Wave functions constructed from an invariant sum over histories satisfy constraints

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Invariance of classical equations of motion under a group parametrized by functions of time implies constraints between canonical coordinates and momenta. In the Dirac formulation of quantum mechanics, invariance is normally imposed by demanding that physical wave functions are annihilated by the operator versions of these constraints. In the sum-over-histories quantum mechanics, however, wave functions are specified, directly, by appropriate functional integrals. It therefore becomes an interesting question whether the wave functions so specified obey the operator constraints of the Dirac theory. In this paper, we show for a wide class of theories, including gauge theories, general relativity, and first-quantized string theories, that wave functions constructed from a sum over histories are, in fact, annihilated by the constraints *provided* that the sum over histories is constructed in a manner which respects the invariance generated by the constraints. By this we mean a sum over histories defined with an invariant action, invariant measure, and an invariant class of paths summed over. We use this result to give three derivations of the Wheeler-DeWitt equation for the wave function of the universe starting from the sum-over-histories representation of it. The first uses Becchi-Rouet-Stora-Tyutin methods and the explicit path-integral construction of Batalin, Fradkin, and Vilkovisky. The second is a direct derivation from the gauge-fixed Hamiltonian path integral. The third exploits the embedding variables introduced by Isham and Kuchař, in terms of which the connection with the constraints representing the four-dimensional diffeomorphism group is most clearly seen. In each case it is found that the symmetry leading to the Wheeler-DeWitt equation is not in fact four-dimensional diffeomorphism invariance; rather, it is the closely connected but slightly larger canonical symmetry of the Hamiltonian form of the action of general relativity. By allowing our path-integral construction to be either Euclidean or Lorentzian, we show that the consequent Wheeler-DeWitt equation is independent of which one is taken as a starting point. Our results are general, in that they do not depend on a particular representation of the sum over histories, but they are also formal, in that we do not address such issues as the operator ordering of the derived constraints. Instead, we isolate those general features of a sum over histories which define an invariant construction of a wave function and show that these imply the operator constraints.

I. INTRODUCTION

In classical dynamics, invariance of the equations of motion under a group parametrized by functions of time implies constraints between the canonical coordinates and their momenta:[1]

$$T_\alpha(p_i,q^i)=0 \ . \tag{1.1}$$

In Dirac's quantum mechanics of such constrained Hamiltonian systems, this invariance is expressed by operator constraints which annihilate the wave functions representing physical states:[2]

$$T_\alpha(\hat{p}_i,\hat{q}^{\,i})\Psi=0 \ . \tag{1.2}$$

In sum-over-histories quantum mechanics wave functions are defined by suitably restricted sums over histories of the form[3]

$$\Psi=\sum_{\text{histories}}\exp[-\sigma S(\text{history})] \ . \tag{1.3}$$

The class of histories summed over determines the wave function. For some purposes a Euclidean construction with $\sigma=1$ is useful. For others a Lorentzian construction with $\sigma=-i$ is more appropriate. Most generally, sums of the form (1.3) over *complex* contours are of interest as in the "wave function of the universe" construction in the "no-boundary" theory of the cosmological initial condition.[4]

If wave functions are defined by sums over histories, it becomes an interesting question whether they satisfy the operator constraints of the Dirac theory. One expects that if the defining sum over histories respects the invariance of the theory, then the resulting wave function should satisfy the operator constraints which implement that invariance. That is, we expect (1.2) to be a *conse-*

quence of (1.3). This paper is concerned with demonstrating that consequence.

The most famous example of a constrained Hamiltonian theory is Einstein's general relativity. In general relativity two metrics which are related by a diffeomorphism are physically equivalent—they describe the same geometry. There are no further observable fields which can supply anything like a preferred system of coordinates. As a consequence, the classical gravitational action is a functional of the metric alone and is invariant under diffeomorphisms. This invariance implies the four constraints of general relativity.

In relativity, canonical coordinates may be taken to be the three-metric of a spacelike surface, $h_{ij}(\mathbf{x})$, and the matter-field configurations on that surface. For simplicity we shall consider the case of a single scalar field $\phi(\mathbf{x},t)$ whose spatial configuration we denote by $\chi(\mathbf{x})$. The constraints following from diffeomorphism invariance are relations between these coordinates and their canonical momenta, $\pi^{ij}(\mathbf{x})$ and $\pi_\chi(\mathbf{x})$, respectively. There are three momentum constraints and one Hamiltonian constraint for each point on the surface. In the case of spatially closed cosmologies, these have the form

$$\mathcal{H}_i = -2D_j \pi_i^j + T_i^n = 0 \ , \tag{1.4a}$$

$$\mathcal{H} = l^2 G_{ijkl}\pi^{ij}\pi^{kl} - l^{-2} h^{1/2}({}^3R - 2\Lambda) + h^{1/2} T_{nn} = 0 \ . \tag{1.4b}$$

Here T_i^n and T_{nn} are the energy-momentum tensor of the matter once and twice projected on the normal to the surface. These are to be viewed as functions of the canonical coordinates and momenta. D_i and ${}^3R$ are the covariant derivative and scalar curvature intrinsic to the three-surface, and G_{ijkl} is defined by

$$G_{ijkl} = \tfrac{1}{2} h^{-1/2}(h_{il}h_{kj} + h_{ik}h_{jl} - h_{ij}h_{kl}) \ . \tag{1.5}$$

In these expressions $l = (16\pi G)^{1/2}$ is the Planck length in the units with $\hbar = c = 1$ we use throughout.

In the quantum mechanics of closed cosmologies, the operator form of the Hamiltonian constraint

$$\hat{\mathcal{H}}(\mathbf{x})\Psi[h_{ij},\chi] = 0 \tag{1.6a}$$

is called the Wheeler-DeWitt equation and summarizes the quantum dynamics. The operator form of the three-momentum constraints

$$\hat{\mathcal{H}}_i(\mathbf{x})\Psi[h_{ij},\chi] = 0 \tag{1.6b}$$

expresses invariance under coordinate transformations in the spacelike surface.

The derivation of the constraints from the sum over histories has previously been considered by a series of authors: Hartle and Hawking[5] gave a formal derivation, but without attention to the inevitable gauge fixing. Barvinsky and Ponomariov[6] and Barvinsky[7] gave a more careful derivation, but using the so-called "canonical" gauges. The use of such gauges has been convincingly criticized by Teitelboim,[8] who also gave a construction of the path integral manifestly satisfying the momentum constraints, but an explicit derivation of the Wheeler-DeWitt equation was not given. Halliwell[9] has given a very detailed treatment, with attention to the path-integral measure and operator ordering, but in the restricted context of minisuperspace models. Implicit in the work of Henneaux[10] is a derivation utilizing Becchi-Rouet-Stora-Tyutin (BRST) invariance and taking advantage of the formal possibility of transforming the constraints into ones which commute among themselves. Woodard[11] has considered the issue of enforcing the Wheeler-DeWitt equation in canonical inner products. Although many of these derivations may be criticized on the grounds of precision and generality, the underlying ideas are useful, and we shall exploit them in what follows.

In this paper we shall present a derivation of the operator constraints for invariantly constructed sum-over-histories wave functions that is general enough to apply to a wide class of invariant theories and to different sum-over-histories representations of them, but specific enough to be investigated in particular models. By studying the connection between invariance and constraints generally, we are able to achieve two things: First, we can isolate the essential requirements for an invariant sum-over-histories construction in a way that is concrete enough for these requirements to be tested in specific cases. These requirements are that the action, measure, and class of histories summed over be invariant under the symmetry generated by the constraints. Second, we can show clearly that invariance so defined is the origin of the operator constraints. Two caveats should be noted. First, we do not demonstrate that sums over histories invariant under *any* notion of symmetry imply wave functions satisfying constraints. Rather, the invariance must be explicitly related to the classical constraints of the theory. Second, nothing here is assumed about the wave functions (for example, their normalizability) beyond the fact that they have a sum-over-histories integral representation. This effort may therefore be regarded as an investigation of the properties of a specific class of integral representations. As we shall see, however, the class is general enough to apply to a very wide variety of interesting cases.

The general lemma exhibiting the connection between invariance and constraints is derived in Sec. II. Using the lemma, we are able to present three different derivations of the constraints of general relativity from three different sum-over-histories representations of the sum over geometries. The first, in Sec. III, is a BRST-invariant representation,[12] following the path integral construction of Batalin, Fradkin, and Vilkovisky[13] (BFV). This has the advantage of formal elegance and simplicity, as well as the sanction arising from the successful use of BRST methods in other areas. The BFV starting point provides perhaps the most explicit representation of the invariant measure. However, because the BFV construction exploits a *global* symmetry, namely, BRST invariance, it reproduces the invariant sum over four geometries only for manifolds with topology $\mathbb{R}\times M^3$, where M^3 is a compact three-manifold. To show that the constraints are satisfied independently of topology, we give in Sec. IV a second demonstration where the lemma of Sec. II is applied directly to a phase-space sum over histories. The invariance here is that of the infinitesimal canonical symmetries generated by the constraints themselves. The result is a direct and conceptually simple derivation.

For neither of these demonstrations, however, is the connection with the underlying diffeomorphism group explicit. This is because, while the commutators of the constraints close, they do not reproduce the algebra of the four-dimensional diffeomorphism group.[14] For related reasons wave functions on superspace do not carry a representation of the four-dimensional diffeomorphism group. They cannot do so because some diffeomorphisms displace a spacelike surface forward or backward in time, while the superspace of three-geometries and spatial matter-field configurations contains no time label. These difficulties and their resolution were clearly discussed by Isham and Kuchař.[15] These authors showed how, by breaking general covariance and augmenting the configuration space of general relativity by the embeddings of a foliating family of spacelike surfaces, one could arrive at a space large enough to carry a representation of the algebra of four-dimensional diffeomorphisms. In Sec. V we use their method to give another derivation of the constraints from invariant sums over histories, which makes explicit the connection with the algebra of diffeomorphisms.[16]

All of our demonstrations are formal in the sense that few details of any specific implementation of functional integrals will be used. As a consequence, no information about such things as operator ordering of the constraints are recovered. However, the possibility of such formal derivations is just a reflection of the underlying generality and elementary nature of the connection between invariance and constraints in the quantum theory. Indeed, we are able to reduce our derivation to just the assumptions of the invariance of the action, and measure and class of histories summed over, together with a few assumptions on the behavior of functional integrals.

The importance of summing over an invariant class of histories to obtain a wave function satisfying operator constraints emerges clearly from this work in all three demonstrations. This connection was stressed by Teitelboim[17] and Hartle,[16,18] and emerges very clearly in the models studied by Halliwell.[9] It becomes an important restriction on the contour of integration defining a no-boundary wave function of the universe.[19] However, in each case the notion of invariance which leads to the operator constraints must be carefully and specifically defined. As we shall see, there are several *different* notions of invariance traceable to the underlying diffeomorphism invariance of spacetime theories. Only one, the canonical symmetry generated by the constraints themselves, defines those invariant sum-over-histories constructions leading to wave functions annihilated by operator versions of the constraints.

II. INVARIANCE AND CONSTRAINTS

A. Classical invariance and classical constraints

In classical dynamics, invariance of the equations of motion under a group with a finite number of parameters that are constant in time implies conservation laws.[1] Invariance under a group parametrized by *functions* of time implies constraints.[1] Let us recall the standard arguement in the Lagrangian framework where symmetries are usually most easily expressed. Consider a system whose histories are paths $q^A(t)$ in an N-dimensional configuration space $A=1,\ldots,N$. Consider an action of the form

$$S[q^A(t)]=\int_{t'}^{t''} dt\, L(\dot q^A,q^A) \ . \tag{2.1}$$

Suppose that the action is invariant under infinitesimal transformations of the form

$$q^A(t)\to q^A(t)+\delta q^A(t) \ , \tag{2.2a}$$

where

$$\delta q^A(t)=\epsilon^\alpha(t) f^A_\alpha(\dot q^A(t),q^A(t)) + \dot\epsilon^\alpha(t) g^A_\alpha(\dot q^A(t),q^A(t)) \ , \tag{2.2b}$$

for functions $\epsilon^\alpha(t)$, $\alpha=1,\ldots,m$, which are arbitrary except for possible restrictions at their end points. We assume that the g^A_α do not vanish identically for $\alpha=1,\ldots,\tilde m$ and the f^A_α do not vanish identically for $\alpha=\tilde m+1,\ldots,m$. Among the transformations (2.2) there will be, in general, those describing the reparametrizations of t. Under (2.2) the change in the action is

$$\delta S=\left[\delta q^A\frac{\partial L}{\partial \dot q^A}\right]_{t'}^{t''}+\int_{t'}^{t''}dt\,\delta q^A E_A \tag{2.3a}$$

$$=\left[\epsilon^\alpha\left[f^A_\alpha\frac{\partial L}{\partial\dot q^A}+g^A_\alpha E_A\right]+\dot\epsilon^\alpha g^A_\alpha\frac{\partial L}{\partial \dot q^A}\right]_{t'}^{t''} + \int_{t'}^{t''}dt\,\epsilon^\alpha(t)\left[f^A_\alpha E_A-\frac{d}{dt}(g^A_\alpha E_A)\right]=0 \ , \tag{2.3b}$$

where E_A are the equations of motion

$$E_A=-\frac{d}{dt}\left[\frac{\partial L}{\partial \dot q^A}\right]+\frac{\partial L}{\partial q^A} \ . \tag{2.4}$$

Invariance of the action means $\delta S=0$. The equations of motion, however, will be invariant under the weaker condition that δS is just a boundary term. Invariance of either kind under a group parametrized by arbitrary functions $\epsilon^\alpha(t)$ requires that the integrand in (2.3) vanish, not just for q^A satisfying the equation of motion $E_A=0$, but for all $q^A(t)$. The action will then be invariant provided the $\epsilon^\alpha(t)$ are restricted at the boundaries so that the remaining surface terms vanish.

