in \mathcal{V}} a_n \begin{pmatrix} \bar{\Pi}_n \\ \Phi_n \end{pmatrix}, \tag{5.8}$$

with $a_{n^*} = a_n^*$. As before, we write $\mathcal{V} = \mathcal{U} \cup \mathcal{U}^*$, so that each pair n, n^* is split between \mathcal{U} and \mathcal{U}^* . The orthonormality relations are (3.16). Using them, we can invert (5.8) as in (3.18), and obtain the expansion of the integrated bosonic Lagrangian, which reads

$$\mathcal{L}_{\text{bos}}' \equiv \int_{\Omega} L_{\text{bos}}' \mathrm{d}^{3} \mathbf{x} = \sum_{n \in \mathcal{U}} i \tau_{n} \omega_{n} (a_{n}^{*} \dot{a}_{n} - \dot{a}_{n}^{*} a_{n}) - 2 \sum_{n \in \mathcal{U}} \tau_{n} \omega_{n}^{2} a_{n}^{*} a_{n}.$$
(5.9)

Since we have six independent fields (for every value of the Lie algebra index *a*), which are the components ϕ , *B*

and A_{μ} of Φ , we can distinguish six classes of frequencies ω_n . Two of them, which we denote by ω_n^{g} and $\omega_n^{g'}$, may depend on the gauge-fixing parameters ξ and λ , while the other four may depend on the parameters $\tilde{\xi}$ and $\tilde{\lambda}$, but not on ξ and λ .

Out of the four gauge independent frequencies, two are physical, denoted by $\omega_n^{\rm ph}$ and $\omega_n^{\rm ph'}$, and two must be quantized as purely virtual, denoted by $\omega_n^{\rm d}$ and $\omega_n^{\rm d'}$.

The distinction between the two classes of gauge independent frequencies is somewhat flexible. In the absence of data (which require us to make experiments about scattering processes where the restrictions to finite τ and compact Ω play crucial roles), the only theoretical constraints we have are that: (a) the eigenfunctions Π_n , Φ_n , associated with each set of frequencies $\omega_n^{\rm g}$, $\omega_n^{\rm g'}$, $\omega_n^{\rm ph}$, $\omega_n^{\rm ph'}$, $\omega_n^{\rm d}$, and $\omega_n^{\rm d'}$, make a complete set for some component of Π , Φ ; (b) altogether, they are a complete set for Π , Φ ; (c) the eigenfunctions have the right limits for $\Omega \to \mathbb{R}^3$. Such limits are $\tilde{\xi}$ and $\tilde{\lambda}$ independent for $\omega_n^{\rm ph}$, $\omega_n^{\rm ph'}$, $\tilde{\xi}$, and $\tilde{\lambda}$ dependent for $\omega_n^{\rm d}$ and $\omega_n^{\rm d'}$.

As an example of the flexibility we are referring to, we can consider linear combinations of solutions whose frequencies have the same limits for $\Omega \to \mathbb{R}^3$. As we show in the examples of Secs. VII and VIII, if the relative coefficients are appropriately oscillating, the mixing disappears when $\Omega \to \mathbb{R}^3$. This ambiguity reflects the large arbitrariness we have, when we formulate quantum field theory in a finite interval of time τ , on a compact space manifold Ω . Like the parameters $\tilde{\xi}$ and $\tilde{\lambda}$, different choices of the basis (7.2) may parametrize, in a way that remains to be clarified, different interplays between the physical process we want to study and the external environment where it is placed, or the apparatus we use to make the measurements.

In several cases, it may be helpful to first set $\tilde{\xi} = \tilde{\lambda} = 1$, where the frequencies and eigenfunctions simplify and can often be written explicitly, make the choices of basis there, and then extend the choices to $\tilde{\xi}, \tilde{\lambda} \neq 1$ by expanding in powers of $\delta_{\tilde{\xi}} = (\tilde{\xi} - 1)/2$ and $\delta_{\tilde{\lambda}} = (\tilde{\lambda} - 1)/2$.

The gauge dependent frequencies ω_n^g and $\omega_n^{g'}$ can be quantized as purely virtual or not, provided we implement this choice consistently everywhere. The physical quantities are unaffected by the choice, because they are gauge independent.

Writing $\mathcal{U} = \mathcal{U}_{g} \cup \mathcal{U}'_{g} \cup \mathcal{U}_{d} \cup \mathcal{U}'_{d} \cup \mathcal{U}_{ph} \cup \mathcal{U}'_{ph} \equiv \bigcup_{I=1}^{6} \mathcal{U}^{I}$, the expansion (5.8) becomes

$$\begin{pmatrix} \bar{\Pi} \\ \Phi \end{pmatrix} = \sum_{I=1}^{6} \sum_{n \in \mathcal{U}^{I}} \left[\begin{pmatrix} \bar{\Pi}_{n}^{I} \\ \Phi_{n}^{I} \end{pmatrix} z_{n}^{I} + \begin{pmatrix} \bar{\Pi}_{n}^{I*} \\ \Phi_{n}^{I*} \end{pmatrix} \bar{z}_{n}^{I} \right].$$
(5.10)

The coefficients are the coherent states

$$Z_n(t) = (z_n^g, z_n^{g'}, z_n^d, z_n^{d'}, z_n^{ph}, z_n^{ph'}) = (z_n^I) = (a_n).$$
(5.11)

The bosonic Lagrangian \mathcal{L}'_{bos} can be split accordingly.

The two gauge dependent frequencies ω_n^g and $\omega_n^{g'}$ are easy to calculate, since they must correspond, by the gauge symmetry, to those of the ghost Lagrangian L'_{gh} . Repeating the procedure described above for L'_{gh} , we find that the eigenfunctions we are talking about solve the standard problem

$$\Delta C_n(\mathbf{x}) = -\xi \omega_n^2 C_n(\mathbf{x}) \text{in} \Omega, \qquad C_n|_{\partial \Omega} = 0,$$

and come in two copies (ghosts and antighosts).

The gauge transformations of the coherent states can be derived from the ones of the fields and the momenta, combined with the expansion (5.10), as explained in Sec. III B. Since $\delta \phi = \theta C$, $\delta \bar{C} = \theta B$, there must be ϕ modes that transform into the ghost ones, and antighost modes that transform into the *B* ones. This means that the ϕ , *B*, *C*, and \bar{C} expansions have the structures

$$\begin{pmatrix} \phi \\ B \end{pmatrix} = \begin{pmatrix} \phi_n \\ 0 \end{pmatrix} z_{\phi n} + \begin{pmatrix} \phi_n^* \\ 0 \end{pmatrix} \bar{z}_{\phi n} + \begin{pmatrix} \psi_n \\ B_n \end{pmatrix} z_{Bn} + \begin{pmatrix} \psi_n^* \\ B_n^* \end{pmatrix} \bar{z}_{Bn} + \cdots$$
$$\begin{pmatrix} C \\ \bar{C} \end{pmatrix} = \begin{pmatrix} \phi_n \\ \psi_n' \end{pmatrix} z_{Cn} + \begin{pmatrix} \phi_n^* \\ \psi_n'^* \end{pmatrix} \bar{z}_{Cn} + \begin{pmatrix} 0 \\ B_n \end{pmatrix} z_{\bar{C}n} + \begin{pmatrix} 0 \\ B_n^* \end{pmatrix} \bar{z}_{\bar{C}n}.$$
(5.12)

where the sums on *n* are understood, the dots collect the contributions of the A^0 and **A** modes, and ψ_n and ψ'_n are unspecified functions. The coherent states denoted by $z_{\phi n}$ and $\bar{z}_{\phi n}$ do not contribute to the expansions of A^0 and **A**; the A^0 , **A** modes may contribute to the expansion of ϕ , but not to the one of *B*.

The only nontrivial gauge transformations of the coherent states are

$$\delta z_{\phi n} = \theta z_{Cn}, \qquad \delta \bar{z}_{\phi n} = \theta \bar{z}_{Cn}, \qquad \delta z_{\bar{C}n} = \theta z_{Bn}, \qquad \delta \bar{z}_{\bar{C}n} = \theta \bar{z}_{Bn}, \tag{5.13}$$

and the $\phi BC\bar{C}$ sector of the Lagrangian reads

$$L'_{\phi BC\bar{C}} = -\sum_{n} i\omega_{n}(\bar{z}_{Bn}\dot{z}_{\phi n} - \dot{\bar{z}}_{Bn}z_{\phi n} + \dot{z}_{Bn}\bar{z}_{\phi n} - z_{Bn}\dot{\bar{z}}_{\phi n}) + 2\sum_{n}\omega_{n}^{2}(\bar{z}_{Bn}z_{\phi n} + z_{Bn}\bar{z}_{\phi n}) + \sum_{n} i\omega_{n}(\bar{z}_{\bar{C}n}\dot{z}_{Cn} - \dot{\bar{z}}_{\bar{C}n}z_{Cn} + \dot{z}_{\bar{C}n}\bar{z}_{Cn} - z_{\bar{C}n}\dot{\bar{z}}_{Cn}) - 2\sum_{n}\omega_{n}^{2}(\bar{z}_{\bar{C}n}z_{Cn} + z_{\bar{C}n}\bar{z}_{Cn}).$$
(5.14)

VI. GAUGE THEORIES: INTERACTIONS

Now that we have taken care of the quadratic part, we are ready to include the interactions. Working out the momenta π_{Φ} from the Lagrangian (4.6), we obtain

$$\begin{aligned} \pi_B^a &= -\xi \tilde{A}^{0a}, \qquad \pi_{A^0}^a = -\frac{\tilde{\xi}^2}{\tilde{\lambda}} \dot{A}^0 - \frac{\tilde{\xi}}{\tilde{\lambda}} \nabla \cdot \mathbf{A}, \qquad \mathbf{\pi}_A^a = \mathbf{F}^a, \\ \pi_{\tilde{C}} &= \xi \frac{1 - \mathrm{e}^{-ig\,\mathrm{ad}_\phi}}{ig\,\mathrm{ad}_\phi} \dot{C}, \qquad \pi_C^a = \xi \frac{\delta \tilde{A}^{0a}}{\delta \phi^b} C^b, \qquad \pi_{\tilde{H}}^a = \tilde{\xi} \dot{H}^a, \qquad \pi_H^a = \tilde{\xi} D_0 H^a. \end{aligned}$$

plus π_{ϕ} , which we do not report here, because its expression can be read from the gauge transformations, which, by (3.4), are still (4.7) and (5.5): $\theta \pi_{\phi} = -\delta \pi_{\bar{C}}$.