The vanishing of the integrand of (2.3b) means, in particular, that the coefficients of the third time derivatives of q^A, which occur linearly for $\alpha=1,\ldots,\tilde m$, and of the second term derivatives of q^A, which occur linearly for $\alpha=\tilde m+1,\ldots,m$, must vanish separately. Thus

$$h^A_\alpha\frac{\partial^2 L}{\partial \dot q^A\partial \dot q^B}=0, \quad \alpha=1,\ldots,m \ , \tag{2.5}$$

where

$$h_\alpha^A = g_\alpha^A, \quad \alpha = 1, \ldots, \tilde{m} \ , \tag{2.6a}$$

$$h_\alpha^A = f_\alpha^A, \quad \alpha = \tilde{m}+1, \ldots, m \ . \tag{2.6b}$$

The degeneracy of the matrix of derivatives (2.5) is the sign of a constrained system. The field equations

$$h_\alpha^A E_A = 0, \quad \alpha = 1, \ldots, m \ , \tag{2.7}$$

involve only q^A and $\dot{q}^A$, not $\ddot{q}^A$. They are thus constraints on the initial data.

When we come to constructing the equivalent Hamiltonian formulation of dynamics, the relation (2.5) means that the equations defining the momenta

$$p_A = \frac{\partial L}{\partial \dot{q}^A} \tag{2.8}$$

are not independent. By themselves, they cannot be solved for the $\dot{q}^A$ as functions of p_A and q^A. The m dependent relations of (2.8) when then expressed in terms of the p_A and q^A become the m constraints of the Hamiltonian theory:

$$T_\alpha(p_A, q^A) = 0, \quad \alpha = 1, \ldots, m \ . \tag{2.9}$$

It is in this way that invariance implies constraints.

It is also easy to see that invariance of the equations of motion under a symmetry such as (2.2), but whose parameters ϵ^α are *independent of time,* implies conservation laws. Suppose the change in the action, necessarily a pure divergence, is written

$$\delta S = [\epsilon^\alpha F_\alpha(\dot{q}^A, q^A)]_{t'}^{t''} \ . \tag{2.10}$$

It then follows from (2.3) that when the equations of motion, $E_A = 0$, are satisfied the quantities

$$f_\alpha^A p_A - F_\alpha(p_A, q^A) \tag{2.11}$$

are conserved.

We shall now show that, in a large and interesting class of theories, wave functions constructed as invariant path integrals satisfy the operator forms of these constraints.

B. A lemma

There is a rich variety of invariant theories and their general characterization is a complex subject.[2] We shall consider a general class characterized by the following properties.

(a) The theory is described by a configuration space consisting of n coordinates q^i, which have nonvanishing conjugate momenta p_i and "multipliers" λ^α with vanishing momenta. We shall consider cases where the theory is described by a Lagrangian action $S[q^i, \lambda^\alpha]$, containing no more than first derivatives in the time, and also cases where it is described by a Hamiltonian action $S[p_i, q^i, \lambda^\alpha]$. Where it is not necessary to distinguish, we shall write $S[z^A]$, with z^A being either the set (q^i, λ^α) or $(p_i, q^i, \lambda^\alpha)$.

(b) There is a set of transformations

$$z^A \to z^A + \delta z^A \ , \tag{2.12}$$

where δz^A depends linearly on m parameters ϵ^α and their derivatives $\dot{\epsilon}^\alpha$ and where the ϵ^α are freely specifiable functions of t for which the following two facts hold. First,

$$\delta q^i = \epsilon^\alpha f_\alpha^i(p_i, q^i) \ , \tag{2.13}$$

for some functions f_α^i, which depend only on q^i and p_i in the Hamiltonian form or on q^i and $p_i = p_i(\dot{q}^i, q^i)$ in the Lagrangian one. In particular, δq^i is independent of any multipliers or $\dot{\epsilon}^\alpha$. Second, we assume that the action changes under (2.12) by at most a boundary term independent of $\dot{\epsilon}^\alpha$ and the multipliers. That is, we assume δS has the form

$$\delta S = [\epsilon^\alpha F_\alpha(p_i, q^i)]_{t'}^{t''} \ . \tag{2.14}$$

The condition (2.14) implies the invariance of the equations of motion. It also implies the invariance of the action if the conditions $\epsilon^\alpha(t') = 0 = \epsilon^\alpha(t'')$ are imposed for those α for which F_α does not vanish identically. However, the derivation of the operator constraints that we shall give requires not just transformations which leave the action invariant, but most generally those for which either (2.13) or (2.14) or both are satisfied in a nontrivial way. As we shall see in Secs. II C and II D below, a large and interesting number of theories possess invariances in this class. They include gauge theories, general relativity, and first-quantized string theories, each in Lagrangian, Hamiltonian, and BRST forms.

We now consider wave functions $\Psi(q^i)$ constructed as invariant path integrals of the form

$$\Psi(q^{i\prime\prime}) = \int_{\mathcal{C}} \mathcal{D}z^A \delta(q^i(t'') - q^{i\prime\prime}) \times \Delta_C[z^A] \delta[C^\alpha(z^A)] \exp(-\sigma S[z^A]) \ . \tag{2.15}$$

The ingredients of this formula are as follows. The variables z^A are the configuration- or phase-space coordinates defined above. $S[z^A]$ is the Lagrangian or Hamiltonian action satisfying the two conditions (a) and (b). $\sigma = -i$ for Lorentzian path integrals and $+1$ for Euclidean ones. $\mathcal{C}$ denotes the class of paths that are integrated over. This integration *includes* an integration over the final values $q^i(t'')$. It is the surface δ function $\delta(q^i(t'') - q^{i\prime\prime})$ that ensures that at $t = t''$ all paths end at the point $q^i(t'') = q^{i\prime\prime}$, which is the argument of the wave function. $C^\alpha(z^A)$ are a set of gauge-fixing conditions, and $\Delta_C[z^A]$ are associated weight factors discussed below. In the case of gauge theories, they are Faddeev-Popov determinants. More generally, they are integrals over the ghosts of the exponential of a suitable ghost action and may not always be interpreted as determinants. Gauge-fixing conditions will not be present in every application. For example, in the BRST construction they will be absent. The form (2.15) thus covers a wide variety of interesting cases. We shall show that if a path-integral construction of the form (2.15) is invariant with a symmetry satisfying (2.13) and (2.14), then the resulting wave function will satisfy operator forms of the constraints.

We now spell out what we mean by an invariant path-integral construction. An invariant path-integral construction involves an action, measure, and class of paths for which the following four properties hold under the transformation (2.12).

(1) The action S changes at the most by a surface term of the form (2.14). It is thus strictly invariant under transformations (2.12) when ϵ vanishes at the end points.

(2) The class of paths, $\mathcal{C}$, is invariant.

(3) The path integral (2.15) is independent of the choice of gauge conditions C^α in a class which includes those generated from a defining C^α by a symmetry transformation, that is, at least all $C^\alpha_\epsilon[z^A]$ of the form

$$C^\alpha_\epsilon[z^A]=C^\alpha[z^A+\delta z^A] \; . \tag{2.16a}$$

(4) The combination of the measure and the gauge-fixing weight factor transform under a symmetry transformation (2.12) according to

$$\mathcal{D}z^A\Delta_C[z^A]\rightarrow\mathcal{D}z^A\Delta_{C_\epsilon}[z^A] \; . \tag{2.16b}$$

In addition to these four properties characterizing the invariance of the path integral (2.15), we will also need to assume the following.

(5) Integrals of the form (2.15) weighted by functions of p_i and q^i on the final surface are equal to corresponding, appropriately ordered, operators acting on $\Psi(q^{i''})$. That is, for a given $\mathcal{F}(p_i,q^i)$,

$$\begin{aligned}\int_{\mathcal{C}}\mathcal{D}z^A\mathcal{F}(p_i(t''),q^i(t''))\delta(q^i(t'')-q^{i''})\\ \times\Delta_C[z^A]\delta[C^\alpha(z^A)]\exp(-\sigma S[z^A])\\ =\mathcal{F}\left[-\frac{1}{\sigma}\frac{\partial}{\partial q^{i''}},q^{i''}\right]\Psi(q^{i''}) \; ,\end{aligned} \tag{2.17}$$

for some deducible operator acting on the right-hand side. Of course, (3)–(5) are usually deemed to be *consequences* of a path-integral construction such as (2.15). In gauge theories, (3) and (4) follow from the standard Faddeev-Popov determinant construction and (5) from explicit implementations of the sum over paths. Consequences or not, these are the minimal criteria necessary to define an invariant construction.

We shall return to a discussion of assumptions (1)–(5) below, but now we show that the operator constraints on an invariantly constructed wave function follow immediately from the above. The argument is standard: We translate the integration variables in (2.15) by a symmetry transformation (2.12) for which $\epsilon^\alpha(t)$ is nonvanishing only in a neighborhood of t''. The overall integral is unchanged because we are merely changing the variables of integration. The class of paths is unchanged because it is invariant. The action changes according to (2.14) with only the surface term at $t=t''$ contributing because $\epsilon^\alpha(t')=0$. The change in measure and gauge-fixing machinary consists of no more than a change of gauge conditions. The integral with translated integrand therefore takes the form

$$\begin{aligned}\Psi(q^{i''})=\int_{\mathcal{C}}\mathcal{D}z^A\delta(q^i(t'')+\delta q^i(t'')-q^{i''})\\ \times\Delta_{C_\epsilon}[z^A]\delta[C^\alpha_\epsilon(z^A)]\\ \times\exp\{-\sigma(S[z^A]+\delta S[z^A])\} \; .\end{aligned} \tag{2.18}$$

Using the assumed independence of gauge-fixing condition, C^α_ϵ may be replaced by C^α in (2.18). Then, subtracting (2.15) from (2.18), expanding to first order in ϵ^α, and using (2.16) and (2.17), we have

$$\begin{aligned}0=\int_{\mathcal{C}}\mathcal{D}z^A\epsilon^\alpha(t'')\left[-f^i_\alpha(p_i(t''),q^i(t''))\frac{\partial}{\partial q^{i''}}\right.\\ \left.-\sigma F_\alpha(p_i(t''),q^i(t''))\right]\\ \times\delta(q^i(t'')-q^{i''})\Delta_C[z^A]\delta[C^\alpha(z^A)]\\ \times\exp(-\sigma S[z^A]) \; .\end{aligned} \tag{2.19}$$

Then, using (2.17), we find, in some suitable operator ordering,

$$[f^i_\alpha(\hat{p}''_i,\hat{q}^{i''})\hat{p}''_i-F_\alpha(\hat{p}''_i,\hat{q}^{i''})]\Psi(q^{i''})=0 \; , \tag{2.20a}$$

where

$$\hat{p}''_i=-\frac{1}{\sigma}\frac{\partial}{\partial q^{i''}}, \quad \hat{q}^{i''}=q^{i''} \; . \tag{2.20b}$$

This is the main result—a differential operator identity for $\Psi(q^i)$ satisfied as a consequence of a path integral satisfying invariance properties (1)–(5).

The derivation of the operator constraints (2.20) made essential the use of the freedom to prescribe ϵ^α as a function of t. Choosing ϵ^α so that $\epsilon^\alpha(t')=0$ eliminated the surface term at $t=t'$ in δS given by (2.14). However, the operator constraints would still follow if $\epsilon^\alpha(0)$ did not vanish, but the *class of paths* was such that the surface term at $t=t'$ vanished. For example, operator constraints would follow for wave-function constructions satisfying (1)–(5) based on global symmetries with parameters ϵ^α independent of time, provided the class of paths, $\mathcal{C}$, was such that $F_\alpha(p_i,q^i)=0$ at $t=t'$. We shall make use of this special extension of the lemma when considering BRST symmetry in Sec. III.

The variety of theories for which the assumptions (1)–(5) are true and operator constraints follow is best illustrated by specific examples. These will be the topic of the following sections. Before proceeding to them, however, we offer some comments on (1)–(5).

First, we note that the assumption (4) is weaker than that which could be imposed on gauge theories based on compact semisimple Lie groups. We do not require that Δ_C be a determinant as mentioned above. Even if it is, we do not require it to be invariant under gauge transformations, but only that it, together with the measure, transform as (2.16). This will allow extension to nonsemisimple cases. Further discussion of this point may be found in Appendix C.

The above derivation relies on formal manipulations of path integrals and in this sense is general and independent of specific implementations, for example, as a limit of integrals over piecewise linear paths parametrized by the values z^A at a discrete number of times (time slicing). One consequence of this is that no information was obtained on the operator ordering of (2.20a). This depends specifically on how the path integral is implemented.

Moreover, the validity of some of the assumptions may depend on the implementation as well. Specifically, consider assumption (5). This might be derived in a time-slicing implementation of a configuration-space path integral as follows: Divide the interval $t=t'$ to $t=t''$ into $N+1$ intervals of width h at points $t_0, t_1, \ldots, t_N$. The sum over paths may then be represented as a sum *in between* the t slices followed by a sum over the values on the slices. If, as h becomes small, a single classical path dominates the sum in between slices, then one can write

$$\Psi(q^{i''}) = \lim_{N\to\infty} \int_{\mathcal{C}} \prod_{J=0}^{N} \prod_{A} dz_J^A \mu(z_K^A) \delta(q_N^i - q^{i''}) \times \delta[C^\alpha(z_K^A)] \Delta_C[z_K^A] \times \exp\left[-\sigma \sum_{J=0}^{N} S_{\rm cl}(z_{J+1}^A, z_J^A)\right], \tag{2.21}$$

where $S_{\rm cl}$ is the action of the classical path connecting z_J^A to z_{J+1}^A. Equation (2.21) gives a specific implementation of the path integral. Relations such as (2.17) then follow from the classical connection

$$p_N^i = \frac{\partial S_{\rm cl}}{\partial q_N^i}(z_N^A, z_{N-1}^A), \tag{2.22}$$

or from approximations to this, valid to leading order in h. Similar connections hold for time-slicing implementations of phase-space path integrals.[20]

The existence of an implementation such as (2.21) may be crucially dependent on the form of the action and gauge conditions. For example, such a time-slicing implementation is generally known only for Lagrangian actions which are quadratic in the t derivatives. Further, for a single classical path to dominate the sum between slices, its action must become large as h becomes small. For a reparametrization-invariant action, this cannot be true in general for the parameter T is arbitrary. It will be true, however, when the sum is restricted by gauge conditions, C^α, which tie t to a physically meaningful time.[21] Such considerations should be kept in mind when considering the generality of formal statements such as (2.21).