Then, we make the redefinition (3.10). The only changes are

$$\bar{\boldsymbol{\pi}}_{A_0}^a = \boldsymbol{\pi}_{A_0}^a + \frac{\tilde{\boldsymbol{\xi}}}{\tilde{\boldsymbol{\lambda}}} \boldsymbol{\nabla} \cdot \mathbf{A}^a = -\frac{\tilde{\boldsymbol{\xi}}^2}{\tilde{\boldsymbol{\lambda}}} \dot{A}^0,$$
$$\bar{\boldsymbol{\pi}}_A^a = \boldsymbol{\pi}_A^a - \boldsymbol{\nabla} A^{0a} = \dot{\mathbf{A}}^a + g f^{abc} A^{0b} \mathbf{A}^c.$$
(6.1)

Since the differences between $\pi_{\hat{\Phi}}$ and $\bar{\pi}_{\hat{\Phi}}$ are gauge invariant, the gauge transformations of the new variables $\bar{\pi}_{\hat{\Phi}}$ and $\hat{\Phi}$ are simply

$$\delta \phi = \Lambda = \theta C, \qquad \delta \bar{C} = \theta B,$$

$$\delta \bar{\pi}_B = -\theta \bar{\pi}_C, \qquad \delta \bar{\pi}_{\bar{C}} = -\theta \bar{\pi}_{\phi}, \qquad (6.2)$$

the other fields $\bar{\pi}_{\hat{\Phi}}$ and $\hat{\Phi}$ being invariant.

The case of trivial boundary conditions $\hat{\Phi}|_{\partial\Omega} = 0$, which are evidently gauge invariant, can be treated straightforwardly. The quadratic Lagrangian, which defines the coherent states and the expansions of the fields, is the one of the previous section. The interacting sector \mathcal{L}'_{int} of the total action (3.23) can be easily expressed in terms of coherent states, since it does not depend on their time derivatives.

The most general boundary conditions are $\hat{\Phi}|_{\partial\Omega} = \hat{f}$, where \hat{f} is a row of given functions on $\partial\Omega$. To build physical amplitudes, we must choose a gauge invariant and gauge nontrivial \hat{f} , which means set $\phi = B = C = \bar{C} = 0$ on $\partial\Omega$. Since there are no theoretical or practical motivations to relax these requirements, from now on we adopt the boundary conditions

$$\hat{\Phi}|_{\partial\Omega} = (0, 0, A_0^0, \mathbf{A}_0, 0, 0, H_0, \bar{H}_0).$$
(6.3)

Then we make the shifts

$$\hat{\Phi} \rightarrow \hat{\Phi} + \hat{\Phi}_0,$$
 (6.4)

where $\hat{\Phi}_0$ are functions defined on the whole of Ω , with the sole requirement that they coincide with the right-hand side of (6.3) on $\partial\Omega$. After the shift, the boundary conditions are $\hat{\Phi}|_{\partial\Omega} = 0$, the gauge transformations are still (4.7), and we can freely integrate the space integrals by parts, to move space derivatives away from any field.

It is important to stress that the conditions (6.3) apply to the Lagrangian (4.6), before even talking about momenta, so we do not have to worry about the behaviors of the momenta on $\partial\Omega$ at this stage.

Take the Lagrangian (4.6), and denote it by $L_{\text{tot}}(\hat{\Phi}) = L_{\text{free}}(\hat{\Phi}) + L_{\text{int}}(\hat{\Phi})$. Once we implement the shift (6.4) on it, we obtain

$$L_{\text{tot}}(\hat{\Phi} + \hat{\Phi}_0) = L_{\text{tot}}(\hat{\Phi}_0) + A(\hat{\Phi}_0)\hat{\Phi} + B(\hat{\Phi}_0)\hat{\Phi} + \nabla(\hat{\Phi}C(\hat{\Phi}_0)) + L(\hat{\Phi}, \hat{\Phi}_0),$$
(6.5)

where $L(\hat{\Phi}, \hat{\Phi}_0) = L_{\text{free}}(\hat{\Phi})$ + interactions. We can ignore the term $\nabla(\hat{\Phi}C(\hat{\Phi}_0))$, since it disappears as soon as we integrate on the space manifold Ω . The quadratic sector of $L_{\text{tot}}(\hat{\Phi} + \hat{\Phi}_0)$ coincides with $L_{\text{free}}(\hat{\Phi})$, which is the one of $L_{\text{tot}}(\hat{\Phi})$, up to interactions.

Next, we proceed as explained in Sec. III C. We define the momenta, redefine them according to (3.42) (that is to say, according to (6.1) with $\pi \to \tilde{\pi}, \bar{\pi} \to \tilde{\pi}$), and get to the extended Lagrangian \tilde{L}'_{φ} . Since the quadratic sector of (6.5) is $L_{\text{free}}(\hat{\Phi})$, the eigenfunctions coincide with those we had with trivial boundary conditions. So do the expansions in terms of coherent states (5.11). Once we integrate the Lagrangian and include endpoint corrections, to have the correct variational problem, the final action is (3.43), which just contains some linear corrections (and possibly different interactions) with respect to the action (3.23).

Once we have the action, the theory can be phrased diagrammatically. The diagrams are of the usual type, apart from the presence of external sources and the discretizations of the loop momenta [1].

When we want a transition amplitude, we must choose initial and final conditions $z_n^I(t_i) = z_{ni}^I$, $\bar{z}_n^I(t_f) = \bar{z}_{nf}^I$ for the coherent states. The physical degrees of freedom are the transverse components of **A**, which must be quantized as physical particles. Their initial and final conditions z_{ni}^{ph} , z_{ni}^{ph} , \bar{z}_{nf}^{ph} , and $\bar{z}_{nf}^{ph'}$ are free.

The gauge degrees of freedom are ϕ , *B*, *C*, and \overline{C} . They can be quantized as purely virtual or not, provided the choice is implemented consistently everywhere. Their initial and final conditions are trivial, i.e.,

$$z_{ni}^{g} = z_{ni}^{g'} = \bar{z}_{nf}^{g} = \bar{z}_{nf}^{g'} = 0,$$
 (6.6)

and similarly for *C* and \overline{C} .

The purely virtual fields are A^0 , H, \bar{H} , and the longitudinal components of **A**. They are quantized as purely virtual particles, by removing their on-shell contributions to the diagrams perturbatively to all orders, according to the rules of Refs. [2,11], and setting the initial and final conditions of the coherent states associated with them to zero. This means

$$z_{ni}^{d} = z_{ni}^{d'} = \bar{z}_{nf}^{d} = \bar{z}_{nf}^{d'} = 0,$$
 (6.7)

and similarly for H and \overline{H} .

The decomposition of **A** into "transverse" and "longitudinal" components is defined by the arrangement (5.10), after identifying the (physical vs purely virtual) eigenfunctions (5.11) and their frequencies. We illustrate these facts in the examples of the next two sections.

Note that we do not need to disentangle the physical and purely virtual degrees of freedom on $\partial\Omega$, because purely virtual particles are not required to have trivial boundary conditions [1]. The freedom associated with their boundary

conditions may describe some sort of interaction between the observer, or the environment, and the physical process we are observing.

The unitarity equation $U^{\dagger}U = 1$ holds under appropriate assumptions (such as the cancellation of the gauge anomalies at one loop). An easy way to prove the statement is to formulate the gauge sector (identified by the fields ϕ , *B*, *C*, and \overline{C}) as purely virtual, as in [21], because then we know that it does not contribute to the product in between U^{\dagger} and *U*.

Normally, instead, the fields of the gauge sector are treated as physical fields (because the gauge symmetry ensures that they mutually compensate inside the physical quantities). Then the product between U^{\dagger} and U is a sum over a complete set of states, which includes the gauge non invariant ones. Those states are studied by relaxing the initial and final conditions (6.6) on the gauge sector.

VII. GAUGE THEORIES ON THE SEMI-INFINITE CYLINDER

In this section and the next one we illustrate the general theory in the cases $\Omega = \text{semi-infinite cylinder}$ and $\Omega = \text{finite cylinder}$, concentrating on the frequencies and the eigenfunctions. We have seen that, once we have those, we can proceed straightforwardly. We choose the special gauges $\xi = \lambda$, $\tilde{\xi} = \tilde{\lambda}$, to simplify the calculations. This allows us to keep one free parameter (λ) in the gauge sector and one ($\tilde{\lambda}$) in the purely virtual sector.

We denote the semi-infinite cylinder by $\Omega = S^1 \times [-\ell, \infty)$, while *r* is the radius of the circle S^1 . Using cylindrical coordinates θ , *z*, we have

$$\mathbf{A}(t,\theta,z) = \hat{\mathbf{\theta}}A_{\theta}(t,\theta,z) + \hat{\mathbf{z}}A_{z}(t,\theta,z), \quad \nabla = \frac{\hat{\mathbf{\theta}}}{r}\frac{\partial}{\partial\theta} + \hat{\mathbf{z}}\frac{\partial}{\partial z}.$$

It is convenient to reach the semi-infinite cylinder from the infinite cylinder ($\ell = \infty$). We recall that the Lagrangian is (5.1) and the momenta are (5.4), while the shifted momenta are (5.7). Defining $\Phi = (\phi, B, A^0, A_{\theta}, A_z)$, we search for eigenfunctions of the form

$$\Phi(t,\theta,z) = \bar{\Phi}_0 e^{i\hat{p}x} e^{in\theta} e^{-it\hat{\omega}/r}, \qquad (7.1)$$

where $\overline{\Phi}_0$ denotes a row of constants, while x = z/r, $n \in \mathbb{Z}$, \hat{p} is a rescaled momentum and $\hat{\omega}$ is a rescaled frequency. Inserting (7.1) into the field equations derived from (5.1), the system has solutions when the frequencies are

$$\hat{\omega}^{\rm g} = \frac{1}{\sqrt{\lambda}} \sqrt{n^2 + \hat{p}^2}, \ \hat{\omega}^{\rm d} = \frac{1}{\sqrt{\tilde{\lambda}}} \sqrt{n^2 + \hat{p}^2}, \ \hat{\omega}^{\rm ph} = \sqrt{n^2 + \hat{p}^2}.$$

Two degeneracies are present, since the gauge-dependent (i.e., λ -dependent) frequencies $\hat{\omega}^{g}$ and the $\tilde{\lambda}$ -dependent frequencies $\hat{\omega}^{d}$ appear twice. Instead, the physical

frequency $\hat{\omega}^{ph}$ appears once. The independent solutions for the five components of Φ are ten: five correspond to the particles and five correspond to the antiparticles. We do not write their expressions explicitly. It is sufficient to recall that the most general solution contains 10 arbitrary constants.