As a final comment, we would like to stress the far-reaching nature of the assumption (2) that the paths are invariant. Commonly, path integrals are used to construct propagators which evolve wave functions in t. The invariance of the action under groups with a functional dependence on t can then be used to show that the constraints are conserved in the sense that, if they are satisfied by the initial wave function, they will be satisfied by the final one. Or, in the case of a symmetry generated by time-independent parameters, it can be shown that an eigenfunction of a conserved quantity remains an eigenfunction. Here a path integral over an invariant set of paths is being used to *construct* wave functions which satisfy the constraints.

We shall now illustrate the application of this lemma in an important class of cases.

C. Constrained Hamiltonian systems

A large and useful class of constrained theories are those theories defined on a phase space (p_i, q^i) for which the constraints $T_\alpha(p_i, q^i)$ are in involution under Poisson brackets:

$$\{T_\alpha, T_\beta\} = U_{\alpha\beta}^{\gamma} T_\gamma, \tag{2.23}$$

where our convention is $\{q^i, p_j\} = \delta_j^i$ and the structure coefficients $U_{\alpha\beta}^\gamma$ may be functions of p_i and q^i. The Hamiltonian action on phase space for such theories takes the standard form

$$S[p_i, q^i, \lambda^\alpha] = \int_{t'}^{t''} dt (p_i \dot{q}^i - H_0 - \lambda^\alpha T_\alpha), \tag{2.24}$$

where λ^α are multipliers which when varied enforce the constraints $T_\alpha = 0$. H_0 is the physical Hamiltonian of the theory and satisfies

$$\{H_0, T_\alpha\} = V_\alpha^\beta T_\beta, \tag{2.25}$$

where V_α^β may depend on p_i and q^i. H_0 vanishes identically when the physical time is included among the dynamical variables q^i (parametrized theories) and the action as a consequence is reparametrization invariant.

Gauge theories, general relativity, and first-quantized string theory are examples of theories of the above type. For gauge theories with four-vector potential, $A_\mu^a(\mathbf{x}, t)$, the q^i represent its spatial components, $q^i \sim A_i^a(\mathbf{x})$, and the λ^α its temporal components, $\lambda^\alpha \sim A_0^a(\mathbf{x})$. The structure coefficients $U_{\alpha\beta}^\gamma$ are constants and $V_\alpha^\beta = 0$. For the case of general relativity described in detail in Sec. IV, the q^i represent the components of the three-metric, $q^i \sim h_{ij}(\mathbf{x})$, and the λ^α represent the lapse and shift, $\lambda^\alpha \sim (N(\mathbf{x}), N^i(\mathbf{x}))$. $H_0 = 0$ and the structure coefficients $U_{\alpha\beta}^\gamma$ depend on q^i, but not p_i.

There exist a great variety of Lagrangian forms of the action corresponding to theories characterized by (2.24). They may be found from (2.24) by using equations of motion to eliminate the momenta or multipliers or both.[21] The result is generally an action of the form (2.1).

The Hamiltonian action (2.24) is invariant under canonical transformations generated by the constraints. To see this, consider the transformations

$$\delta p_i = \{p_i, \epsilon^\alpha T_\alpha\}, \tag{2.26a}$$

$$\delta q^i = \{q^i, \epsilon^\alpha T_\alpha\}, \tag{2.26b}$$

where $\epsilon^\alpha(t)$ is a function of time. An elementary calculation[22] shows that if

$$\delta\lambda^\alpha = \dot{\epsilon}^\alpha - U_{\beta\gamma}^\alpha \lambda^\beta \epsilon^\gamma - V_\beta^\alpha \epsilon^\beta, \tag{2.27}$$

then

$$\delta S = [\epsilon^\alpha F_\alpha(p_i, q^i)]_{t'}^{t''}, \tag{2.28}$$

where

$$F_\alpha = p_i \frac{\partial T_\alpha}{\partial p_i} - T_\alpha. \tag{2.29}$$

Equation (2.28) shows that the equations of motion are invariant under the transformations (2.26) and (2.27) because the action changes by a pure divergence. The action itself is invariant in general only with the additional restrictions[22,23] $\epsilon^\alpha(t')=0=\epsilon^\alpha(t'')$. The exception is when the constraints are linear in the momenta and F_α vanishes identically.

Equation (2.26b) implies

$$\delta q^i=\epsilon^\alpha \frac{\partial T_\alpha}{\partial p_i}\equiv \epsilon^\alpha f^i_\alpha(p_i,q^i) \ . \tag{2.30}$$

This and (2.28) show that constrained Hamiltonian systems fall into the class of theories, satisfying conditions (a) and (b), with which the lemma is concerned. It follows that wave functions Ψ constructed from a path integral satisfying (1)–(5) obey the operator constraint (2.20). Using (2.29) and (2.30), this takes the form

$$T_\alpha(\hat{p}_i,\hat{q}^i)\Psi(q^i)=0 \ . \tag{2.31}$$

All the constraints are therefore satisfied as operator identities. As already mentioned, the explicit construction of path integrals for Ψ satisfying the assumptions is the task of the following sections.

A word is probably in order concerning the connection between the Euclidean and Lorentzian forms of the constraints of the same theory. Consider a theory of the class under discussion defined by an action

$$S[q^i,\lambda^\alpha]=\int_{t'}^{t''} dt\, L(\dot{q}^i,q^i,\lambda^\alpha) \ . \tag{2.32}$$

Suppose now that there is a continuation of the variables $\dot{q}^i,\lambda^\alpha$ *alone* to new real or purely imaginary values such that L becomes a purely imaginary function on the continued values. That is,

$$L(\dot{q}^i,q^i,\lambda^\alpha)=iL^E(\dot{q}^i,q^i,\lambda^\alpha) \ , \tag{2.33}$$

where L^E is purely real on the continued ranges. Such a continuation in some cases can be effected by sending $t\rightarrow -it$, but in other interesting problems (e.g., gauge theories, general relativity) will involve continuation of the λ^α instead or as well.

The Lagrangian L^E defines the Euclidean version of the theory. Clearly,

$$p_i=\frac{\partial L}{\partial \dot{q}^i}=i\frac{\partial L^E}{\partial \dot{q}^i}\equiv ip_i^E \ . \tag{2.34}$$

The Euclidean constraints are found by differentiating L^E with respect to λ^α:

$$T^E_\alpha(p_i^E,q^i)=\frac{\partial L^E}{\partial\lambda^\alpha}\propto\frac{\partial L}{\partial\lambda^\alpha}=T_\alpha(ip_i^E,q^i) \ , \tag{2.35}$$

where the factor of proportionality is ± 1 or $\pm i$, depending on whether or not λ^α was continued to imaginary values. In obtaining this result it was important that the q^i were not continued. The form of the Euclidean constraints expressed in terms of coordinates and momenta will therefore differ in the Euclidean and Lorentzian cases. However, taking note of the operator forms of the momenta in (2.20),

$$p_i=-i\frac{\partial}{\partial q^i},\quad p_i^E=-\frac{\partial}{\partial q^i} \ , \tag{2.36}$$

we see that the operator forms of the constraints are identical up to constant factors of proportionality:

$$T^E_\alpha\left[-\frac{\partial}{\partial q^i},q^i\right]\propto T_\alpha\left[-i\frac{\partial}{\partial q^i},q^i\right] \ . \tag{2.37}$$

Specifically, the operator form of the Hamiltonian constraint for general relativity (the Wheeler-DeWitt equation) will be the same whether the wave function is constructed from a Euclidean or Lorentzian path integral.

It goes without saying that in order for a functional integral to define a wave function satisfying constraints, the functional integral must exist. The Euclidean action for most matter fields is positive definite, and the Euclidean functional integral (1.3) is convergent when the integration is over real field configurations. For gravity, however, the Euclidean Einstein-Hilbert action is unbounded from below and the integral over purely real metrics will not converge. In the gravitational case integrals of the form (2.15) with $\sigma=1$ must be understood to be taken over a *complex* contour such that the integral is convergent. *Any* convergent contour that is invariant, in the sense discussed above, will generate a wave function annihilated by the constraints. The issues involved in identifying suitable contours for a wave function of the universe are discused in Ref. 19.

Having shown generally in this section that the Euclidean and Lorentzian sums over histories yield essentially equivalent operator constraints, we shall, for simplicity, restrict attention to purely Lorentzian examples in what follows.

III. BRST DERIVATION

In the previous section we defined, through a list of four requirements, the notion of an invariant path-integral construction for a wave function and demonstrated, with one further requirement, that a wave function so constructed satisfies operator constraints. In the next sections we shall apply this derivation to wave functions constructed as sums over geometries obeying the dynamics of Einstein's general relativity. We shall be concerned, in particular, with the wave function of the universe defined by the Euclidean sum over geometries of the "no-boundary" proposal. The burden of the demonstration will be to show explicitly that requirements (1)–(5) are satisfied.

General relativity has a well-known Hamiltonian formulation.[24] It might, therefore, seem conceptually most natural to begin considering sums over geometries expressed as Hamiltonian path integrals and applying the derivation of the constraints arising from the Hamiltonian symmetry (2.26) and (2.27) that was discussed in Sec. II C. The immediate task in such an approach would be to demonstrate the invariance (2.16) of the combination of measure and gauge-fixing weight factor Δ_C. As argued by Fradkin and Vilkovisky,[25] when the constraints T_α are not the infinitesimal generators of a group, the factors Δ_C will not, for arbitrary gauges, be determinants of the familiar Faddeev-Popov type.[26] Rather, the factors Δ_C are most easily defined starting from a BRST-invariant form of the sum over geometries and integrating out the ghosts. General relativity is a theory of this kind. The structure functions $U^{\gamma}_{\alpha\beta}$ defining the "algebra" of constraints in general relativity are functions of the canonical coordinates; the constraints are therefore not the generators of a group; and the Δ_C are not Faddeev-Popov determinants for a general gauge. To understand the transformation properties of the Δ_C, we therefore begin with a review of the BRST-invariant path-integral construction of Batalin, Fradkin, and Vilkovisky.[14,27] We shall apply this understanding to a direct derivation of the operator constraints based on the Hamiltonian symmetry of the action in the next section. However, the development of the BFV construction yields an additional dividend: An application of the extension of the general lemma discussed in Sec. II yields an alternative derivation of the operator constraints for invariantly constructed wave functions, as a consequence of the global BRST symmetry of the defining path integral. This BRST derivation of the constraints is the topic of the present section.

Recall that we are interested in wave functions defined by invariantly constructed path integrals for a class of constrained systems described by an action of the form

$$S_0=\int_{t'}^{t''} dt(p_i\dot{q}^{\,i}-H_0-\lambda^{\alpha}T_{\alpha}) , \tag{3.1}$$

where the constraints and the canonical Hamiltonian H_0 are taken to satisfy

$$\{T_{\alpha},T_{\beta}\}=U^{\gamma}_{\alpha\beta}T_{\gamma}, \quad \{H_0,T_{\alpha}\}=V^{\beta}_{\alpha}T_{\beta} . \tag{3.2}$$

The structure coefficients $U^{\gamma}_{\alpha\beta}, V^{\beta}_{\alpha}$ may depend on p_i and q^i. We are primarily interested in the case of general relativity with closed three-surfaces, for which $H_0=0$, but for completeness we will retain H_0.

The T_{α} generate a symmetry of the action S_0. In particular, under the transformations

$$\delta q^i=\epsilon^{\alpha}\{q^i,T_{\alpha}\}, \quad \delta p_i=\epsilon^{\alpha}\{p_i,T_{\alpha}\} , \tag{3.3}$$

$$\delta\lambda^{\alpha}=\dot{\epsilon}^{\,\alpha}-U^{\alpha}_{\beta\gamma}\lambda^{\beta}\epsilon^{\gamma}-V^{\alpha}_{\beta}\epsilon^{\beta} , \tag{3.4}$$

the action changes by an amount

$$\delta S_0=\left[\epsilon^{\alpha}(t)\left[p_i\frac{\partial T_{\alpha}}{\partial p_i}-T_{\alpha}\right]\right]_{t'}^{t''} . \tag{3.5}$$

Equation (3.5) vanishes only if the otherwise arbitrary parameter $\epsilon^{\alpha}(t)$ satisfies the boundary conditions

$$\epsilon^{\alpha}(t')=0=\epsilon^{\alpha}(t'') , \tag{3.6}$$

for those values of α corresponding to T_{α} not strictly linear in the momenta.