Now we move to the semi-infinite cylinder. Since the *x* dependence of the solutions (7.1) is as simple as $e^{i\hat{p}x}$, they cannot satisfy the boundary conditions $\Phi(t, \theta, -\ell) = 0$ on $\Omega = S^1 \times [-\ell, \infty)$, if they are taken separately. However, if we take linear combinations of functions (7.1) with the same $\hat{\omega}$, we can impose the conditions $\Phi(t, \theta, -\ell) = 0$ on them. This way, the number of arbitrary coefficients gets reduced to a half. Ultimately, we obtain five independent solutions, or a solution with five arbitrary coefficients.

Omitting the overall factor $e^{in\theta}e^{-it\hat{\omega}/r}$ and the arbitrary constant in front, the physical solution reads

$$\phi = 0, \qquad B = \frac{(\lambda - \tilde{\lambda})\hat{\omega}^2}{\tilde{\lambda}\hat{p}_{\beta}}\sin\beta, \qquad A_0 = -\frac{i\lambda\hat{\omega}}{\tilde{\lambda}\hat{p}_{\beta}}\sin\beta,$$
$$A_{\theta} = -\frac{i}{n}\left(\hat{p}_{\alpha}\sin\alpha + \frac{n^2}{\hat{p}_{\beta}}\sin\beta\right), \qquad A_z = \cos\alpha - \cos\beta,$$

where

$$\begin{split} \alpha &= (z+\ell)\frac{\hat{p}_{\alpha}}{r}, \qquad \beta = (z+\ell)\frac{\hat{p}_{\beta}}{r}\\ \hat{\omega}^2 &= \hat{p}_{\alpha}^2 + n^2 = \frac{1}{\lambda}(\hat{p}_{\beta}^2 + n^2). \end{split}$$

We see that λ -dependent contributions are present, but they are just pure gauge, since the field strength $F = \partial_z A_\theta - \partial_\theta (A_z/r)$ is λ independent. It would be impossible to fulfill the boundary conditions of the semi-infinite cylinder without a pure gauge part.

To study the limit $\ell \to \infty$, we multiply the solution by factors such as $2e^{\pm i\ell \hat{p}_a}$, and drop all the oscillating terms when ℓ gets large. The results are

$$\phi, B, A^0 \to 0, \qquad A_\theta \to \mp \frac{\hat{p}_\alpha}{n} e^{\pm i x \hat{p}_\alpha}, \qquad A_z \to e^{\pm i x \hat{p}_\alpha},$$

which coincide with the physical solutions at $\ell = \infty$. If, instead, we multiply by $2e^{\mp i\ell \hat{p}_{\beta}}$ and repeat the same procedure, we obtain an $\ell = \infty$ pure-gauge solution. The other $\ell = \infty$ solutions are obtained in similar ways from the general $\ell < \infty$ solution.

We can identify a solution by the integer *n*, a momentum \hat{p} (e.g., \hat{p}_{α} in the example above) and a dispersion relation giving the frequency $\hat{\omega}$ in terms of *n* and \hat{p} . When we switch to coherent states, we can label them as

$$Z_{\hat{p}n} = (z_{\hat{p}n}^{g}, z_{\hat{p}n}^{g'}, z_{\hat{p}n}^{d}, z_{\hat{p}n}^{d'}, z_{\hat{p}n}^{ph}).$$
(7.2)

The physical solutions correspond to $z_{\hat{p}n}^{\text{ph}}$, and are quantized as physical particles. We can quantize all the other components of $Z_{\hat{p}n}$ as purely virtual particles. This means that we give them trivial initial and final conditions, and remove the on-shell contributions due to them, inside the diagrams, perturbatively to all orders, with the procedures of [2,11].

The free action is

$$S_{\text{free}} = -i \int \frac{\mathrm{d}\hat{p}}{2\pi} \sum_{n \in \mathbb{Z}} (\bar{Z}_{\hat{p}nf} \Theta_{\hat{p}n} \Omega_{\hat{p}n} Z_{\hat{p}n}(t_{\text{f}}) + \bar{Z}_{\hat{p}n}(t_{\text{i}}) \Theta_{\hat{p}n} \Omega_{\hat{p}n} Z_{\hat{p}n\text{i}}) + \int_{t_{\text{i}}}^{t_{\text{f}}} \mathrm{d}t \int \frac{\mathrm{d}\hat{p}}{2\pi} \sum_{n \in \mathbb{Z}} [i(\bar{Z}_{\hat{p}n} \Theta_{\hat{p}n} \Omega_{\hat{p}n} \dot{Z}_{\hat{p}n} - \dot{\bar{Z}}_{\hat{p}n} \Theta_{\hat{p}n} \Omega_{\hat{p}n} Z_{\hat{p}n}) - 2\bar{Z}_{\hat{p}n} \Theta_{\hat{p}n} \Omega_{\hat{p}n}^2 Z_{\hat{p}n}],$$
(7.3)

where $\Omega_{\hat{p}n}$ is the diagonal matrix of the frequencies, while $\Theta_{\hat{p}n}$ is the diagonal matrix of the factors $\tau_n = \pm 1$ of (3.16).

As we have explained in the previous sections, there is a certain liberty in choosing the decomposition (7.2), since the only constraints are that: (a) each set is complete for some field Φ (i.e., it can be used to expand the field, in order to functionally integrate over it); (b) altogether, the eigenfunctions form a complete set for the fields Φ and the momenta $\bar{\pi}_{\Phi}$; and (c) the eigenfunctions have the right limits for $\ell \to \infty$.

Note that the solutions of the semi-infinite cylinder contain five arbitrary real constants, while those of the infinite cylinder contain twice as many. They are doubled by the sign choices in the multiplying factors $e^{\pm i\ell \hat{p}_a}$, $e^{\pm i\ell \hat{p}_{\beta}}$, etc., which are used for the large ℓ limit.

It may be puzzling that the number of integration variables of the functional integral "doubles" in the limit $\ell \to \infty$, so to speak. Actually, the number of variables is infinite, so we cannot really say that it doubles. It is convenient to explain what happens in detail, since similar instances are met frequently. Consider the Laplacian on the segment $[0, \ell]$ with Dirichlet boundary conditions. We have the eigenfunctions $\sin(\pi nx/\ell)$, $n \in \mathbb{Z}$, $x \in [0, \ell]$. They "double" in the limit $\ell \to \infty$, because, after centering the segment by means of the shift $x = y + (\ell/2)$, one has to distinguish the cases n = even and n = odd, which give different eigenfunctions for $\ell \to \infty$ (sines and cosines, respectively). Similarly, $\sin(\ell \hat{p}_{\alpha}) = \cos(\ell (\hat{p}_{\alpha} - \pi/(2\ell)))$, so the doubling comes from negligible shifts of \hat{p}_{α} , or ω , which give other eigenfunctions with the same dispersion relation for $\ell \to \infty$.

The experimental data we have today, which mainly concern *S* matrix amplitudes, are not sufficient to guide us uniquely through the wide freedom we face when $\tau < \infty$ on a compact Ω . Probably, changing the basis of physical and purely virtual frequencies in (7.2) is equivalent to twisting the boundary conditions, or having different interplays between the experimental setup and the physical process. At any rate, once we make our choices of initial, final and boundary conditions, as well as the basis (7.2), everything else is uniquely determined.

VIII. GAUGE THEORIES ON A CYLINDER

In this section we study gauge theories on a cylinder $\Omega = S^1 \times [-\ell/2, \ell/2]$. We start again from the parametrization (7.1) for the solutions of the field equations of the infinite cylinder. Then we superpose solutions with the same frequency, and impose the boundary conditions $\Phi(t, \theta, -\ell/2) = \Phi(t, \theta, \ell/2) = 0$. We find, as expected, that it is not sufficient to reduce the set of independent coefficients, as it was for the semi-infinite cylinder, but we must also discretize the frequencies.

Specifically, we insert

$$\Phi(t,\theta,z) = \tilde{\Phi}(x) \mathrm{e}^{in\theta} \mathrm{e}^{-it\hat{\omega}/r}$$

into the equations, where x = z/r, $n \in \mathbb{Z}$, and $\tilde{\Phi}(x)$ are linear combinations of

 $e^{\pm ix\sqrt{\hat{\omega}^2 - n^2}}, \qquad e^{\pm ix\sqrt{\hat{\lambda}\hat{\omega}^2 - n^2}}, \qquad e^{\pm ix\sqrt{\hat{\lambda}\hat{\omega}^2 - n^2}}.$

We fix the coefficients of the linear combinations by means of the boundary conditions, after determining the frequencies $\hat{\omega}$ that admit nontrivial solutions.

The \tilde{B} equation is independent of the other variables, and just reads

$$\tilde{B}'' = (n^2 - \lambda \hat{\omega}^2) \tilde{B}, \qquad (8.1)$$

where the prime denotes the derivative with respect to x. Moreover, $\tilde{\phi}$ does not enter any equation apart from its own, which reads

$$\tilde{\phi}'' = (n^2 - \lambda \hat{\omega}^2) \tilde{\phi} + \Delta_{\tilde{\phi}}, \qquad (8.2)$$

where $\Delta_{\tilde{\phi}}$ vanishes when all the other fields vanish. The \tilde{A}_0 equation depends on \tilde{A}_0 and \tilde{B} , while the equations of \tilde{A}_{θ} and \tilde{A}_z depend on \tilde{A}_{θ} , \tilde{A}_z , and \tilde{B} .

The gauge-dependent frequencies are

$$\hat{\omega}_{kn}^{\mathsf{g}} = \frac{1}{\sqrt{\lambda}} \sqrt{k^2 \frac{\pi^2 r^2}{\ell^2} + n^2}, \qquad n \in \mathbb{Z}, \qquad k \in \mathbb{N}_+.$$

They are associated with two eigenfunctions. One is

$$\tilde{\phi}_{kn} = \sin\left(k\pi\frac{\hat{z}}{\ell}\right), \qquad \tilde{B}_{kn} = \tilde{A}^0_{kn} = \tilde{A}_{\theta kn} = \tilde{A}_{zkn} = 0,$$
(8.3)

where $\hat{z} = z - (\ell/2)$, and the other one is

$$\tilde{B}_{kn} = \sin\left(k\pi \frac{\hat{z}}{\ell}\right),$$

with nontrivial $\tilde{\phi}_{kn}, \tilde{A}^0_{kn}, \tilde{A}_{\theta kn}$, and \tilde{A}_{zkn} . (8.4)

We omit the expressions of the nontrivial fields here, since they are not crucial for our discussion. The solutions (8.4) are the only ones with a nontrivial \tilde{B} .