The above symmetry of the action may be broken by adding a gauge-fixing term

$$S_{\rm GF}=\int_{t'}^{t''} dt\, \Pi_{\alpha}(\dot{\lambda}^{\alpha}-\chi^{\alpha}(p_i,q^i,\lambda^{\alpha})) . \tag{3.7}$$

Here Π_{α} is a Lagrange multiplier enforcing the gauge-fixing conditions $\dot{\lambda}^{\alpha}=\chi^{\alpha}$ and χ^{α} is an arbitrary function of p_i, q^i, and λ^{α}. Before putting the gauge-fixed action into a path integral, it is necessary to add ghost terms to give the correct measure and so ensure independence of the choice of gauge-fixing condition. The ghost terms are added in such a way that, subject to certain boundary conditions, the total action is invariant under the global symmetry of BRST. According to BFV, the appropriate ghost action is

$$S_{\rm ghost}=\int_{t'}^{t''} dt\left[\bar{\rho}_{\alpha}\dot{c}^{\,\alpha}+\rho^{\alpha}\dot{\bar{c}}_{\alpha}-\bar{\rho}_{\alpha}\rho^{\alpha}-\bar{c}_{\alpha}\{\chi^{\alpha},T_{\beta}\}c^{\beta}-\bar{c}_{\alpha}\frac{\partial\chi^{\alpha}}{\partial\lambda^{\beta}}\rho^{\beta}-\bar{\rho}_{\alpha}V^{\alpha}_{\beta}c^{\beta}-\bar{\rho}_{\alpha}U^{\alpha}_{\beta\gamma}\lambda^{\beta}c^{\gamma}-\frac{1}{2}\bar{c}_{\alpha}c^{\gamma}\{\chi^{\alpha},U^{\beta}_{\gamma\sigma}\}\bar{\rho}_{\beta}c^{\sigma}\right] . \tag{3.8}$$

The ghost fields $c^{\alpha},\bar{\rho}_{\alpha},\bar{c}_{\alpha},\rho^{\alpha}$ and the Lagrange multipliers $\lambda^{\alpha},\Pi_{\alpha}$ satisfy the Poisson-brackets relations

$$\{\bar{\rho}_{\alpha},c^{\beta}\}=\delta^{\beta}_{\alpha}, \quad \{\rho^{\alpha},\bar{c}_{\beta}\}=\delta^{\alpha}_{\beta}, \quad \{\lambda^{\alpha},\Pi_{\beta}\}=\delta^{\alpha}_{\beta} . \tag{3.9}$$

We will use the conventions of Henneaux[10] for the anticommuting variables. In what follows all derivatives are *left* derivatives; e.g., $\delta f(c^{\alpha})=\delta c^{\alpha}(\partial f/\partial c^{\alpha})$.

It is convenient to define an extended phase space including the ghosts and Lagrange multipliers, with coordinates (P_A,Q^A), where

$$Q^A=(q^i,\lambda^{\alpha},c^{\alpha},\bar{c}_{\alpha}), \quad P_A=(p_i,\Pi_{\alpha},\bar{\rho}_{\alpha},\rho^{\alpha}) . \tag{3.10}$$

A BRST transformation on any function F on the extended phase space is then defined to be a canonical transformation of the form

$$\delta F=\{F,\Lambda\Omega\} . \tag{3.11}$$

Here Λ is a constant anticommuting parameter and Ω is the BRST charge

$$\Omega=c^{\alpha}T_{\alpha}+\rho^{\alpha}\Pi_{\alpha}-\tfrac{1}{2}U^{\alpha}_{\beta\gamma}c^{\beta}c^{\gamma}\bar{\rho}_{\alpha} . \tag{3.12}$$

It has the important property that it is nilpotent, $\{\Omega,\Omega\}=0$. This follows from the Jacobi identities derivable from (3.2) (see Appendix B). The BRST charge (3.12) is that appropriate to theories of rank 1 (as defined by Henneaux[10]), which includes gauge theories and general relativity. Extra terms in (3.12) are nescessary for theories of higher rank. Although the following analysis deals explicitly only with the rank-1 case, we expect the extension to the case of higher-rank theories to be straightforward.

The total action may now be concisely written:

$$\begin{aligned}S_T&=S_0+S_{\rm GF}+S_{\rm ghost}\\&=\int_{t'}^{t''} dt[P_A\dot{Q}^{\,A}-H_0-\bar{\rho}_{\alpha}V^{\alpha}_{\beta}c^{\beta}-\{\bar{\rho}_{\alpha}\lambda^{\alpha}+\bar{c}_{\alpha}\chi^{\alpha},\Omega\}] .\end{aligned} \tag{3.13}$$

In this form the BRST invariance of the action is relatively straightforward to demonstrate. The Poisson-brackets term in (3.13) is BRST invariant by virtue of the Jacobi identity and the nilpotency of Ω. The term $H_0+\bar{p}_\alpha V^\alpha_\beta c^\beta$, absent in the case of general relativity, may be shown, at some length, to have zero Poisson brackets with Ω using one of the Jacobi identities derivable from (3.2) (see Appendix B). Finally, since the BRST transformation is just a canonical transformation on the extended phase space, the change coming from $P_A\dot{Q}^A$ is just a boundary term. The total change in the action under a BRST transformation is therefore given by

$$\delta S_T=\left[P_A\frac{\partial(\Lambda\Omega)}{\partial P_A}-\Lambda\Omega\right]_{t'}^{t''} . \tag{3.14}$$

By choosing suitable boundary conditions, this boundary term can be made to vanish, and thus the action will be BRST invariant. A set of boundary conditions which do the job are

$$\begin{aligned} &q^i(t')=q^{i'},\quad \Pi_\alpha(t')=0 ,\\ &c^\alpha(t')=0,\quad \bar{c}_\alpha(t')=0 ,\end{aligned} \tag{3.15}$$

$$\begin{aligned} &q^i(t'')=q^{i''},\quad \Pi_\alpha(t'')=0 ,\\ &c^\alpha(t'')=0,\quad \bar{c}_\alpha(t'')=0 .\end{aligned} \tag{3.16}$$

Other choices of boundary conditions are also possible, but here we will consider only this choice. Note that they are themselves BRST invariant. We shall return to their discussion below.

We may now write down the BFV path integral. It is

$$\Psi(q^{i''})=\int \mathcal{D}P_A\mathcal{D}Q^A\exp(iS_T) . \tag{3.17}$$

The path integral is over all histories $(P_A(t),Q^A(t))$ satisfying the BRST-invariant boundary conditions (3.15) and (3.16). For convenience, we do not exhibit the dependence on $q^{i'}$ in Ψ explicitly. The integral may be defined by a time-slicing procedure, and the measure is then taken to be the canonically invariant Liouville measure on each time slice. For example, an explicit time-slicing definition is

$$\Psi(q^{i''})=\int \prod_{k=1}^{n} dP_A(k)dQ^A(k)\delta(q^i(n)-q^{i''})\times\delta(\Pi_\alpha(n))\delta(c^\alpha(n))\delta(\bar{c}_\alpha(n))\exp(iS_T) . \tag{3.18}$$

On the initial slice $k=0$, the field satisfy the boundary conditions (3.15). There are no integrations of any of the fields on the initial slice. This is because the skeletonization of the action S_T is assumed to be such that, on the $k=0$ slice, it is independent of the fields conjugate to those fixed there.

The whole point of constructing the path integral in this way may now be stated: It is that the path integral (3.17) can be shown to be independent of the choice of gauge-fixing condition. This result is known as the Fradkin-Vilkovisky theorem, and an outline of its proof is given in Appendix A.

Given the BRST-invariant path-integral construction (3.17), we may now apply the extension of the lemma of Sec. II and demonstrate that the BRST symmetry of the construction (3.17) implies that $\Psi(q^{i''})$ is annihilated by the constraints. However, an immediate application of the lemma would lead to a vacuous result. This is because under a BRST transformation with the boundary conditions (3.15) and (3.16), the action and the end-point value of $q^i(t)$ are in fact totally unchanged, $\delta S=0$, $\delta q^i(t'')=0$. It is therefore necessary to relax the boundary conditions a little and first consider the wave function $\tilde{\Psi}(q^{i''},c^{\alpha''})$, defined on an extended configuration space including the ghost fields. This wave function is defined by a path integral of the form (3.17) in which the boundary conditions on the initial surface are the same, but on final the surface (3.16) is replaced by

$$\begin{aligned} &q^i(t'')=q^{i''},\quad \Pi_\alpha(t'')=0 ,\\ &c^\alpha(t'')=c^{\alpha''},\quad \bar{c}_\alpha(t'')=0 .\end{aligned} \tag{3.19}$$

Explicitly,

$$\tilde{\Psi}(q^{i''},c^{\alpha''})=\int \mathcal{D}P_A\mathcal{D}Q^A\delta(q^i(t'')-q^{i''})\delta(\Pi_\alpha(t''))\times\delta(c^\alpha(t'')-c^{\alpha''})\delta(\bar{c}_\alpha(t''))\exp(iS_T) . \tag{3.20}$$

The object of ultimate interest, $\Psi(q^{i''})$, is, of course, obtained by setting the ghosts to zero in (3.20) as the boundary conditions (3.15) or the δ functions in (3.18) show:

$$\Psi(q^{i''})=\tilde{\Psi}(q^{i''},0) . \tag{3.21}$$

Now we apply the lemma of Sec. II to the path integral (3.20), where the transformation δ is taken to be a BRST transformation [Eq. (3.11)]. Under the BRST transformation, the action changes according to (3.14). The contribution from the initial surface vanishes because of the boundary conditions (3.15). The class of paths integrated over will be invariant if, as we assume to be the case, the domains of integration are BRST invariant (this is in fact necessary to assume to prove independence of gauge fixing; see Appendix A). In particular, the Lagrange multipliers must be integrated over an infinite range. This will be discussed in more detail in Sec. IV. There is no gauge-fixing machinery to worry about in the prefactor. Finally, the measure is clearly invariant, because it is the Liouville measure and the BRST transformation is a cononical transformation. The assumptions of the extension of the lemma are therefore straightforwardly satisfied, and the operator identity (2.20) holds.

The terms appearing in the operator identity (2.20) are given by

$$\begin{aligned}(-P_A\delta Q^A)_{t=t''}+\delta S_T &=\left[-P_A\delta Q^A+P_A\frac{\partial(\Lambda\Omega)}{\partial P_A}-\Lambda\Omega\right]_{t=t''}\\ &=-\Lambda\Omega\Big|_{t=t''} ,\end{aligned} \tag{3.22}$$

where we have used the fact that $\delta Q^A=\partial(\Lambda\Omega)/\partial P_A$ (and the derivative is a left derivative, as explained above). Note that (2.20) would strictly only hold for amplitudes with fixed final Q^A, whereas the boundary conditions used here involve fixed final Π_α. However, $\Pi_\alpha(t'')=0$, and so Eq. (3.22) is consistent as it stands. It follows from (3.22) that the wave function $\tilde{\Psi}$ is annihilated by the operator version of the BRST charge (3.12), with $\Pi_\alpha=0$. That is,

$$\hat{\Omega}\tilde{\Psi}(q^i,c^\alpha)\equiv\left[c^\alpha T_\alpha+\frac{i}{2}U^\alpha_{\beta\gamma}c^\beta c^\gamma\frac{\partial}{\partial c^\alpha}\right]\Psi(q^i,c^\alpha)=0\ . \tag{3.23}$$

In (3.23) the momenta p_i have been replaced by the usual operators in T_α and in $U^\alpha_{\beta\gamma}$, and the ghost momenta $\bar{\rho}_\alpha$ have been replaced by the operators $-i\partial/\partial c^\alpha$.

There is, of course, the usual operator-ordering ambiguity in making these replacements. To resolve this one normally demands that $\hat{\Omega}^2=0$. The operator ordering issue then becomes the comparatively trivial issue of finding an ordering for the ghosts, and the distinctly nontrivial issue of finding orderings such that the algebra (3.2) is preserved at the quantum level. We have nothing to say about this latter issue. However, *if* a suitable ordering for the p_i and q^i in T_α and $U^\alpha_{\beta\gamma}$ may be found, *then* the chosen ordering for the ghosts in (3.23) guarantees that $\hat{\Omega}^2=0$.

To complete the derivation, $\tilde{\Psi}(q^i,c^\alpha)$ is expanded in the ghosts. One has

$$\tilde{\Psi}(q^i,c^\alpha)=\Psi(q^i)+c^\alpha A_\alpha(q^i)+c^\alpha c^\beta B_{\alpha\beta}(q^i)+\cdots\ , \tag{3.24}$$

for some coefficients $\Psi, A_\alpha, B_{\alpha\beta},\ldots$ depending only on q^i. By virtue of (3.21), the first coefficient $\Psi(q^i)$ is identified with the physically interesting wave function generated by the sum over histories (3.17). Inserting (3.24) into (3.23) and equating coefficients of the ghosts, one immediately obtains, from the coefficient of c^α,

$$T_\alpha(\hat{q}^i,\hat{p}_i)\Psi(q^i)=0\ . \tag{3.25}$$

This completes the derivation.

It should be noted that this sort of derivation may be carried out in a number of different ways. For example, by choosing suitable boundary conditions, one could use the path integral to generate an object of the form $\Psi(q^i,\Pi_\alpha,c^\alpha,\bar{c}_\alpha)$, show that it is annihilated by the appropriate BRST operator (which would now include Π_α), and then examine the consequences for the coefficient in the ghost expansion obtained by setting $\Pi_\alpha, c^\alpha, \bar{c}_\alpha$ to zero. Alternatively, one could consider the object $\Psi(q^i,\lambda^\alpha,\bar{\rho}_\alpha,\rho^\alpha)$, from which $\Psi(q^i)$ is obtained by integrating over λ^α, $\bar{\rho}_\alpha$, and ρ^α. This particular representation emphasizes the dependence of the derivation of the constraints on the domains of integration. Numerous other choices exist. The particular one we used appeared to be the simplest.

Elegant though the above BRST derivation of the constraints is, it is not without its limitations, especially when applied to sums over geometries. To write the action in the form (3.1), one must assume that the topology of the manifold is $\mathbb{R}\times M^3$, where M^3 is a three-manifold. Then the q^i are the components of the three-metric of a family of foliating surfaces and the p_i then conjugate momenta. The action of the BRST symmetry [Eq. (3.11)] is not local in time, but operates globally at all times. The product structure $\mathbb{R}\times M^3$ must therefore hold for the whole four-manifold.

In many situations in quantum gravity, manifolds more general than products are of interest. The sum over geometries for the no-boundary wave function, for the amplitudes for topology change, and for wormhole processes are among these cases. The no-boundary wave function of the universe, for example, is defined by a sum over geometries on compact four-manifolds with only that boundary necessary to define the argument of the wave function. There is considerable evidence from minisuperspace models[5,9,28,29] that the problem of summing over metrics on some compact manifolds can be mapped onto an equivalent sum of functions on $\mathbb{R}\times M^3$ with *two* boundaries and suitable boundary conditions on the paths at one of the boundaries which are equivalent to compactness. For these situations this BRST derivation of the constraints applies directly. For more general situations, however, it is important to have a derivation of the constraints which does not assume the topology $\mathbb{R}\times M^3$ for the whole manifold. This is provided by the direct derivation based on the *local* Hamiltonian symmetry of the action, which we give the next section.