The solutions (8.3) and (8.4) are those which, by gauge invariance, match the eigenfunctions of the ghosts C and \bar{C} . Let us recall that the gauge transformations are $\delta_{\Lambda}\phi = \Lambda =$ θC and $\delta_{\Lambda}\bar{C} = \theta B$. This means that there must exist Φ eigenfunctions that are made of ϕ only, and match the Ceigenfunctions: these are (8.3). Moreover, there must exist Φ eigenfunctions where B matches the \bar{C} eigenfunctions: these are (8.4). Said in different words, the coherent states that multiply the solution (8.3) transform into the Ccoherent states, while the \bar{C} coherent states transform into the coherent states that multiply the solution (8.4), as explained in the last part of Sec. V.

The other frequencies are gauge independent, but depend on $\tilde{\lambda}$. Among those, we have the simple frequencies

$$\hat{\omega}_{kn}^{\mathrm{d}} = \frac{1}{\sqrt{\lambda}} \sqrt{k^2 \frac{\pi^2 r^2}{\ell^2} + n^2}, \qquad n \in \mathbb{Z}, \qquad k \in \mathbb{N}_+, \quad (8.5)$$

with solutions

$$\begin{split} \tilde{\phi}_{kn} &= \frac{i\lambda \tilde{A}_{kn}^{0}}{\hat{\omega}_{kn}^{d}(\tilde{\lambda}-\lambda)}, \qquad \tilde{A}_{kn}^{0} = \sin\left(k\pi \frac{\hat{z}}{\ell}\right), \\ \tilde{B}_{kn} &= \tilde{A}_{\theta kn} = \tilde{A}_{zkn} = 0. \end{split}$$

Then we have two other $\tilde{\lambda}$ -dependent frequencies, which are more involved. Their eigenfunctions have $\tilde{B}_{kn} = \tilde{A}_{kn}^0 = 0$, and nontrivial $\tilde{A}_{\theta kn}$, \tilde{A}_{zkn} and $\tilde{\phi}_{kn}$. It is straightforward to work them out at $\tilde{\lambda} = 1$, where the frequencies coincide with (8.5). We find $A_{\theta} = \sin(k\pi \hat{z}/\ell)$, $A_z = 0$, and $A_{\theta} = 0$, $A_z = \sin(k\pi \hat{z}/\ell)$.

When $\tilde{\lambda} \neq 1$ it is convenient to expand in powers of $\delta = (\tilde{\lambda} - 1)/2$. The frequencies are

$$\hat{\omega}_{kn}^{\text{ph}} = \sqrt{k^2 \frac{\pi^2 r^2}{\ell^2} + \frac{n^2}{\tilde{\lambda}(1+\delta^2)}} + O(\delta^3),$$
$$\hat{\omega}_{kn}^{d\prime} = \sqrt{k^2 \frac{\pi^2 r^2}{\tilde{\lambda}\ell^2} + \frac{n^2}{1+\delta^2}} + O(\delta^3),$$

and the solutions read

$$\begin{split} A_{\theta} &= \sin\left(\frac{k\pi\hat{z}}{\ell}\right) + O(\delta^2), \\ A_z &= i\left[\cos\left(\frac{k\pi\hat{z}}{\ell}\right) - \cos\left(\frac{k\pi\hat{z}}{\ell} + \frac{nz\delta}{r}\right)\right] + O(\delta^2), \end{split}$$

and

$$\begin{split} A_{\theta} &= i(-1)^{k} \bigg[\cos \bigg(\frac{k \pi \hat{z}}{\ell} \bigg) - \cos \bigg(\frac{k \pi \hat{z}}{\ell} + (-1)^{k} \frac{n z \delta}{r} \bigg) \bigg] \\ &+ O(\delta^{2}), \\ A_{z} &= \sin \bigg(\frac{k \pi \hat{z}}{\ell} \bigg) + O(\delta^{2}), \end{split}$$

respectively. For the reasons we have explained before, the distinction between the physical frequencies $\hat{\omega}_{kn}^{\text{ph}}$ and the purely virtual frequencies $\hat{\omega}_{kn}^{d'}$ is to some extent arbitrary.

Once we have the frequencies and the eigenfunctions, we can proceed as in Secs. III, IV, V, and VI, obtain the coherent-state action (3.43), and work out the evolution operator $U(t_{\rm f}, t_{\rm i})$ diagrammatically with the procedure of Ref. [1].

IX. EINSTEIN GRAVITY

In this section we study Einstein gravity. The Hilbert-Einstein action

$$-\frac{1}{16\pi G}\int \mathrm{d}^4x\sqrt{-g}R\tag{9.1}$$

contains double derivatives of the metric tensor, so it cannot be used as is to study quantum field theory in a finite interval of time τ on a compact manifold Ω . The wellknown "TT" action does not have this problem, but differs from (9.1) by a boundary term, which must be treated cautiously, in order to preserve general covariance. Moreover, in Sec. III we have emphasized that we need an orthodox symmetry. In particular, the Lagrangian must be invariant without adding total derivatives, which is not true for the Hilbert Lagrangian of (9.1).

The solution of these problems is as follows. First, we perform the purely virtual extension of ref. [4], at $\tau = \infty$, $\Omega = \mathbb{R}^3$. Then, we switch to the invariant metric tensor and trivialize the symmetry by means of a field redefinition. Third, we add (invariant) total derivatives and switch to the

 $\Gamma\Gamma$ action (built with the invariant metric tensor). Fourth, we restrict to finite τ and compact Ω with the procedure of Sec. III, introduce the coherent states, and work out the final action (3.43). Having trivialized the symmetry, these operations are invariant.

We begin by recalling the purely virtual extension of gravity at $\tau = \infty$, $\Omega = \mathbb{R}^3$, from [4]. The gauge-fixed action is⁶

$$\tilde{S}_{gf} = -\frac{1}{16\pi G} \int d^4x \sqrt{-g}R + \int B_{\mu}(G^{\mu}(g) - \lambda g^{\mu\nu}B_{\nu}) - \int \bar{C}_{\mu}\delta_{\xi}(G^{\mu}(g) - \lambda g^{\mu\nu}B_{\nu})|_{\xi^{\mu} \to C^{\mu}}, \qquad (9.2)$$

where λ is a gauge-fixing parameter, $G^{\mu}(g)$ is the gauge-fixing function, $\delta_{\xi}g^{\mu\nu} = \xi^{\rho}\partial_{\rho}g^{\mu\nu} - g^{\nu\rho}\partial_{\rho}\xi^{\mu} - g^{\mu\rho}\partial_{\rho}\xi^{\nu}$ is the variation of the inverse metric tensor under an infinitesimal diffeomorphism $\delta x^{\mu} = -\xi^{\mu}(x)$, C^{μ} are the Faddeev-Popov ghosts, \bar{C}_{μ} are the antighosts, and B_{μ} are Lagrange multipliers. For example, we can take $G^{\mu}(g) = \partial_{\nu}g^{\mu\nu}$, or the special gauge of Ref. [19], which is more convenient for various purposes, as it is in Yang-Mills theory.

Next, we introduce the extra vector $\zeta^{\mu}(x)$, which by definition transforms as

$$\delta_{\xi}\zeta^{\mu}(x) = \xi^{\mu}(x - \zeta(x)). \tag{9.3}$$

The right-hand side of (9.3) must be understood as a perturbative expansion in powers of ζ^{μ} . As usual, the Faddeev-Popov ghosts C^{μ} are introduced by writing $\xi^{\mu} = \theta C^{\mu}(x)$, where θ is a constant anticommuting parameter. Using ζ^{μ} , we can build the invariant metric tensor

$$g_{\mu\nu d}(x) = (\delta^{\rho}_{\mu} - \zeta^{\rho}_{,\mu}(x))(\delta^{\sigma}_{\nu} - \zeta^{\sigma}_{,\nu}(x))g_{\rho\sigma}(x - \zeta), \quad (9.4)$$

where $\zeta^{\rho}_{,\mu} \equiv \partial_{\mu} \zeta^{\rho}$.

The field ζ^{μ} must be accompanied by anticommuting partners \bar{H}_{μ} and H^{μ} , as well as Lagrange multipliers E_{μ} . To preserve unitarity, we require ζ^{μ} , \bar{H}_{μ} , H^{μ} , and E_{μ} to be purely virtual. As in the case of Yang-Mills theories, the extension amounts to introducing a certain expression in the functional integral, which is equivalent to "1" on the *S* matrix scattering amplitudes, and on the correlation functions of ordinary (which means ζ^{μ} -independent) insertions of invariant composite fields. However, it allows us to build new, physical correlation functions, such as those that contain insertions of the invariant metric tensor (9.4).

Inside the functional integral, the extension is a correction to the action, which reads

$$\begin{split} \tilde{S}_{\text{ext}} &= \int \mathrm{d}^4 x \, E_\mu (V^\mu(g,\zeta) - \tilde{\lambda} g^{\mu\nu}_{\mathrm{d}} E_\nu) \\ &+ \int \mathrm{d}^4 x \, \bar{H}_\mu \frac{\delta}{\delta \zeta^\rho} (V^\mu - \tilde{\lambda} g^{\mu\nu}_{\mathrm{d}} E_\nu) H^\rho, \quad (9.5) \end{split}$$

where $g_d^{\mu\nu}$ is the inverse of $g_{\mu\nu d}$, $V^{\mu}(g, \zeta)$ is an invariant function ($\delta_{\xi}V^{\mu} = 0$), and $\tilde{\lambda}$ is a free parameter. For example, we can take $V^{\mu} = \partial_{\nu}g_d^{\mu\nu}$, or a mirror of the special gauge. At this point, we make a change of field variables⁷

$$\begin{split} \zeta_{\rm d}^{\mu}(x) &= \zeta^{\mu}(x + \zeta_{\rm d}(x)), \qquad C_{\rm d}^{\mu} = (\delta_{\nu}^{\mu} + \zeta_{{\rm d},\nu}^{\mu})C^{\nu}, \\ H^{\mu} &= (\delta_{\nu}^{\mu} - \zeta_{,\nu}^{\mu})H_{\rm d}^{\nu}, \end{split} \tag{9.6}$$

on the total action $\tilde{S}_{\rm gf} + \tilde{S}_{\rm ext}$, to switch from $g_{\mu\nu}$, ζ^{μ} , C^{μ} , H^{μ} to $g_{\mu\nu d}$, $\zeta^{\mu}_{\rm d}$, $C^{\mu}_{\rm d}$, $H^{\mu}_{\rm d}$. We do not change the other fields. This way, we abandon the original metric tensor $g_{\mu\nu}$ in favor of the invariant one, $g_{\mu\nu d}$. Moreover, we trivialize the symmetry, since in the new variables the transformation of $\zeta^{\mu}_{\rm d}$ is just $\delta\zeta^{\mu}_{\rm d} = \xi^{\mu}_{\rm d} \equiv \theta C^{\mu}_{\rm d}$, while $g_{\mu\nu d}$, $C^{\mu}_{\rm d}$ and $H^{\mu}_{\rm d}$ are invariant by construction. The trivialized symmetry thus reads

$$\delta \zeta_{\rm d}^{\mu} = \theta C_{\rm d}^{\mu}, \quad \delta C_{\rm d}^{\mu} = 0, \quad \delta \bar{C}_{\mu} = \theta B_{\mu}, \quad \delta B_{\mu} = 0, \quad (9.7)$$

all the other fields being invariant.