IV. DIRECT HAMILTONIAN DERIVATION

In its Hamiltonian form, general relativity is an example of a constrained theory whose constraints are in involution. The results of Sec. II C can therefore be applied to yield a direct derivation of the operator constraints for wave functions defined by invariantly constructed sums over histories. In this section we spell out this derivation explicitly.

Recall the standard Hamiltonian formulation of general relativity in the form due to Dirac, and Arnowitt, Deser, and Misner.[24] Since it is the most interesting case for further application, we restrict attention to the case of manifolds M with closed boundaries ∂M, e.g., spatially closed cosmologies. Asymptotically flat spacetimes are therefore specifically excluded. In some neighborhood of the boundary, the topology is $\mathbb{R}\times\partial M$, and the geometry can be foliated by a family of closed spacelike surfaces. Choosing coordinates so these surfaces are labeled by a constant value of the coordinate t, any metric in this neighborhood can be written in standard $3+1$ form:

$$ds^2=-N^2dt^2+h_{ij}(dx^i+N^idt)(dx^j+N^jdt)\ . \tag{4.1}$$

In a region where (4.1) is valid, the action for gravity may be written

$$S_g[N,N^i,h_{ij}]=\int dt\, d^3x\, h^{1/2}N \times[K_{ij}K^{ij}-K^2-(2\Lambda-{}^3R)]\ , \tag{4.2}$$

where K_{ij} is the extrinsic curvature of the constant t surfaces and ^3R is their intrinsic curvature scalar. Explicitly,

$$K_{ij}=\frac{1}{2N}(\dot{h}_{ij}+D_{(i}N_{j)}) , \tag{4.3}$$

where D_i is the derivative in the constant-t surfaces and an overdot denotes a t derivative. The action of matter fields may similarly be expressed in terms of N, N^i, h_{ij} and the field variables through (4.1). For illustrative purposes we shall use a single scalar field $\phi(\mathbf{x},t)$ to represent the matter whose value on a constant-t surface we denote by $\chi(\mathbf{x})$. The field's action may be taken to be

$$S_m[N,N^i,h_{ij},\chi]=-\tfrac{1}{2}\int d^4x\sqrt{-g}\,[(\nabla\phi)^2+V(\phi)] . \tag{4.4}$$

The momenta $\pi^{ij}(\mathbf{x})$ conjugate to $h_{ij}(\mathbf{x})$ can be constructed straightforwardly from (4.2). Similarly, the momentum $\pi_\chi(\mathbf{x})$ conjugate to $\chi(\mathbf{x})$ can be constructed from the matter action. In the total action the multipliers N and N^i occur undifferentiated with respect to time. Variation of the total action with respect to them gives the four constraints of general relativity coupled to matter. These are the $\mathcal{H}(\mathbf{x})$ and $\mathcal{H}_i(\mathbf{x})$ of Eq. (1.4), respectively. There are four constraints for each point $\mathbf{x}$ in the constant-t surfaces.

Classically, the constraints of general relativity are in involution. That is, if we write in an abbreviated notation $\mathcal{H}_\alpha(\mathbf{x})=(\mathcal{H}(\mathbf{x}),\mathcal{H}_i(\mathbf{x}))$,

$$\{\mathcal{H}_\alpha(\mathbf{x}),\mathcal{H}_\beta(\mathbf{x}')\}=\int d^3x''\,U^\gamma_{\alpha\beta}(\mathbf{x},\mathbf{x}';\mathbf{x}'')\mathcal{H}_\gamma(\mathbf{x}'') . \tag{4.5}$$

The explicit form of the structure functions can be found in Ref. 24, but will not be important for us. Just their existence is enough to show that general relativity is a theory of the type discussed in Sec. II C. We note, however, that the structure coefficients are not constants, but depend on the three-metric.

General relativity is a constrained Hamiltonian system of the form discussed in Sec. II C. The coordinates q^i are the three metric $h_{ij}(\mathbf{x})$ and the matter fields $\chi(\mathbf{x})$. There are thus an infinity of them—seven for each spatial point. The momenta p_i are the $\pi^{ij}(\mathbf{x})$ and $\pi_\chi(\mathbf{x})$. The Hamiltonian $H_0=0$ and the constraints T_α are the $\mathcal{H}_\alpha(\mathbf{x})$. On the phase space $(h_{ij},\pi^{ij},\chi,\pi_\chi)$, the Arnowitt-Deser-Misner (ADM) action for the general relativity of closed cosmologies coupled to matter is

$$S[\pi^{ij},h_{ij},\pi_\chi,\chi,N^\alpha]=\int dt\int_{\partial M} d^3x\,[\pi^{ij}(\mathbf{x},t)\dot{h}_{ij}(\mathbf{x},t)+\pi_\chi(\mathbf{x},t)\dot{\chi}(\mathbf{x},t)-N^\alpha(\mathbf{x},t)\mathcal{H}_\alpha(\mathbf{x},t)] . \tag{4.6}$$

This action is invariant under the transformations (2.26) and (2.27):

$$\delta h_{ij}(\mathbf{x},t)=\{h_{ij}(\mathbf{x},t),\int_{\partial M} d^3x'\epsilon^\alpha(\mathbf{x}',t)\mathcal{H}_\alpha(\mathbf{x}',t)\} , \tag{4.7a}$$

$$\delta \pi^{ij}(\mathbf{x},t)=\{\pi^{ij}(\mathbf{x},t),\int_{\partial M} d^3x'\epsilon^\alpha(\mathbf{x}',t)\mathcal{H}_\alpha(\mathbf{x}',t)\} , \tag{4.7b}$$

$$\delta N^\alpha(\mathbf{x},t)=\dot{\epsilon}^\alpha(\mathbf{x},t)-\int_{\partial M} d^3x'd^3x''\,U^\alpha_{\beta\gamma}(\mathbf{x}',\mathbf{x}'';\mathbf{x})N^\beta(\mathbf{x}',t)\epsilon^\gamma(\mathbf{x}'',t) , \tag{4.7c}$$

with matter fields transforming similarly. For example, a scalar field transforms as

$$\delta\chi(\mathbf{x},t)=\{\chi(\mathbf{x},t),\int_{\partial M} d^3x'\epsilon^\alpha(\mathbf{x}',t)\mathcal{H}_\alpha(\mathbf{x}',t)\} . \tag{4.7d}$$

The action is invariant *provided,* as stressed by Teitelboim,[8] that $\epsilon^0(\mathbf{x},t)$ vanishes on all components of the boundary ∂M. If $\epsilon^0(\mathbf{x},t)$ is nonvanishing on a single connected component of ∂M, then the action changes by an amount given by (2.28) and (2.29):

$$\delta S[\pi^{ij},h_{ij},\pi_\chi,\chi,N^\alpha]=\int_{\partial M} d^3x\,\epsilon^0(\mathbf{x})\left[\int d^3y\,\pi^{ij}(\mathbf{y})\frac{\delta\mathcal{H}(\mathbf{x})}{\delta\pi^{ij}(\mathbf{y})}-\mathcal{H}(\mathbf{x})\right] . \tag{4.7e}$$

Since $\mathcal{H}$ is quadratic in the momenta, this is easily expressed in terms of π^{ij}, ^3R, Λ, and the components of the stress-energy tensor of the matter field projected onto the boundary. Specific expressions will not be needed for our argument. The important point is that the change in the action is of the form (2.28) with a function F_α, which depends only on the canonical coordinates and momenta, and not on the multipliers.

The canonical symmetry of the action displayed in Eqs. (4.7) is closely connected with diffeomorphism invariance, but does not coincide with it.[14] Indeed, they act on different spaces. The canonical symmetry acts on the space of extended phase-space histories, while diffeomorphisms act on the space of four-dimensional metrics and field configurations. Under an infinitesimal diffeomorphism generated by a vector field $\xi^\alpha(x)$, the metric and matter field change by

$$\delta g_{\alpha\beta}(x)=2\nabla_{(\alpha}\xi_{\beta)}(x) , \tag{4.8a}$$

$$\delta\phi(x)=\xi^\alpha(x)\nabla_\alpha\phi(x) . \tag{4.8b}$$

However, Eqs. (4.7a), (4.7c), and (4.7d) coincide with Eqs.

(4.8) if ϵ^μ and ξ^μ are identified according to

$$\xi^0=\frac{\epsilon^0}{N}, \quad \xi^i=\epsilon^i-\frac{N^i}{N}\epsilon^0 , \tag{4.9}$$

and *provided* the equations of motion relating time derivatives of coordinates to momenta are satisfied. Thus, when the canonical symmetry of $\mathbb{R}\times$(extended phase space) is projected onto the configuration space of four-dimensional metric and field configurations in this sense, it coincides with diffeomorphism invariance. This connection, however, exists only when an infinitesimal ϵ^α yields an infinitesimal ξ^α and in particular can be expected to fail in those regions of extended phase space near where $N=0$. The failure of the two invariances (4.7) and (4.8) to coincide in the absence of (some of) the equations of motion is common to reparametrization-invariant theories with quadratic constraints. It happens, for example, with the free relativistic particle.[30] The existence of a different symmetry of the action written in canonical form from that of the same action in Lagrangian form, however, does not mean that there are two separate sets of constraints which can be derived from the general results of Sec. II. One way to see this is to note that in a time-slicing implementation of the functional integral, the equations of motion are used to compute the skeletonized action in between slices. For the skeletonized action, therefore, the two symmetries coincide. Another way is to note that for actions which are quadratic in momenta as here, doing the integrals over the momenta gives the same result as substituting the relation between time derivatives and momenta as would arise from the relevant equations of motion. Either way, only one set of constraints are derived. However, when considering the requirements (1)–(5) for an invariant path-integral construction, it is important to keep in mind that the invariance which defines the requirements is the canonical symmetry of (4.7). This will have important consequences for the definition of an invariant class of paths, as we discuss below.

Since relativity is a particular case of a Hamiltonian theory whose constraints are in involution as discussed in Sec. II C, the constraints follow immediately from Eq. (2.31):

$$\mathcal{H}_\alpha(\hat{\pi}_{ij},\hat{h}_{ij},\hat{\pi}_\chi,\hat{\chi})\Psi[h_{ij},\chi]=0 , \tag{4.10}$$

for Ψ's constructed according to the invariant sum-over-histories prescription summarized by assumptions (1)–(5) of Sec. II. We now discuss those requirements. Requirement (1) follows immediately from the form of the action as discussed in Sec. II C and as exhibited explicitly in Eq. (4.7). Requirement (5) we shall assume without further discussion. Requirement (3), independence of gauge fixing, is a consequence of the explicit path-integral construction described in Sec. III, and will be discussed no further. Requirements (2) and (4) merit further comment.

A. Range of the lapse

To satisfy requirement (2) the class of histories must be invariant under the transformation (4.7). In the formulation of this section, that issue chiefly concerns the range of integration over the lapse, $N(\mathbf{x},t)$. Equation (4.7c) shows that the symmetry transformation essentially translates the lapse. The integration range $N=-\infty$ to $+\infty$ is therefore invariant. The range $N=0$ to $+\infty$ is not. Specifically, there is no reason that $\dot{\epsilon}^0$ cannot be negative and thus, near $N=0$, connect positive lapse with negative lapse. To derive the constraints the lapse must be integrated over an infinite range. This conclusion was clearly reached by Teitelboim[17] and is supported by several models and explicit examples.[9,16,17]

Some confusion can arise because positive lapse *is* a range invariant under diffeomorphisms. After all, it follows from (4.1) that $+N(\mathbf{x},t)$ corresponds to the *same* metric as $-N(\mathbf{x},t)$ and, therefore, *a fortiori* to the same geometry. We could *by convention* choose to describe a geometry by a positive lapse function and a diffeomorphism-invariant sum over geometries by an integration over positive lapses. The invariance of the positive lapse range can also be seen explicitly from Eqs. (4.8). Consider a simple reparametrization of t, $t\to f(t)$. A diffeomorphism of the interval [0,1] is a one-to-one mapping of the interval onto itself. The function $f(t)$ must therefore leave the end points unchanged and be monotonic, $\dot{f}(t)>0$. For infinitesimal transformations, $f(t)=t+\xi^0(t)$. Work in the gauge $\dot{N}=0$ and ask, how is the range $N>0$ changed under a diffeomorphism generated by ξ^0? It follows from (4.9) that

$$\dot{\epsilon}^0=N\dot{\xi}^0 . \tag{4.11}$$

The derivative $\dot{\xi}^0$ is finite, and $\dot{\epsilon}^0$ will therefore vanish when N is near zero. Positive lapse is sent into positive lapse for those ϵ^0, which correspond to diffeomorphisms.

Although the positive lapse range is invariant under diffeomorphisms, diffeomorphisms are not the relevant symmetry for deriving the constraints by applying the general lemma of Sec. II. Rather, it is the closely related "canonical" symmetry of Eqs. (4.7). This can be seen in two ways. First, the symmetry (4.7) *is* the symmetry generated by the constraints whose derivation is being attempted. Second, inspection of (2.14) shows that to effect the derivation the $\epsilon^\mu(x)$ must be freely prescribable functions, *independent* of N. For the relevant canonical symmetry, positive lapse is not an invariant range. The requirement that histories be summed over an infinite range of the lapse can be stated in a geometrically invariant way which is independent of any 3+1 decomposition as follows: When the action is written in 3+1 form [Eqs. (4.2) and (4.4)], a change in the sign of the lapse results in a change in the sign of the action S. Each half-range of the lapse corresponds to a diffeomorphism-invariant sum over geometries. Including both positive and negative lapse is therefore equivalent to first summing $\exp(iS)$ over *geometries* where S is defined with a fixed sign for N and adding it to the corresponding sum over $\exp(-iS)$ over the same class of geometries.

B. Invariance of the measure

The second requirement which merits discussion is (4). A Hamiltonian form of the sum over histories to which the lemma can be applied to derive (2.31) can itself be derived, at least locally, from the BFV form of the path integral summarized by Eq. (3.17). It has the form (2.15) where z^A corresponds to $(p_i, q^i, \lambda^\alpha)$ and the action is (2.24). The gauge-fixing conditions are limited to the form

$$C^\alpha(p_i, q^i, \lambda^\alpha) = \dot{\lambda}^\alpha - \chi^\alpha(p_i, q^i, \lambda^\alpha) , \tag{4.12}$$

and the gauge-fixing δ function arises from the integration over Π_α. The associated factor Δ_C is then

$$\Delta_C[p_i, q^i, \lambda^\alpha] = \int \mathcal{D}\bar{\rho}_\alpha \mathcal{D}\rho^\alpha \mathcal{D}c^\alpha \mathcal{D}\bar{c}_\alpha \exp(iS_{\text{ghost}}) , \tag{4.13}$$

where S_{ghost} is given by (3.8). The integral over ghost momenta $\bar{\rho}_\alpha, \rho^\alpha$ can be carried out, yielding

$$\Delta_C[p_i, q^i, \lambda^\alpha] = \int \mathcal{D}c^\alpha \mathcal{D}\bar{c}_\alpha \exp(iS_{\text{ghost}}[c^\alpha, \bar{c}_\alpha, p_i, q^i, \lambda^\alpha]) , \tag{4.14a}$$

where S_{ghost} is the ghost action in the ghost configuration space,

$$S_{\text{ghost}} = \int dt \left[\dot{\bar{c}}_\alpha \delta_c(\dot{\lambda}^\alpha - \chi^\alpha) + \frac{1}{2} \left[\dot{\bar{c}}_\alpha + \frac{\partial \chi^\nu}{\partial \lambda^\alpha} \bar{c}_\nu \right] \bar{c}_\beta \{\chi^\beta, U^\alpha_{\gamma\sigma}\} c^\gamma c^\sigma \right] . \tag{4.14b}$$

Here δ_c denotes a transformation of the form (2.26) and (2.27), in which the parameter ϵ^α has been replaced by the ghost field c^α.

With such an explicit representation, the question naturally arises, does the action of a symmetry transformation (4.7) change the combination of measure and Δ_C in accordance with (2.16b)? More specifically, since the Liouville measure $dp_i dq^i$ is invariant under (4.7), the question is whether under (4.7) one has

$$\mathcal{D}\lambda^\alpha \Delta_C[p_i, q^i, \lambda^\alpha] \rightarrow \mathcal{D}\lambda^\alpha \Delta_{C+\delta C}[p_i, q^i, \lambda^\alpha] \tag{4.15}$$

for some $\delta C[p_i, q^i, \lambda^\alpha]$. This question cannot be answered by the usual "Faddeev-Popov" formal arguments developed for gauge theories for two reasons. First of all, Eq. (4.13) does not define a determinant because S_{ghost} is not quadratic in the ghosts. There is a four-ghost term, which arises as a result of the fact that the structure coefficients for gravity depend on the three-metric. Even for those gauges where the gauge-fixing function χ is independent of p_i, and Δ_C therefore, *is* a determinant, the usual formal argument applies only to semisimple compact Lie groups for which $U^\alpha_{\alpha\beta} = 0$. This is discussed in Appendix C. An explicit calculation is required to verify (4.14). The necessary calculation is carried out in Appendix B. We do not check the invariance (4.15) for all gauges, although it would be reassuring to do so. The Ψ defined by (2.15) is assumed to be independent of the gauge-fixing condition. Indeed, this is explicitly verified in Appendix A. It therefore suffices to check (4.15) in one specific gauge to provide a derivation of the operator form of the constraints. In Appendix B we carry out such a check in the cases of the gauge $\dot{\lambda}^\alpha = 0$ for gravity, and in the more general class of gauge conditions $\dot{\lambda}^\alpha = \chi^\alpha(p_i, q^i, \lambda^\alpha)$ for ordinary gauge theories. The result is that while $\mathcal{D}\lambda^\alpha$ and Δ_C are not separately invariant, their combination is. Requirement (4) is thus satisfied.

Thus, by assumption or calculation, the four requirements for an invariant Hamiltonian path integral for Ψ are satisfied, and we derive

$$\mathcal{H}_\alpha(\hat{\pi}^{ij}, \hat{h}_{ij}, \hat{\pi}_\chi, \hat{\chi}) \Psi[h_{ij}, \chi] = 0 . \tag{4.16}$$

As discussed in Sec. II C [cf. Eq. (2.37)], the *operator* form of the constraints are independent of whether Ψ is constructed from a Euclidean or Lorentzian path integral.

This derivation of the constraints (like the purely Lagrangian one following) has one important advantage over the BRST-BFV derivation given in the previous section. That derivation exploited global BRST symmetry and therefore implicitly assumes the topology $\mathbb{R} \times M^3$ for the manifold M. By contrast, this derivation exploits the local symmetry of diffeomorphism invariance. To obtain the result, the $\epsilon^\mu(\mathbf{x}, t)$ can be taken to vanish outside a neighborhood of the boundary ∂M. A sufficiently small neighborhood has the topology $\mathbb{R} \times M^3$ assumed in this derivation. Indeed, this argument shows that if the boundary ∂M consists of n disconnected compact three-manifolds $\partial M^{(k)}$, $k = 1, 2, \ldots, n$, then the constraints must be satisfied for each boundary *separately*. That is,

$$\mathcal{H}^{(k)}_\alpha(\hat{\pi}^{(k)ij}, \hat{h}^{(k)}_{ij}, \hat{\pi}^{(k)}_\chi, \hat{\chi}^{(k)}) \Psi[h^{(1)}_{ij}, \chi^{(1)}, \partial M^{(1)}, \ldots, h^{(n)}_{ij}, \chi^{(n)}, \partial M^{(n)}] = 0 . \tag{4.17}$$

V. EMBEDDINGS AND DIFFEOMORPHISMS

The results of the preceding two sections show that wave functions constructed from sums over histories which respect the canonical symmetry arising from diffeomorphism invariance satisfy operator equations representing the Dirac constraints generating this symmetry. However, these constraints do not themselves give an operator representation of the algebra of diffeomorphisms; the Dirac "algebra" is *not* the algebra of four-dimensional diffeomorphism, although it is connected to it.[14] Intimately related to this is the fact that the space of wave functions on three-metrics is not large enough to admit a representation of the full algebra of diffeomorphisms in the way that it does for spatial diffeomorphisms. Crudely, this is because, classically, the remaining diffeomorphisms are concerned with displacing the three-surface on which the wave function is defined forward or backward in coordinate time. A three-geometry by itself, however, contains no explicit reference to a coordinate time.

The connection between the "algebra" of constraints and four-dimensional diffeomorphisms has recently been fully discussed in a series of papers by Isham and Kuchař.[15] These authors find a formulation of the classical theory of relativity in which the algebra of constraints *is* the full algebra of four-dimensional diffeomorphisms. The theme of this paper has been the connection between the diffeomorphism invariance of classical general relativity and the operator constraints satisfied by invariantly constructed wave functions in the quantum theory. It seems only appropriate, therefore, to investigate a derivation of constraints which actually implement the algebra of diffeomorphism using the ideas of Isham and Kuchař. We shall sketch such a derivation in this section. In certain respects this derivation will be even more formal than those of the preceding sections. Less attention will be paid to the technical details of establishing the validity of assumptions (1)–(5) of Sec. II. Despite this, this derivation is useful in a number of different ways. (i) It provides a direct and transparent connection between an invariant sum over histories and operator constraints on an extended space which do represent the algebra of four-dimensional diffeomorphisms. (ii) It shows the connection between the operator constraints representing diffeomorphisms on the extended space and the Dirac constraints on familiar superspace. (iii) It introduces new and potentially powerful tools for the construction of geometrical sums over histories. (iv) It makes explicit in an invariant way the "sum over time," which is a part of certain generalizations of quantum mechanics that have been proposed for quantum theories of spacetimes.[31]

A. Extended configuration space

The idea of Isham and Kuchař is to enlarge the configuration space of three-metrics and the spatial matter-field configuration so that the enlarged space *can* carry representations of the full four-dimensional diffeomorphism group. They do this by augmenting the superspace of three-metrics and spatial matter-field configurations by embedding variables which explicitly describe how the spacelike hypersurface on which the wave function is defined is lodged in four-dimensional space. Displacements of this surface in time can be described in terms of these embedding variables and operators effecting these displacements introduced. These new operators represent the nonspatial diffeomorphisms. Of course, such embedding labels are not physically measurable for there are no matter fields in nature which exactly define such an embedding. They must be, therefore, integrated out to form physical amplitudes such as the wave function $\Psi[h_{ij}(\mathbf{x}),\chi(\mathbf{x})]$. However, by understanding the representation of diffeomorphisms on the extended configuration space before this integration is performed, one can understand the connection between constraints and diffeomorphisms in a more transparent way.

A family of spatial hypersurfaces which foilates spacetime may be described by giving four scalar functions $X^\mu(x)$. The function $T(x)\equiv X^0(x)$ labels the surface that the point with spacetime coordinates x^α lies upon. The functions $X^m(x)$ are four coordinates which locate the point within the surface $T(x)$. The inverse functions $x^\alpha(T,X^m)$ are a map from positions X^m on the hypersurface T to the spacetime. They are the embedding variables of Isham and Kuchař (although not in the same notation).

Some words on the notation are probably in order. The $X^\mu=(T,X^m)$ are four scalar functions on spacetime. The indices μ and m are thus not tensorial indices, but serve to list these functions. In this section we shall reserve the latter half of the Greek and Roman alphabets beginning with μ and m for this purpose. Indices in the former half of these alphabets will be usual tensorial ones. In both cases Greek indices range over the values 0 to 3, while Roman indices range from 1 to 3. Finally, it should be noted that our notation for the embedding variables is different from that employed by Isham and Kuchař. They use X^α for our x^α and vice versa.

A metric on spacetime may be specified either by giving its components $g_{\alpha\beta}(x)$ in the coordinates x^α or by giving the lapse $N(x)$, shift $N^m(x)$, and spatial metric $s_{mn}(x)$ in a $3+1$ decomposition appropriate to a foliating family of spatial hypersurfaces together with the embedding variables $X^\mu(x)$, which locate these surfaces in spacetime. Such a description in terms of 14 scalar functionals is, of course, highly redundant. Many sets of these 14 functions correspond to the same metric. We could fix the redundancy by demanding, for example, that the X^μ coincide with the x^α. That would lead back to the description of Sec. IV with no freedom to represent displacements of the spacelike hypersurface in time. Rather, we follow Isham and Kuchař and instead fix the four functions (N,N^m). The freely specifiable $X^\mu(x)$ can then describe displacements of the hypersurfaces. The metric is described by the ten functions $(X^\mu(x),s_{mn}(x))$ with much less, although still some, redundancy. There are a variety[32] of suitable ways of fixing the (N,N^m). The precise way will not be especially important for us. When definiteness is needed, however, we can focus on the "Gaussian coordinate conditions" originally employed by Isham and Kuchař. Then the spacetime metric can be written

$$ds^2=-dT^2+s_{mn}(X)dX^m dX^n\equiv s_{\mu\nu}dX^\mu dX^\nu , \qquad (5.1)$$

or in a general system of spacetime coordinates $x^\alpha=(\tau,x^i)$ as

$$ds^2=[-\nabla_\alpha T\nabla_\beta T+s_{mn}\nabla_\alpha X^m\nabla_\beta X^n]dx^\alpha dx^\beta . \qquad (5.2)$$

The ten scalars $X^\mu(x)$ and $s_{mn}(x)$ describe spacetime geometry. The action can be expressed in terms of these variables by substituting (5.2) for the metric in the familiar form (4.2) and (4.4). Then

$$I=I[X^\mu(x),s_{mn}(x),\phi(x)] . \qquad (5.3)$$

This is the action for a parametrized theory in which the special coordinates $X^\mu(x)$ have been elevated to the status of dynamical variables. By varying the s_{mn} keeping the three-*geometries* fixed on two boundary hypersurfaces, one obtains six Einstein equations. In varying the X^μ one obtains the rest. The correct boundary conditions for this latter variation are to fix X^μ on one boundary surface, but allow it to vary freely on the other. This is correct because, given a metric $g_{\alpha\beta}$, a set of first-order partial differential equations must be solved to find the $X^\mu(x)$, which represent it in the form (5.2). The value of $X^\mu(x)$ may be conventionally prescribed on, say, the initial spacelike surface bounding the region for which the action is to be computed. But then it must be allowed to vary freely on the final surface to reproduce the space of all metrics $g_{\alpha\beta}$. Put differently, extremizing the action (5.3), keeping the X^μ fixed on the boundaries, results in field equations which are derivatives of four of the Einstein equations. The Einstein equations themselves result from the free variation of $X^\mu(x)$ on one boundary. The same conclusion can be reached by considering the Hamiltonian form of the action (5.3).