Note that

$$-\frac{1}{16\pi G}\int \mathrm{d}^4x\sqrt{-g}R(g) = -\frac{1}{16\pi G}\int \mathrm{d}^4x\sqrt{-g_\mathrm{d}}R(g_\mathrm{d}),$$

by construction, where g_d inside $\sqrt{-g_d}$ is the determinant of $g_{\mu\nu d}$. At this point, we eliminate the double derivatives by switching to the $\Gamma\Gamma$ action, and restrict to a finite interval of time τ and a compact space manifold Ω :

$$S_{\Gamma\Gamma} = -\frac{1}{16\pi G} \int_{t_{\rm i}}^{t_{\rm f}} \mathrm{d}t \int_{\Omega} \mathrm{d}^3 \mathbf{x} \sqrt{-g_{\rm d}} g_{\rm d}^{\mu\nu} (\Gamma^{\alpha}_{\mu\lambda\mathrm{d}} \Gamma^{\lambda}_{\nu\alpha\mathrm{d}} - \Gamma^{\alpha}_{\mu\nu\mathrm{d}} \Gamma^{\lambda}_{\alpha\lambda\mathrm{d}}).$$

Note that the Lagrangian of this $\Gamma\Gamma$ action, which is built with the invariant metric tensor, is manifestly invariant, so it satisfies the identity (3.2).

The gauge-fixing sector must be rewritten as well, by adding total derivatives, in order to become invariant at the Lagrangian level. Taking $G^{\mu}(g) = \partial_{\nu}g^{\mu\nu}$ for definiteness, we write

$$S_{\rm gf} = S_{\Gamma\Gamma} - \int (g^{\mu\nu} - \eta^{\mu\nu})(\partial_{\nu}B_{\mu}) - \int \lambda B_{\mu}g^{\mu\nu}B_{\nu} + \int [\partial_{\nu}\bar{C}_{\mu} + \lambda\bar{C}_{\mu}B_{\nu}]\delta_{\xi}g^{\mu\nu}|_{\xi^{\mu}\to C^{\mu}}, \qquad (9.8)$$

where $g_{\mu\nu}$ and C^{μ} must be understood as functions of ζ_{d}^{μ} and C_{d}^{μ} , according to the change of variables defined by (9.6), and $\eta^{\mu\nu}$ is the flat-space metric. In (9.8) and (9.9) below, the

⁶Note some changes of notation with respect to Ref. [4].

⁷Note some different signs with respect to the notation of Ref. [4].

integral symbol stands for the dtd^3x integral restricted to the interval τ and the manifold Ω .

The extension (9.5) is rearranged as

$$S_{\text{ext}} = \int E_{\mu} (\partial_{\nu} g_{\text{d}}^{\mu\nu} - \tilde{\lambda} g_{\text{d}}^{\mu\nu} E_{\nu}) + \int (\partial_{\nu} \bar{H}_{\mu} + \tilde{\lambda} \bar{H}_{\mu} E_{\nu}) \delta_{\xi} g^{\mu\nu} |_{g^{\mu\nu} \to g_{\text{d}}^{\mu\nu}, \xi^{\mu} \to H_{\text{d}}^{\mu}}, \quad (9.9)$$

for $V^{\mu} = \partial_{\nu} g_{d}^{\mu\nu}$, after which we integrate E_{μ} away, and proceed as in the case of gauge theories.

We have taken $G^{\mu}(g) = \partial_{\nu}g^{\mu\nu}$ and $V^{\mu} = \partial_{\nu}g^{\mu\nu}_{d}$, for concreteness, but it is easy to adapt the formulas to the special gauge and its mirror, or other choices.

The total action is

$$S_{\rm tot} = S_{\rm gf} + S_{\rm ext}$$

and its symmetry is (9.7). At this point, we read the Lagrangian *L* from S_{tot} , and observe that it is orthodoxically symmetric, as is evident from the expression of (9.8), while the Lagrangian of (9.9) is manifestly invariant. Yet, *L* contains infinitely many time derivatives, due to the expansion of expressions like (9.3) in powers of ζ^{μ} .

The expansion around flat space is defined by writing $g_d^{\mu\nu} = \eta^{\mu\nu} + 2\kappa h_d^{\mu\nu}$, where $\kappa = \sqrt{8\pi G}$ and G is Newton's constant. If we make the replacements

$$\begin{split} C^{\mu}_{\rm d} &\to \kappa C^{\mu}_{\rm d}, \quad B_{\mu} \to \kappa^{-1} B_{\mu}, \quad \bar{C}_{\mu} \to \kappa^{-1} \bar{C}_{\mu}, \quad \lambda \to \lambda \kappa^{2}, \\ \zeta^{\mu}_{\rm d} \to \kappa \zeta^{\mu}_{\rm d}, \quad H^{\mu}_{\rm d} \to \kappa H^{\mu}_{\rm d}, \quad E_{\mu} \to \kappa^{-1} E_{\mu}, \quad \bar{H}_{\mu} \to \kappa^{-1} \bar{H}_{\mu} \\ \tilde{\lambda} \to \tilde{\lambda} \kappa^{2}, \end{split}$$

the perturbative expansion is the expansion in powers of κ .

Equations (9.6) show that $\zeta^{\mu} \to \kappa \zeta^{\mu}$ plus higher order corrections. The Taylor expansions of arguments such as $x^{\mu} - \zeta^{\mu}$ and $x^{\mu} + \zeta^{\mu}_{d}$ inside (9.3), (9.4) and (9.6) raise the

powers of κ by one unit for each derivative they generate on the fields. This means that we are in the situation described in appendix B. Applying the construction of Sec. III, with the rearrangement of appendix B, we build the correct action (3.43) for gravity restricted to a finite interval of time τ , on a compact space manifold Ω . Applying the procedure of [1], we build the evolution operator $U(t_{\rm f}, t_{\rm i})$ between arbitrary initial and final states, with arbitrary boundary conditions, preserving general covariance.

X. QUANTUM GRAVITY WITH PURELY VIRTUAL PARTICLES

The results of the previous section extend to quantum gravity with purely virtual particles, provided we replace the Hilbert-Einstein action with the appropriate action.

Since coherent states are "enemies" of higher derivatives, as we have learned repeatedly, we cannot adopt the higherderivative formulation of Ref. [8], where the Lagrangian density is made of the Hilbert-Einstein term *R*, plus the cosmological term, plus the quadratic terms R^2 and $R_{\mu\nu}R^{\mu\nu}$. We must start from the two-derivative formulation of ref. [22] at $\tau = \infty$, $\Omega = \mathbb{R}^3$, which we briefly recall here.

Besides the metric tensor $g_{\mu\nu}$, the theory contains a scalar field ϕ of mass m_{ϕ} (the inflaton) and a spin-2 purely virtual particle $\chi_{\mu\nu}$ of a certain mass m_{γ} . The action is

$$\begin{split} S_{\rm QG}(g,\phi,\chi,\Phi) &= S_{\rm HE}(g) + S_{\chi}(g,\chi) + S_{\phi}(g+\psi,\phi), \end{split} \eqno(10.1)$$

where

$$S_{\rm HE}(g) = -\frac{r}{16\pi G} \int \sqrt{-g} (2\Lambda_C + R), \quad r = \frac{m_\chi^2}{m_\phi^2} \frac{3m_\phi^2 + 4\Lambda_C}{3m_\chi^2 - 2\Lambda_C},$$

is the Hilbert-Einstein action with a cosmological constant Λ_C ,

$$S_{\phi}(g,\phi) = \frac{3}{4} \left(1 + \frac{4\Lambda_C}{3m_{\phi}^2} \right) \int \sqrt{-g} \left[D_{\mu}\phi D^{\mu}\phi - \frac{m_{\phi}^2}{8\pi G} (1 - e^{\phi\sqrt{8\pi G}})^2 \right]$$

is the inflaton action, and

$$S_{\chi}(g,\chi) = S_{\rm HE}(g+\psi) - S_{\rm HE}(g) + \int \left[-2\chi_{\mu\nu} \frac{\delta S_{\rm HE}(g)}{\delta g_{\mu\nu}} + \frac{rm_{\chi}^2}{16\pi G} \sqrt{-g} (\chi_{\mu\nu}\chi^{\mu\nu} - \chi^2) \right]_{g \to g+\psi}$$

is the $\chi_{\mu\nu}$ action, with

$$\psi_{\mu
u} = 2\chi_{\mu
u} + \chi_{\mu
u}\chi - 2\chi_{\mu
ho}\chi^{
ho}_{
u}, \qquad \chi = \chi_{\mu
u}g^{\mu
u}.$$

We gauge-fix (10.1) as in (9.2), and make the purely virtual extension as in (9.5). Then we switch from the variables $g_{\mu\nu}$, ϕ , $\chi_{\mu\nu}$, ζ^{μ} , C^{μ} , H^{μ} to the variables $g_{\mu\nu d}$, ϕ_{d} , $\chi_{\mu\nu d}$, ζ^{μ}_{d} , C^{μ}_{d} , H^{μ}_{d} , by means of (9.4), (9.6) and

$$\phi_{\rm d}(x) = \phi(x - \zeta(x)), \qquad \chi_{\mu\nu\rm d}(x) = (\delta^{\rho}_{\mu} - \zeta^{\rho}_{,\mu}(x))(\delta^{\sigma}_{\nu} - \zeta^{\sigma}_{,\nu}(x))\chi_{\rho\sigma}(x - \zeta)$$

The action (10.1) is invariant under the change of variables $g_{\mu\nu}, \phi, \chi_{\mu\nu} \rightarrow g_{\mu\nu d}, \phi_d, \chi_{\mu\nu d}$, which is just a diffeomorphism. This means that we can simply view (10.1) as a function of $g_{\mu\nu d}, \phi_d, \text{and } \chi_{\mu\nu d}$. Next, we add total derivatives to eliminate the terms like $\varphi_{1d} \cdots \varphi_{n-1d} \partial \partial \varphi_{dn}$ in favor of terms like $\varphi_{1d} \cdots \varphi_{n-2d} \partial \varphi_{n-1d} \partial \varphi_{nd}$, in the quadratic sector of the Lagrangian. Moreover, we rearrange the gauge-fixing part as in (9.8) and the purely virtual extension as in (9.9). At that point, we can identify the eigenfunctions and the coherent states. As far as the interaction sector is concerned, we rearrange it as explained in appendix B. Then we use the procedure of Sec. III to build the final action (3.43) for the restriction to finite τ and compact Ω . From that point onward, we can proceed as explained in Sec. III and Ref. [1], and build the evolution operator $U(t_{\rm f}, t_{\rm i})$ between arbitrary initial and final states, with arbitrary boundary conditions.