The action (5.3) is as invariant under diffeomorphisms when expressed in terms of $(X^\mu(x), s_{mn}(x), \phi(x))$ as it was when expressed in terms of $(g_{\alpha\beta}(x), \phi(x))$. The coordinates x^α are completely general. Classically, this invariance of the action under diffeomorphisms implies four constraints between the coordinates and momenta on a spacelike surface. These include not only the three-metric $h_{ij}(\mathbf{x})$ and its conjugate momentum $\pi^{ij}(\mathbf{x})$, but also the values of $X^\mu(\mathbf{x})$ on this surface, which we denote by $Y^\mu(\mathbf{x})$, and their conjugate momentum $P_\mu(\mathbf{x})$. These relations are straightforward to find. Write the metric in standard $3+1$ form

$$ds^2 = -N^2 d\tau^2 + h_{ij}(dx^i + N^i d\tau)(dx^j + N^j d\tau) \ . \quad (5.4)$$

Express N and N^i in terms of X^μ using (5.2). Calculate the momenta conjugate to X^μ. Since the X^μ enter only through the lapse and shift, and since these enter undifferentiated into the action for general relativity, we have

$$P_\mu(\mathbf{x}) = \frac{\partial \mathcal{L}}{\partial N(\mathbf{x})} \frac{\partial N(\mathbf{x})}{\partial \dot{X}^\mu(\mathbf{x})} + \frac{\partial \mathcal{L}}{\partial N^i(\mathbf{x})} \frac{\partial N^i(\mathbf{x})}{\partial \dot{X}^\mu(\mathbf{x})} \ . \quad (5.5)$$

Here $\mathcal{L}$ denotes the Lagrangian density expressed in $3+1$ form and a dot denotes a τ derivative. $\partial\mathcal{L}/\partial N$ and $\partial\mathcal{L}/\partial N^i$ are the standard Hamiltonian and momentum constraints of general relativity $\mathcal{H}$ and $\mathcal{H}_i$, respectively. Calculating the derivatives following Isham and Kuchař, we find the constraints

$$\Pi_\mu(\mathbf{x}) = P_\mu(\mathbf{x}) - n_\mu(\mathbf{x})\mathcal{H}(\mathbf{x}) + Y^i_\mu(\mathbf{x})\mathcal{H}_i(\mathbf{x}) = 0 \ , \quad (5.6)$$

where $n_\mu(\mathbf{x})$ is the unit normal to constant τ surfaces and $Y^i_\mu(\mathbf{x})$ are the three tangent vectors to this surface, $Y^i_\mu = s_{\mu\nu} h^{ij} D_j Y^\nu$. In this expression, $\mathcal{H}(\mathbf{x})$ and $\mathcal{H}_i(\mathbf{x})$ can be regarded as functionals of h_{ij}, π^{ij}, χ, and π_χ. n_μ and Y^i_μ can be expressed entirely in terms of $X^\mu(\mathbf{x})$, its derivatives in the surface, and the metric h_{ij}. For n_μ this follows from

$$n_\mu \propto \epsilon_{\mu\nu\sigma\tau} D_1 Y^\nu D_2 Y^\sigma D_3 Y^\tau \ , \quad (5.7)$$

and the fact that the metric $s_{\mu\nu}$ needed to effect the normalization of n_μ [Eqs. (5.1) and (5.2)] involves no time derivatives. For Y^i_μ it follows from its definition and the same facts. The constraints (5.6) are quadratic in all momenta except P_μ, in which they are linear.

The most important fact concerning the constraints $\Pi_\mu(\mathbf{x})$ on the extended configuration space is that their Poisson-brackets algebra is Abelian:[33]

$$\{\Pi_\mu(\mathbf{x}), \Pi_\nu(\mathbf{x}')\} = 0 \ . \quad (5.8)$$

This, as shown by Isham and Kuchař, is the same as saying the constraints Π_μ generate the algebra of the diffeomorphism group. The generators of diffeomorphisms are vector fields. In the special coordinates of Eq. (5.1), we may represent these as $U^\mu(X^\nu)$, $V^\mu(X^\nu)$, etc. Isham and Kuchař show that the smeared constraints

$$\Pi(U) = \int d^3\mathbf{x}\, U^\mu(X^\nu(\mathbf{x}))\Pi_\mu(\mathbf{x}) \quad (5.9)$$

generate the algebra of the full diffeomorphism group, viz.,

$$\{\Pi(U), \Pi(V)\} = \Pi([U,V]) \ . \quad (5.10)$$

Here $\{\ ,\ \}$ are the canonical Poisson brackets and $[\ ,\ ]$ is the Lie brackets between two vector fields. Explicitly,

$$[U,V] = -(U^\nu \nabla_\nu V^\mu - V^\nu \nabla_\nu U^\mu)\frac{\partial}{\partial X^\mu} \ . \quad (5.11)$$

The constraints on the augmented space of variables generate the algebra of four-dimensional diffeomorphisms.

B. Quantum operator constraints

The fact that a spacetime metric $g_{\alpha\beta}(x)$ may be represented through (5.2) in terms of the fields $(X^\mu(x), s_{mn}(x))$ means that the sum over geometries may be represented as sums over the $(X^\mu(x), s_{mn}(x))$. The sum over the three-metric s_{mn} on surfaces of constant T can be conveniently exchanged for a sum over the three-metrics γ_{ij} on the surface of constant τ since these are related by

$$\gamma_{ij} = s_{mn} D_i X^m D_j X^n - D_i T D_j T \ , \quad (5.12)$$

where D_i is the derivative in the surface. The action (5.3) is invariant under diffeomorphisms and so the familiar gauge-fixing machinery is required in constructing the sum. Thus, in particular, (1.3) can be represented in the neighborhood of ∂M as

$$\Psi[h_{ij}(\mathbf{x}), \chi(\mathbf{x})] = \int_{\mathcal{C}} \mathcal{D}X\, \mathcal{D}\gamma\, \mathcal{D}\phi\, \Delta_C[X,\gamma]\delta(C^\alpha[X,\gamma]) \times \exp(iS[X,\gamma,\phi]) \ . \quad (5.13)$$

The integration is over three-metrices γ_{ij} which induce the metric h_{ij} on the boundary, over matter fields ϕ which induce χ in the boundary, and over the fields X^μ. This integration *includes* an integration over the value of $Y^\mu(\mathbf{x})$ on the boundary. To see why this is so, imagine that the conditions $\mathcal{C}$ were fixed on one boundary while Ψ is calculated on another, ∂M. The values of $X^\mu(x)$ may be conveniently fixed on the boundary associated with $\mathcal{C}$, but they are then determined on ∂M by the metric. An integration over the metric thus includes an integration over the $Y^\mu(\mathbf{x})$ whose range we shall discuss below. The gauge condition $C^\alpha = 0$ must ensure that the functions

$X^{\mu}(x)$ are not only single valued on M, but also form a good coordinate system on M. That is they must be in one-to-one correspondence with the coordinates x^{α}. The easiest way to do this is to make the X^{α} coincide with the x^{α} up to scale. Equation (5.5) is not as unfamiliar as it looks. The integrations over γ and X are essentially the integration over three-metric, lapse, and shift in a $3+1$ decompositions of each four-metric of the form (5.2).

The integration over the $X^{\mu}(x)$ can be carried out in two steps. First, an integration in which the values of $X^{\mu}(x)$ are kept fixed on the boundary and, second, an integration over these values. For the first integration we write

$$\psi[Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})] = \int_{\mathcal{C}} \mathcal{D}X\,\mathcal{D}\gamma\,\mathcal{D}\phi\,\Delta_C[X,\gamma]\delta(C^{\alpha}[X,\gamma]) \times \exp(iS[X,\gamma,\phi]) \,, \tag{5.14}$$

where the integration is as before except that the integration over X^{μ} must match the values $Y^{\mu}(\mathbf{x})$ prescribed on ∂M by the arguments of ψ. The second integration is then

$$\Psi[h_{ij}(\mathbf{x}),\chi(\mathbf{x})] = \int \mathcal{D}Y\,\psi[Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})] \,. \tag{5.15}$$

This integration is over the class of functions $Y^{\mu}(\mathbf{x})$, which induce a good coordinate system on the boundary, that is, say, for which there is a one-to-one correspondence between the values of x^i and $Y^i(\mathbf{x})$.

A physical picture can be associated with the mathematical decomposition of the sum over geometries represented by Eqs. (5.14) and (5.15). Suppose there *were* matter fields $X^{\mu}(x)$ defining a preferred system of coordinates—a system of ideal rods and clocks—so that the spacetime intervals were connected to their values by (5.1). Such fields would necessarily couple to spacetime and other matter as in (5.3). The amplitude $\psi[Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})]$ would then be the physical amplitude for the values $(Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x}))$ to be assumed on a spacelike surface. Or, since the embedding variables $Y^{\mu}(\mathbf{x})$ label a unique spacelike surface, one could say that $\psi[Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})]$ is the amplitude for the three-metric and matter fields to have the values $h_{ij}(\mathbf{x})$ and $\chi(\mathbf{x})$ on the spacelike surface $Y^{\mu}(\mathbf{x})$. The amplitude ψ is then the wave function on that spacelike surface in a familiar sense and, as we shall see below, obeys a familiar Schrödinger equation [Eq. (5.24)]. Of course, there are no such matter fields defining a preferred system of coordinates. However, one can introduce such fields as unphysical labels for convenience in computation *provided* their values are summed over in computing physical amplitudes. This is exactly the significance of (5.15). The use of labels for individual particles which are in fact indistinguishable, or proper time in theories of a relativistic particle, are other examples of the use of unobservable labels in physics. Their hallmark in the theory is that *amplitudes* are summed over their values before computing probabilities. Were they potentially observable quantities, then *probabilities* should be summed over their values when they are not involved.

We shall now show formally that the appropriate invariance of the functional integral defining the amplitude $\psi[Y_{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})]$ implies operator forms of the constraints associated with this invariance in the classical theory on the extended configuration space, that is

$$\hat{\Pi}_{\nu}(\mathbf{x})\psi[Y^{\mu}(\mathbf{x}),h_{ij}(\mathbf{x}),\chi(\mathbf{x})]=0 \,. \tag{5.16}$$

Further, we shall argue that (5.16) and (5.15) together imply the constraints of general relativity on the wave functions $\Psi[h_{ij}(\mathbf{x}),\chi(\mathbf{x})]$, that is

$$\hat{\mathcal{H}}_{\alpha}(\mathbf{x})\Psi[h_{ij}(\mathbf{x}),\chi(\mathbf{x})]=0 \,. \tag{5.17}$$

Yet another derivation of the operator constraints will thus have been achieved.

Indeed, several different derivations of the constraints $\hat{\Pi}_{\mu}\psi=0$ on the extended phase space can be given. For example, we could give a standard canonical derivation following the methods of Sec. IV. However, since the algebra of constraints is *Abelian* [Eq. (5.8)], the familiar Faddeev-Popov construction (Appendix C) applies directly and a derivation from the Lagrangian form of the path integral (5.14) can be given. It is instructive to follow this route first.

To implement the general lemma of Sec. II, we must identify the symmetry of the Lagrangian action which satisfies assumptions (1)–(5). Under an infinitesimal diffeomorphism generated by a vector field $\xi^{\alpha}(x)$, metric and field variables change as follows:

$$\delta g_{\alpha\beta}=2\nabla_{(\alpha}\xi_{\beta)} \,, \tag{5.18a}$$

$$\delta\phi=\xi^{\alpha}\nabla_{\alpha}\phi \,, \tag{5.18b}$$

$$\delta X^{\mu}=\xi^{\alpha}\nabla_{\alpha}X^{\mu} \tag{5.18c}$$

(recall that the X^{μ} are four scalar fields). ∇_{α} is the four-dimensional derivative. The change in the action is easy to calculate. The action is invariant under diffeomorphisms which leave the ends of the range of integration unchanged. However, in order to make use of the results of Sec. II, we consider diffeomorphisms where ξ^{α} may not vanish on the final surface. The change in the action is then entirely the change resulting from the displacement of the final surface. Specifically, for the gravitational action,

$$\delta S_g=(\xi\cdot n)h^{1/2}[K_{ij}K^{ij}-K^2-(2\Lambda-{}^3R)] \,, \tag{5.19}$$

and for the matter action from (4.4),

$$\delta S_m=\tfrac{1}{2}(\xi\cdot n)h^{1/2}[(\nabla\phi)^2+V(\phi)] \,. \tag{5.20}$$

Here n_{μ} is the normal to the final surface. Equations (5.18) and (5.19) can be expressed in $3+1$ form in terms of π^{ij}, h_{ij}, π_{χ}, χ, and the projections of ξ^{α} in the surface and normal to it. These we define by

$$\epsilon^0=(\xi\cdot n)=N\xi^0 \,, \tag{5.21a}$$

$$\epsilon^i=\xi^i+N^i(\xi\cdot n)=\xi^i+N^i\xi^0 \,. \tag{5.21b}$$

The result is

$$\delta S_g = \epsilon^{\perp}[\pi_{ij}\pi^{ij} - \tfrac{1}{2}\pi^2 - h^{1/2}(2\Lambda - {}^3R)] , \tag{5.22a}$$

$$\delta S_m = \tfrac{1}{2}\epsilon^{\perp}[\pi_\chi^2 + V(\chi)] . \tag{5.22b}$$

Similarly, for Eqs. (5.18),

$$\delta h_{ij} = 2D_{(i}\epsilon_{j)} + \epsilon^0 h^{-1/2}(\pi_{ij} - \tfrac{1}{2}h_{ij}\pi) , \tag{5.23a}$$

$$\delta\chi = \epsilon^i D_i\chi + \epsilon^0 h^{-1/2}\pi_\chi , \tag{5.23b}$$

$$\delta X^\mu = \epsilon^i D_i X^\mu + \epsilon^0 n^\mu . \tag{5.23c}$$

Equation (5.22) and (5.23) are of the general form of Eqs. (2.14) and (2.13) *provided* we identify the symmetry of the action with that generated by the *projected* components of the diffeomorphism vector field ξ^α and allow the $\epsilon^\mu(x)$ to be arbitrary infinitesimal functions of x. It will not escape the reader that (5.21) coincides with (4.9), and an elementary calculation shows (5.23) coincides with (4.7). We have thus recovered, in this Lagrangian form, the canonical symmetry of preceding sections.

The action is invariant under diffeomorphisms which preserve the end points no matter how they are parametrized. However, only if written in terms of the 3+1 projections ϵ^μ will the changes in coordinates and action have the special form of (2.13) and (2.14), that is, the form (parameter)$\times$(function of coordinates and momenta alone). Only using this form, can we deduce the constraints. To see this more clearly, imagine using the ξ^α as the parameters. The result would be (2.19) with the brackets multiplied by N. Since N is integrated over, we could not then use (2.17) and conclude (2.20).

Thus, even in this Lagrangian, demonstration, even though we are considering constraints which actually implement the algebra of diffeomorphisms, we conclude that it is the larger canonical symmetry which defines the necessary invariance of the sum-over-histories construction. The ranges of integration, gauge-fixing factors, and measure must be invariant under this symmetry.