A. Unitarity in the presence of a cosmological constant

The cosmological constant Λ_C is nonvanishing, because renormalization turns it on anyway, even if we start from a vanishing Λ_C . A nonzero Λ_C raises some issues that we must address.

First of all, flat space is not a solution of the field equations (with $\phi = 0$, $\chi_{\mu\nu} = 0$), so it would be better to formulate perturbation theory by expanding the metric tensor $g_{\mu\nu}$ around a de Sitter or anti-de Sitter metric, according to the sign of Λ_C , rather than the flat-space metric. However, an expansion of that type does not allow an easy switch to energy/momentum space by means of Fourier transforms, and makes the calculations of loop diagrams, and the proofs of general theorems, very hard.

Since the physical results do not depend on the expansion we make, we may insist on using the expansion around flat space, in spite of its non standard features. For example, it generates one-leg vertices and a spurious graviton mass term, which can even be of tachyonic type, depending on the sign of Λ_C .

Whatever difficulties the expansion may generate, they are of a spurious nature, which means that they must compensate, and ultimately cancel out. In this spirit, the expansion around flat space is preferable, because its unusual features are simpler to deal with.

The other problem concerns the S matrix: we do not know how to define asymptotic states and S matrix amplitudes on nonflat spacetimes [23]. What about unitarity, then?

Although we cannot claim that the *S* matrix is unitary in a strict sense, when $\Lambda_C \neq 0$, we can still claim that it is unitary up to effects due to the cosmological constant [21]. Those effects are small for all practical purposes: a scattering process should involve wavelengths as large as the universe to be affected by Λ_C in a non negligible way.

Besides, now we have a simpler way out. Thanks to the results of this paper and [1], we are less dependent on the

paradigms that have dominated the scene since the birth of quantum field theory. In particular, we can study unitarity without being tied to the *S* matrix, by concentrating on the evolution operator $U(t_{\rm f}, t_{\rm i})$.

We have shown that we can build a unitary $U(t_{\rm f}, t_{\rm i})$ diagrammatically in a finite interval of time $\tau = t_{\rm f} - t_{\rm i}$, on a compact space manifold Ω , with arbitrary initial and final states, and arbitrary boundary conditions. The goal has been achieved both in Einstein gravity (which is not renormalizable, but this does not jeopardize its perturbative unitarity) and in quantum gravity with purely virtual particles (which is renormalizable and unitary). In the first case the cosmological constant can be added with no difficulty, and $U(t_{\rm f}, t_{\rm i})$ remains well-defined and unitary for every $\tau < \infty$. In the second case, the cosmological constant is already present by default.

This means that the cosmological constant does not have a problem with unitarity. It does have problems with the very notions of *S* matrix and asymptotic states. Given that the difficulties only appear in the $\tau \to \infty$ limit, the $\tau < \infty$ formalism we have developed here might suggest new ways to investigate asymptotic states in gravity with a cosmological constant.

XI. CONCLUSIONS

When we study gauge theories and gravity on a compact manifold, possibly with boundary, and on a finite interval of time, we face the nontrivial task of formulating the initial, final, and boundary conditions in invariant ways. The ordinary gauge potential A^{μ} and the metric tensor $g_{\mu\nu}$ are not straightforward to handle, in this respect. Nor are the field strength $F^{\mu\nu a}$, in non-Abelian gauge theories, or the curvature tensors R, $R_{\mu\nu}$, $R_{\mu\nu\rho\sigma}$, in gravity, because none of them is invariant.

The purely virtual extensions of gauge theories and gravity formulated in ref.s [3,4] come to the rescue, because they allow us to define invariant matter and gauge fields ψ_d and A_d^{μ} , and an invariant metric tensor $g_{\mu\nu d}$, without changing the ordinary physical quantities, such as the *S* matrix amplitudes and the correlation functions of non-linear invariant composite fields, like $F_{\mu\nu}^a F^{\mu\nu a}, \bar{\psi}\psi$, etc. Yet, they allow us to study new correlation functions, like those of the invariant fields ψ_d , A_d^{μ} , and $g_{\mu\nu d}$. They also provide a way of formulating invariant initial, final and boundary conditions in gauge theories and gravity on a compact manifold Ω , in a finite interval of time τ .

Switching to the invariant variables ψ_d , A_d^{μ} , and $g_{\mu\nu d}$, it is also possible to "trivialize" the symmetries. Then it is relatively straightforward to organize the action properly, and work out the eigenfunctions and the frequencies for the expansions of the fields. The functional integral is defined as the integral on the coefficients of those expansions. Coherent states are introduced, and the evolution operator $U(t_f, t_i)$ is worked out between arbitrary initial and final states. The formalism we have developed allows us to calculate $U(t_{\rm f}, t_{\rm i})$ diagrammatically, and perturbatively, for arbitrary boundary conditions on $\partial \Omega$. In all the operations we make, the local symmetries are under control, so $U(t_{\rm f}, t_{\rm i})$ is gauge invariant and invariant under general coordinate transformations.

We have illustrated the basic properties of the formalism in Yang-Mills theory on two relatively simple manifolds: the semi-infinite cylinder and the cylinder.

The limit $\tau \to \infty, \Omega \to \mathbb{R}^3$ (which would give the usual S matrix) is only regular when the cosmological constant Λ_C vanishes, due to the problems related to the definitions of asymptotic states and S matrix amplitudes at $\Lambda_C \neq 0$. Yet, such problems are not problems of unitarity *per se*, because the evolution operator $U(t_f, t_i)$ of quantum gravity is unitary for every $\tau < \infty$.

It might be impossible to test the S matrix predictions for a long time, in quantum gravity. Hopefully, working with $U(t_{\rm f}, t_{\rm i})$ at finite τ on a compact Ω can allow us to explore more options, and figure out experimental setups that could amplify tiny effects like those of quantum gravity till they become detectable.

ACKNOWLEDGMENTS

We are grateful to U. Aglietti for helpful discussions.

APPENDIX A: FORMAL PROPERTIES OF $\delta = \theta \Delta$

In this appendix we study the key formal properties of the operator δ of the gauge transformations, and give a very economic proof of theorem (3.25).

Adopting the notation (3.26), (3.27), (3.28) of Sec. III B, we can write $\delta = \theta \Delta$,

$$\Delta = \sum_{a} \sum_{n \in \hat{\mathcal{U}}} v_n^{aT} \sigma_1 \frac{\delta_l}{\delta u_n^a} + \text{c.c.}, \quad (A1)$$

where "c.c." denotes the complex conjugate. It is easy to prove the properties

$$\Delta^2 = 0, \quad \Delta u_n^{aT} = v_n^{aT} \sigma_1 + u_n^{aT} \sigma_3 \Delta, \quad \Delta v_n^{aT} = v_n^{aT} \sigma_3 \Delta,$$

$$\frac{\delta_l}{\delta u_n^a} \Delta = \Delta \sigma_3 \frac{\delta_l}{\delta u_n^a}, \quad \frac{\delta_l}{\delta v_n^a} \Delta = \Delta \sigma_3 \frac{\delta_l}{\delta v_n^a} + \sigma_1 \frac{\delta_l}{\delta u_n^a}, \tag{A2}$$

where Δ is meant to act everywhere to its right.

Now we prove theorem (3.25), stating that a local function X that solves $\Delta X = 0$ can be written as X = $X_0 + Y$, where $X_0 = X|_{u=v=\bar{u}=\bar{v}=0}$ and Y is a local function.

Define the operators

$$\hat{\Delta} = \sum_{a} \sum_{n \in \hat{\mathcal{U}}} u_n^{aT} \sigma_1 \frac{\delta_l}{\delta v_n^a} + \text{c.c.},$$
$$\mathcal{D} = \sum_{a} \sum_{n \in \hat{\mathcal{U}}} \left(u_n^{aT} \frac{\delta_l}{\delta u_n^a} + v_n^{aT} \frac{\delta_l}{\delta v_n^a} \right) + \text{c.c}$$

Using (A2), it is straightforward to prove the identities

$$[\mathcal{D}, \Delta] = [\mathcal{D}, \hat{\Delta}] = 0, \qquad \{\Delta, \hat{\Delta}\} = \mathcal{D}.$$
 (A3)

The former is a consequence of homogeneity.

Now, decompose X as $X = X_0 + X'$. Clearly, $\Delta X_0 =$ $\Delta X' = 0$. Moreover, $\mathcal{D}^{-1}X'$ is well-defined, by homogeneity. Using (A3), we immediately find

$$\begin{aligned} X' &= \mathcal{D}\mathcal{D}^{-1}X' = \{\Delta, \hat{\Delta}\}\mathcal{D}^{-1}X' = \Delta\hat{\Delta}\mathcal{D}^{-1}X' \\ &+ \hat{\Delta}\mathcal{D}^{-1}\Delta X' = \Delta Y, \qquad Y = \hat{\Delta}\mathcal{D}^{-1}X', \end{aligned}$$

which proves the theorem.

Note that we never have to involve, discard, or pay attention to total derivatives, so the theorem applies to functions, not just functionals.

APPENDIX B: HIGHER-DERIVATIVE INTERACTIONS

In this appendix we extend the results of Sec. III to interaction Lagrangians that contain arbitrarily many derivatives of the fields, as long as their number grows together with the power of some coupling. This part is only needed for gravity. We show that we can rearrange the Lagrangian \mathcal{L}' so as to finally have an action with the form and the properties of (3.43).

We assume that the Lagrangian $L(\phi, \dot{\phi})$ is decomposed as (3.1), that the symmetry is orthodox and linear, that the quadratic sector $L_{\text{free}}(\phi, \phi)$ has the same structure as in Sec. III (no more than one derivative on each field, no more that two derivatives in each term), but we allow $L_{\rm int}(\phi, \dot{\phi})$ to contain arbitrary monomials $\partial^{m_1}\phi_1\cdots\partial^{m_n}\phi_n$ of the fields, differentiated arbitrary numbers of times $m_1, \ldots m_n$. For definiteness, we assume that $L_{\text{int}}(\phi, \dot{\phi})$ is proportional to some coupling λ , which we use to trace the interaction terms. We write them as $\mathcal{O}(\lambda)$, or $\mathcal{O}(\lambda^n)$, n > 1, when we mean higher orders.

We proceed as in Sec. III up to the integrated Lagrangian \mathcal{L}' , expressed in terms of coherent states. This means that: we make the shift (3.34) with the conditions (3.44); then we work out the momenta $\tilde{\pi}^{I}_{\omega}$, make the redefinition (3.42), and expand $\bar{\tilde{\pi}}^{I}_{\varphi}, \varphi^{I}$ in coherent states. We obtain the same quadratic part we had before, then the linear terms due to $\Delta L'_{\varphi}$, plus interactions $\mathcal{L}'_{int}(z, \bar{z}) = \mathcal{O}(\lambda)$.

Before the expansion in coherent states, we have a wide freedom. For example, we can change the interaction sector of the Lagrangian by adding gauge invariant total space derivatives. After the switch from $\tilde{\pi}^{I}_{\varphi}, \varphi^{I}$ to coherent states, these corrections give legit vertices. Moreover, the expansion takes care of the space sector, so we do not need to worry about the space derivatives any longer. What we have to do, instead, is rearrange the interaction part $\mathcal{L}'_{int}(z, \bar{z})$, to remove the time derivatives of z and \bar{z} , which are still there, and can be arbitrarily many. We achieve this goal by adding (gauge invariant) total time derivatives to \mathcal{L}'_{int} .

We can arrange $\mathcal{L}'(z, \bar{z})$ into a sum

$$\mathcal{L}'(z,\bar{z}) = \mathcal{L}'_{\text{free}}(z,\bar{z}) + \mathcal{L}'_{\text{int 0}}(z,\bar{z}) + \mathcal{L}'_{\text{int der}}(z,\bar{z}), \qquad (B1)$$

where $\mathcal{L}'_{\text{free}}(z, \bar{z})$ includes the quadratic terms, as well as the linear terms due to $\Delta L'_{\varphi}$, $\mathcal{L}'_{\text{int 0}}(z, \bar{z}) = \mathcal{O}(\lambda)$ is free of time derivatives, while $\mathcal{L}'_{\text{int der}}(z, \bar{z}) = \mathcal{O}(\lambda)$ vanishes when all the time derivatives are set to zero.

We also assume that the each term of $\mathcal{L}'_{int der}$ has a power of λ that is equal to the number of its time derivatives, at least. We remove $\mathcal{L}'_{int der}$ iteratively by means of field redefinitions and dropping gauge invariant total derivatives, without affecting the symmetry and the other properties of the Lagrangian \mathcal{L}' .

We proceed by induction. We assume that $\mathcal{L}'_{\text{int der}}$ has N powers of λ more than one for each time derivative, and write $\mathcal{L}'_{\text{int der}} = \mathcal{O}(\lambda^N)\mathcal{O}(\lambda\partial_t)$ to mean this. We give a procedure to rearrange the Lagrangian so that the new $\mathcal{L}'_{\text{int der}}$ is $\mathcal{O}(\lambda^{N+1})\mathcal{O}(\lambda\partial_t)$. Since we are able to do so for arbitrary N, starting from N = 0, we remove $\mathcal{L}'_{\text{int der}}$ entirely.

Replacing the functional derivatives of (A1) with ordinary derivatives, we can write the operator Δ as

$$\Delta \equiv \sum_{j=0}^{\infty} \sum_{a} \sum_{n \in \hat{\mathcal{U}}} v_{jn}^{aT} \sigma_1 \frac{\partial_l}{\partial u_{jn}^a} + \text{c.c.}, \quad (B2)$$

where u_{jn}^a and v_{jn}^a denote the *j*-th time derivatives of u_n^a and v_n^a , respectively.

We know that $\mathcal{L}'_{\text{int der}}$ must be gauge invariant by itself $(\Delta \mathcal{L}'_{\text{int der}} = 0)$, since Δ does not mix derivatives and orders of the interactions. Using theorem (3.25), we can write

$$\mathcal{L}'_{\text{int der}} = X_0 + \Delta Y_s$$

where X_0 is a function that depends only on w_{jn}^{α} and \bar{w}_{jn}^{α} (the *j*th time derivatives of w_n^{α} and \bar{w}_n^{α}), and *Y* is another function.

Since every term $\mathcal{L}'_{\text{int der}}$ must contain time derivatives, X_0 has the form

$$X_0 = \sum_{j>0} \sum_{\alpha} \sum_{n \in \hat{\mathcal{U}}} w_{jn}^{\alpha} X_n^{\alpha j} + \text{c.c.},$$

for certain Δ invariant functions $X_n^{\alpha j}$, and their conjugates. We can write

$$X_0 = \sum_{lpha} \sum_{n \in \hat{\mathcal{U}}} \dot{w}_n^{lpha} X_n^{lpha} + X_0^{ ext{tder}} + ext{c.c.},$$

where X_n^{α} are other Δ invariant functions, and X_0^{tder} are gauge invariant total derivatives. As part of the rearrangement to get to the correct final action, we drop X_0^{tder} .

Now we consider *Y*. Since it must contain time derivatives, its form is

$$Y = \sum_{j>0} \sum_{n \in \hat{\mathcal{U}}} \left[\sum_{\alpha} w_{jn}^{\alpha} Y_{n}^{\alpha j} + \sum_{a} (u_{jn}^{aT} Y_{n+}^{aj} + v_{jn}^{aT} Y_{n-}^{aj}) \right] + \text{c.c.}$$

The only thing that matters is ΔY , so we can replace Y with

$$\begin{split} Y' &= \sum_{j>0} \sum_{n \in \hat{\mathcal{U}}} \left(\sum_{\alpha} w_{jn}^{\alpha} Y_n^{\alpha j} + \sum_{a} u_{jn}^{aT} \tilde{Y}_{n+}^{aj} \right) + \text{c.c.},\\ \tilde{Y}_{n+}^{aj} &= Y_{n+}^{aj} + \sigma_1 \sigma_3 \Delta Y_{n-}^{aj}, \end{split}$$

since $\Delta Y = \Delta Y'$, by the first and third identities of (A2). Subtracting gauge invariant total derivatives from $\mathcal{L}'_{int der}$, we rearrange this expression as

$$Y' \to \sum_{n \in \hat{\mathcal{U}}} \left(\sum_{\alpha} \dot{w}_n^{\alpha} Y_n^{\alpha} + \sum_{a} \dot{u}_n^{aT} \tilde{Y}_{n+}^{a} \right) + \text{c.c.},$$

for some Y_n^{α} and \tilde{Y}_{n+}^{α} .

So far, the rearrangement gives

$$\mathcal{L}_{\text{int der}}' \to \bar{X} \equiv \sum_{n \in \hat{\mathcal{U}}} \left[\sum_{\alpha} \dot{w}_{n}^{\alpha} (X_{n}^{\alpha} + (-1)^{\epsilon_{n}^{\alpha}} \Delta Y_{n}^{\alpha}) + \Delta \sum_{a} \dot{u}_{n}^{aT} \tilde{Y}_{n+}^{a} \right] + \text{c.c.}, \qquad (B3)$$

where ϵ_n^{α} is the statistics of w_n^{α} . Note that X_n^{α} , Y_n^{α} and \tilde{Y}_{n+1}^{α} are $\mathcal{O}(\lambda^{N+1})\mathcal{O}(1)$.

At this point, we remove \bar{X} by means of the field redefinitions,

$$\begin{split} \bar{w}_{n}^{\alpha} &\to \bar{w}_{n}^{\alpha} - \frac{(-1)^{\epsilon_{n}^{\alpha}} X_{n}^{\alpha} + \Delta Y_{n}^{\alpha}}{2\tau_{n}^{\alpha} i \omega_{n}^{\alpha}}, \qquad \bar{u}_{n}^{a} \to \bar{u}_{n}^{a} - \frac{\sigma_{1} \tilde{Y}_{n+}^{a}}{2\tau_{n}^{a} i \omega_{n}^{a}}, \\ \bar{v}_{n}^{a} &\to \bar{v}_{n}^{a} - \frac{\Delta \tilde{Y}_{n+}^{a}}{2\tau_{n}^{a} i \omega_{n}^{a}}, \end{split}$$
(B4)

and their conjugates. We show that this operation replaces $\mathcal{L}'_{\text{int der}}$ with higher-order derivative interactions $\mathcal{O}(\lambda^{N+1})\mathcal{O}(\lambda\partial_t)$, and preserves the key properties of $\mathcal{L}'_{\text{free}}$ and $\mathcal{L}'_{\text{int 0}}$.

When we apply the redefinition (B4) to $\mathcal{L}'_{int der}$ we obtain $\mathcal{O}(\lambda^{N+1})\mathcal{O}(\lambda\partial_t)$ at least, which go into the new $\mathcal{L}'_{int der}$. When we apply (B4) to \mathcal{L}'_{free} minus the universal kinetic terms (3.31) and (3.32), we obtain: (a) interaction terms with no derivatives, which go into the new \mathcal{L}'_{int0} ; plus (b) $\mathcal{O}(\lambda^{N+1})\mathcal{O}(\lambda\partial_t)$, which go into the new \mathcal{L}'_{int0} . The same occurs when we apply (B4) to \mathcal{L}'_{int0} .

It remains to apply the redefinition (B4) to (3.31) and (3.32). The second orders of the Taylor expansions give

 $\mathcal{O}(\lambda^{N+1})\mathcal{O}(\lambda\partial_t)$. So, it is sufficient to focus on the first orders of the Taylor expansions.

From (3.31) we get the correction

$$-\sum_{\alpha}\sum_{n\in\hat{\mathcal{U}}}\dot{w}_{n}^{\alpha}(X_{n}^{\alpha}+(-1)^{\epsilon_{n}^{\alpha}}\Delta Y_{n}^{\alpha}) \\ +\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{\alpha}\sum_{n\in\hat{\mathcal{U}}}\left[(-1)^{\epsilon_{n}^{\alpha}}X_{n}^{\alpha}+\Delta Y_{n}^{\alpha}\right]w_{n}^{\alpha}+\mathrm{c.c.}$$

The first term subtracts the first one of (B3). The rest is a gauge invariant total derivative, which we remove.

From (3.32) we get the correction

$$-\sum_{a}\sum_{n\in\hat{\mathcal{U}}}\Delta(\dot{u}_{n}^{aT}\tilde{Y}_{n+}^{a})+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{a}\sum_{n\in\hat{\mathcal{U}}}\Delta(u_{n}^{aT}\tilde{Y}_{n+}^{a})+\mathrm{c.c.},$$

which cancels the rest of (B3), plus gauge invariant total derivatives.

In the end, we remain with a $\mathcal{L}'_{int der}$ that is $\mathcal{O}(\lambda^{N+1}) \times \mathcal{O}(\lambda \partial_t)$. That is to say, we have raised its λ power by one unit. Iterating in *N*, we can make $\mathcal{L}'_{int der}$ disappear entirely.

Summarizing, the effects of the iterated redefinitions (B4), the rearrangements and the droppings of gauge invariant total derivatives in the interaction sector are: (1) they cancel the term $\mathcal{L}'_{int der}$; (2) they do not affect the symmetry transformations (3.28); this is evident from (B4), using $\delta = \theta \Delta$; (3) they do not affect the universal kinetic terms (3.31) and (3.32); (4) they do not affect \mathcal{L}'_{free} ; (5) they do not change the structure of \mathcal{L}'_{int0} ; (6) they leave the Lagrangian \mathcal{L}' orthodoxically symmetric. In the end, we have the correct \mathcal{L}' :

$$\mathcal{L}'(z,\bar{z}) = \mathcal{L}'_{\text{free}}(z,\bar{z}) + \mathcal{L}'_{\text{int}\,0}(z,\bar{z}). \tag{B5}$$

Note that point (6) is tautologically true now: a gauge invariant Lagrangian of the form (B5) is necessarily orthodoxically invariant, if the symmetry is linear, since the universal kinetic terms are invariant by themselves, and the rest does not contain time derivatives.

The field redefinitions (B4) are perturbative, so their Jacobian determinant is trivial, if we use the analytic or dimensional regularization techniques [20].

To get to the action (3.23), we integrate on time, add the usual endpoint corrections, as in (3.23) and (3.43), and we are done.

- D. Anselmi, Quantum field theory of physical and purely virtual particles in a finite time interval on a compact space manifold: Diagrams, amplitudes and unitarity, J. High Energy Phys. 07 (2023) 209.
- [2] D. Anselmi, Diagrammar of physical and fake particles and spectral optical theorem, J. High Energy Phys. 11 (2021) 030.
- [3] D. Anselmi, Purely virtual extension of quantum field theory for gauge invariant fields: Yang-Mills theory, Eur. Phys. J. C 83, 544 (2023).
- [4] D. Anselmi, Purely virtual extension of quantum field theory for gauge invariant fields: Quantum gravity, Eur. Phys. J. C 83, 1066 (2023).
- [5] J. Schwinger, The theory of quantized fields. III, Phys. Rev. 91, 728 (1953); J. R. Klauder, The action option and a Feynman quantization of spinor fields in terms of ordinary c-numbers, Ann. Phys. (N.Y.) 11, 123 (1960); E. C. G. Sudarshan, Equivalence of semiclassical and quantum mechanical descriptions of statistical light beams, Phys. Rev. Lett. 10, 277 (1963); R. J. Glauber, Coherent and incoherent states of the radiation field, Phys. Rev. 131, 2766 (1963).
- [6] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill Inc, New York, 1980).
- [7] D. Anselmi and M. Piva, A new formulation of Lee-Wick quantum field theory, J. High Energy Phys. 06 (2017) 066.
- [8] D. Anselmi, On the quantum field theory of the gravitational interactions, J. High Energy Phys. 06 (2017) 086.

- [9] R. E. Cutkosky, Singularities and discontinuities of Feynman amplitudes, J. Math. Phys. (N.Y.) 1, 429 (1960); M. Veltman, Unitarity and causality in a renormalizable field theory with unstable particles, Physica (Amsterdam) 29, 186 (1963).
- [10] G. 't Hooft, Renormalization of massless Yang-Mills fields, Nucl. Phys. B33, 173 (1971); Renormalizable Lagrangians for massive Yang-Mills fields, Nucl. Phys. B35, 167 (1971); G. 't Hooft and M. Veltman, Diagrammar, CERN Report No. CERN-73-09; M. Veltman, *Diagrammatica. The Path to Feynman Rules* (Cambridge University Press, New York, 1994).
- [11] D. Anselmi, A new quantization principle from a minimally non time-ordered product, J. High Energy Phys. 12 (2022) 088.
- [12] T. D. Lee and G. C. Wick, Negative metric and the unitarity of the S-matrix, Nucl. Phys. B9, 209 (1969); Finite theory of quantum electrodynamics, Phys. Rev. D 2, 1033 (1970); R. E. Cutkosky, P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, A non-analytic S matrix, Nucl. Phys. B12, 281 (1969); T. D. Lee, A relativistic complex pole model with indefinite metric, in *Quanta: Essays in Theoretical Physics Dedicated to Gregor Wentzel* (Chicago University Press, Chicago, 1970), p. 260; N. Nakanishi, Lorentz noninvariance of the complex-ghost relativistic field theory, Phys. Rev. D 3, 811 (1971); B. Grinstein, D. O'Connell, and M. B. Wise, Causality as an emergent macroscopic phenomenon: The Lee-Wick O(N) model, Phys. Rev. D 79, 105019 (2009).

- [13] E. Tomboulis, 1/N expansion and renormalization in quantum gravity, Phys. Lett. B 70, 361 (1977); E. Tomboulis, Renormalizability and asymptotic freedom in quantum gravity, Phys. Lett. B 97, 77 (1980); Shapiro and L. Modesto, Superrenormalizable quantum gravity with complex ghosts, Phys. Lett. B 755, 279 (2016); L. Modesto, Super-renormalizable or finite Lee–Wick quantum gravity, Nucl. Phys. B909, 584 (2016); J. F. Donoghue and G. Menezes, Unitarity, stability and loops of unstable ghosts, Phys. Rev. D 100, 105006 (2019).
- [14] D. Anselmi, E. Bianchi, and M. Piva, Predictions of quantum gravity in inflationary cosmology: Effects of the Weyl-squared term, J. High Energy Phys. 07 (2020) 211.
- [15] K. N. Abazajian *et al.*, CMB-S4 science book, first edition, arXiv:1610.02743.
- [16] A. Melis and M. Piva, One-loop integrals for purely virtual particles, Phys. Rev. D 108, 096021 (2023).
- G. J. van Oldenborgh and J. A. M. Vermaseren, New algo-[17] rithms for one loop integrals, Z. Phys. C 46, 425 (1990); J. Kublbeck, M. Bohm, and A. Denner, Feyn arts: Computer algebraic generation of Feynman graphs and amplitudes, Comput. Phys. Commun. 60, 165 (1990); A. Denner, Techniques for calculation of electroweak radiative corrections at the one loop level and results for W physics at LEP-200, Fortschr. Phys. 41, 307 (1993); T. Hahn, Loop calculations with FeynArts, FormCalc, and LoopTools, Acta Phys. Pol. B 30, 3469 (1999); T. Hahn, Generating Feynman diagrams and amplitudes with FeynArts 3, Comput. Phys. Commun. 140, 418 (2001); A. Alloul, N.D. Christensen, C. Degrande, C. Duhr, and B. Fuks, FeynRules 2.0 - A complete toolbox for tree-level phenomenology, Comput. Phys. Commun. 185, 2250 (2014); H. H. Patel, Package-X: A Mathematica package for the analytic calculation of one-loop integrals, Comput. Phys. Commun. 197, 276 (2015).

- [18] K. Nomoto and R. Fukuda, Quantum field theory with finite time interval, Prog. Theor. Phys. 86, 269 (1991).
- [19] D. Anselmi, Aspects of perturbative unitarity, Phys. Rev. D 94, 025028 (2016).
- [20] C. G. Bollini, J. J. Giambiagi, and A. Gonzáles Domínguez, Analytic regularization and the divergences of quantum field theories, Nuovo Cimento **31**, 550 (1964); C. G. Bollini and J. J. Giambiagi, The number of dimensions as a regularizing parameter, Nuovo Cimento Soc. Ital. Fis. **12B**, 20 (1972); Lowest order divergent graphs in ν-dimensional space, Phys. Lett. **40B**, 566 (1972); G. t Hooft and M. Veltman, Regularization and renormalization of gauge fields, Nucl. Phys. **B44**, 189 (1972); G. M. Cicuta and E. Montaldi, Analytic renormalization via continuous space dimension, Lett. Nuovo Cimento **4**, 329 (1972).
- [21] D. Anselmi, Fakeons, unitarity, massive gravitons and the cosmological constant, J. High Energy Phys. 12 (2019) 027.
- [22] D. Anselmi and M. Piva, Quantum gravity, fakeons and microcausality, J. High Energy Phys. 11 (2018) 021.
- See for example the discussions in S.B. Giddings, The [23] boundary S-matrix and the AdS to CFT dictionary, Phys. Rev. Lett. 83, 2707 (1999); V. Balasubramanian, S. B. Giddings, and A. Lawrence, What do CFTs tell us about anti-de Sitter spacetimes?, J. High Energy Phys. 03 (1999) 001; J. Bros, H. Epstein, M. Gaudin, U. Moschella, and V. Pasquier, Triangular invariants, three-point functions and particle stability on the de Sitter universe, Commun. Math. Phys. 295, 261 (2010); E. T. Akhmedov and P. V. Buividovich, Interacting field theories in de Sitter space are non-unitary, Phys. Rev. D 78, 104005 (2008); E.T. Akhmedov, Lecture notes on interacting quantum fields in de Sitter space, Int. J. Mod. Phys. D 23, 1430001 (2014); D. Marolf, I. A. Morrison, and M. Srednicki, Perturbative S-matrix for massive scalar fields in global de Sitter space, Classical Quantum Gravity 30, 155023 (2013).