An important advantage of the Isham-Kuchař formulation is that the constraints generate an Abelian algebra [Eq. (5.8)]. The method of Faddeev and Popov reviewed briefly in Appendix C may, therefore, be applied directly. The result of the formal argument adumbrated in Appendix C is that Δ_C, the Faddeev-Popov determinant, is *invariant* under the symmetry transformations (5.18). The measure in the sum over histories (5.14) must therefore also be invariant. We have not constructed this measure. It plausibly could be found by beginning with the canonical sum over histories defined with the invariant "Liouville" measure and integrating out the momenta as in the treatments of Leutwyler,[34] and Fradkin and Vilkovisky.[35] The important point is that the measure should be invariant under diffeomorphisms parametrized as in Eq. (5.23). The seeming "noncovariant" nature of this parametrization may well lead to a similar "noncovariant" appearance of the measure, as in the familiar case.[34,35]

The above informal analysis indicates how assumptions (1)–(5) of Sec. II can be satisfied for a sum over histories of the form (5.14) on the expanded configuration space of Isham and Kuchař. We may conclude the operator form of the constraints (5.16). More explicitly, but still formally,

$$i\frac{\delta\psi}{\delta Y^\mu} = \left[n_\mu \mathcal{H}\left[-i\frac{\delta}{\delta h_{ij}}, h_{ij}, -i\frac{\delta}{\delta\chi}, \chi\right] - Y^i_\mu \mathcal{H}_i\left[-\frac{\delta}{\delta h_{ij}}, h_{ij}, \frac{\delta}{\delta\chi}, \chi\right]\right]\psi . \tag{5.24}$$

The n_μ here are regarded as functionals of $Y^\mu(\mathbf{x})$ and $h_{ij}(\mathbf{x})$ defined by (5.7) and the normalization condition. The relations

$$(D_i Y^\mu) Y^j_\mu = \delta^j_i , \tag{5.25a}$$

$$n_\mu D_i Y^\mu = n^\mu Y^i_\mu = 0 , \tag{5.25b}$$

$$n_\mu n^\mu = -1 , \tag{5.25c}$$

where indices μ are raised and lowered with the metric $g_{\alpha\beta}(Y^\mu, h_{ij})$ defined by (5.2) enable the constraints (5.24) to be written in the form

$$in^\mu \frac{\delta\psi}{\delta Y^\mu} = \mathcal{H}(\hat{\pi}^{ij}, \hat{h}_{ij}, \hat{\pi}_\chi, \hat{\chi})\psi , \tag{5.26a}$$

$$iD_i Y^\mu \frac{\delta\psi}{\delta Y^\mu} = \mathcal{H}_i(\hat{\pi}^{ij}, \hat{h}_{ij}, \hat{\pi}_\chi, \hat{\chi})\psi . \tag{5.26b}$$

The operator constraint (5.26a) has a physical interpretation as a Schrödinger equation (or Schwinger-Tomonaga equation) describing evolution in the special hypersurfaces picked out by the fields $X^\mu(x)$. Indeed, yet another way of deriving this constraint would be to repeat the original argument of Feynman for deriving the Schrödinger equation from the path integral for nonrelativistic quantum mechanics.[3] To do this we would need to introduce an explicit implementation of the sum in (5.14), say, by skeletonizing the integral on a coordinate lattice in the x^α. We can then study the "evolution" between the penultimate and final surfaces of constant τ as the lattice spacing is made small.[36]

We now investigate the consequences of the constraints (5.26) for the wave function of the universe Ψ connected with ψ by (5.15). To do this we integrate both sides of (5.26) over all possible spacelike hypersurfaces specified by $Y^\mu(\mathbf{x})$. This integration should be restricted to surfaces which are members of a foliation of spacetime. It should not include, for example, surfaces which are self-intersecting. The range of integration must be invariant under the symmetry (5.23). In particular, this will mean that the values of $n_\mu Y^\mu$ will have to cover an infinite range, over both positive and negative values. The label "time" of the spacelike surfaces must be integrated over an infinite range to recover physical amplitudes [cf. Ref. 18]. In keeping with the adumbrative spirit of this section, we shall propose no explicit implementation of the integral over $Y^\mu(\mathbf{x})$. Rather, we proceed formally and write, using (5.15),

$$\mathcal{H}\Psi[h_{ij}(\mathbf{x}), \chi(\mathbf{x})] = i\int \mathcal{D}Y\, n^\mu \frac{\delta\psi}{\delta Y^\mu} , \tag{5.27a}$$

$$\mathcal{H}\Psi[h_{ij}(\mathbf{x}), \chi(\mathbf{x})] = i\int \mathcal{D}Y\, D_i Y^\mu \frac{\delta\psi}{\delta Y^\mu} . \tag{5.27b}$$

The right-hand sides of Eqs. (5.27) may be integrated by parts. We assume that the sum over histories defining ψ is such that the "surface" terms in this integration vanish. The remaining integrals involve the formal quantities $\delta n^{\mu}(\mathbf{x})/\delta Y^{\mu}(\mathbf{x})$ and $\delta(D_i Y^{\mu}(\mathbf{x}))/\delta Y^{\mu}(\mathbf{x})$. Continuing formally,

$$\frac{\delta(D_i Y^{\mu}(\mathbf{x}))}{\delta Y^{\mu}(\mathbf{x})}=D_i\delta(\mathbf{x},\mathbf{x})=0 \ . \tag{5.28a}$$

A similar expression for the functional derivative of n^{μ} may be found by varying the expressions (5.25) using (5.2) and keeping $h_{ij}(\mathbf{x})$ fixed. Again, one finds

$$\frac{\delta n^{\mu}(\mathbf{x})}{\delta Y^{\mu}(\mathbf{x})}\propto D_i\delta(\mathbf{x},\mathbf{x})=0 \ . \tag{5.28b}$$

Thus, formally, the right-hand sides of Eqs. (5.27) vanish and the constraints

$$\hat{\mathcal{H}}_{\alpha}(\mathbf{x})\Psi[h_{ij}(\mathbf{x}),\chi(\mathbf{x})]=0 \tag{5.29}$$

are recovered for the invariantly constructed wave function of the universe.

VI. SUMMARY AND CONCLUSIONS

The object of this paper has been to elucidate the connection between operator constraints on wave functions in the Dirac quantization procedure and the symmetry properties of a sum-over-histories representation of such wave functions. In particular, we proved, in Sec. II, a lemma showing very generally that wave functions constructed from a sum over histories satisfy a set of operator constraints *provided* the sum over histories is constructed in an *invariant* manner. That is, the path integral should involve, in specific senses, an invariant action, invariant class of paths summed over, and invariant measure, and gauge-fixing machinery.

Applied to gauge theories, the lemma readily shows that a gauge-invariant path-integral construction for a wave function (of the Faddeev-Popov type, for example) satisfies the Gauss-law constraints. When applied to an invariant sum-over-geometries construction for the wave function of the universe, the consequent operator constraints were found to be the Wheeler-DeWitt equation and momentum constraints of canonical quantum gravity. Sections III–V were devoted to constructing three different path-integral representations of the wave function and verifying, in each case, that they were indeed invariant. However, for the case of general relativity, with which this paper is primarily concerned, it was necessary to be precise about exactly which symmetry it is that leads to the constraints.

The Hamiltonian form of the action for general relativity is invariant under the canonical symmetry generated by the constraints. This symmetry transformation may be projected down from extended phase space onto configuration space, by invoking the usual relationship between velocities and momenta. The resulting symmetry transformation on configuration space is not exactly four-dimensional diffeomorphism invariance, but is in fact a larger, more restrictive symmetry. In particular, although a half-infinite range for the lapse N is diffeomorphism invariant, it is not invariant under the canonical symmetry. In each of the three derivations, the constraints were found to follow from the path integral only if the larger canonical symmetry was fully exploited: Invariance of the path-integral construction under four-dimensional diffeomorphisms alone was not sufficient to derive the constraints. In turn, consideration of the canonical symmetry was made necessary by the structure of the general lemma of Sec. II. There the constraints arose from free variations in the action and coordinates arising from the symmetries *projected* into the boundary surfaces. These were the canonical symmetries in the case of canonical forms of the action and coincided with them in the case of the Lagrangian forms.

Our first derivation of the constraints, in Sec. III, was perhaps the most elegant from the technical point of view. There, we gave an explicit construction of the gauge-fixed path integral in Hamiltonian form, using the BFV method. With the gauge-fixing machinery exponentiated using ghost fields and Lagrange multipliers, the path-integral construction is invariant under the global symmetry of BRST. Application of the lemma led immediately to the discovery that wave functions on an extended configuration space including the ghosts are annihilated by the BRST generator. Wave functions on the usual configuration space annihilated by the usual constraints were readily obtained by expanding out in the ghost fields. However, one can still say that it is the canonical symmetry of the Hamiltonian form of the action that leads to the constraints, and not four-dimensional diffeomorphisms, in that the method is a *Hamiltonian* BRST method, and the global BRST symmetry is based on local canonical symmetry.

The most direct derivation of the constraints was that given in Sec. IV. Here the symmetry utilized was the canonical symmetry of the Hamiltonian form of the action, and in this derivation it is most clearly seen that it is this symmetry, and not diffeomorphism invariance, that leads to the constraints. This derivation was technically more cumbersome than the previous one, in that it was necessary to demonstrate the invariance of the gauge-fixing machinery not present in the BRST derivation. The gauge-fixing weight factor Δ_C in the BFV construction could not be regarded as a Faddeev-Popov determinant because in a general gauge, the ghost action from which it is constructed involves a four-ghost coupling. In fact, even in a gauge with no four-ghost term, we found that Δ_C is still not of the Faddeev-Popov type in that it is not gauge invariant. This is because, as explained in Appendix C the usual proof of gauge invariance of the Faddeev-Popov measure relies on the assumption of a compact semisimple Lie group, which does not hold for gravity. We were able to show, however, in Appendix B, that Δ_C combined with the functional integral measure on the Lagrange multipliers $\mathcal{D}\lambda^{\alpha}$ *is* invariant, and this is sufficient for the derivation of the constraints.

Although the derivations of Secs. III and IV establish the connection between invariant sums over histories and the constraints, they fail to make explicit the contact with four-dimensional diffeomorphisms. The canonical symmetry of the Hamiltonian theory, when projected down onto configuration space, is certainly closely related to spacetime diffeomorphisms, but the *algebra* of the constraints of the Hamiltonian theory on the full phase space is *not* the algebra of four-dimensional diffeomorphisms. For this reason we gave, in Sec. V, a derivation which rectified this shortcoming. There, we went to an enlarged phase space which included the embedding variables of a foliating family of spacelike surfaces. As shown by Isham and Kuchař, the (suitably smeared) constraints of this new formulation, linearly related to the old ones, *do* obey the algebra of four-dimensional diffeomorphisms. We gave a sum-over-histories representation of the wave function using this enlarged set of variables and once again derived the constraints. This derivation was less detailed than the previous two, in that we did not devote much attention to, for example, the issue of the construction of the gauge-fixing weight factor, or to the measure and range for the integration over embeddings. These points we hope to return to in a future publication.

It is, however, important to emphasize the following concerning this derivation: Although the *algebra* of the constraints on the enlarged phase space is the algebra of four-dimensional diffeomorphisms, the infinitesimal symmetry transformations generated by the constraints, when projected down onto configuration space, are not quite spacetime diffeomorphisms, but, as we found in the previous sections, constitute a slightly larger symmetry. Once again, we found that the constraints could be derived only if this larger symmetry was fully exploited.

In just two sentences the conclusion of this paper is as follows. Classically invariance implies constraints. Wave functions defined by invariant sums over histories satisfy operator constraints *provided* the notion of an invariant sum over histories is carefully and suitably defined.

Note added. Since the completion of this paper, one of us (J.J.H.) has elaborated on these ideas for the case of global spacetime symmetries—see J. J. Halliwell, MIT CTP Report No. 1927, 1991 (unpublished). This paper considers parametrized scalar field theory in a fixed spacetime background, in which the embedding variables describing the location of the three-surfaces in the spacetime (as introduced in Sec. V above) are raised to the status of dynamical variables. The parametrized field theory is used to give a path-integral representation of the wave functionals for scalar field theory in curved spacetime backgrounds. It is shown that if this path integral is invariant under the isometry group of the spacetime, then the wave functionals so constructed are annihilated by the corresponding global symmetry generators. This result is used to discuss de Sitter–invariant states in the de Sitter spacetime. It is found that only through the embedding variables can one obtain the fullest appreciation of the spacetime symmetries of the wave functionals in the functional Schrödinger picture, a situation reminiscent of that encountered in Sec. V above. In particular, introduction of the embeddings turns out to be essential for the derivation of the global constraints.

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APPENDIX A: FRADKIN-VILKOVISKY THEOREM

The crucial point of the BFV path-integral construction described in Sec. III is that the path integral is independent of the gauge-fixing function. This result is known as the Fradkin-Vilkovisky theorem[10,13] and will be used explicitly in Appendix C, to show that the measure and gauge-fixing machinery have the correct transformation properties for the derivation of the constraints. In fact, the version of the theorem we need is actually a modest generalization of that explicitly written down in Refs. 10 and 13. But before describing this generalization, let us first indicate how the proof of the theorem goes.

So that we can understand the ideas without getting obscured by details, let us consider a finite-dimensional system with (commuting) phase-space coordinates $z^A=(x^i,p_i)$, and consider the path integral

$$\Psi=\int \mathcal{D}x^i(t)\mathcal{D}p_i(t)e^{iS} , \tag{A1}$$

for some action S. We imagine that the path integral is defined by a time-slicing procedure, and $\mathcal{D}x^i(t)\mathcal{D}p_i(t)$ is taken to be the Liouville measure on every time slice. Suppose the action is invariant under a single global symmetry generated by a generating function $F(p,q)$; that is, it is unchanged by the transformation

$$\delta x^i=\epsilon\{x^i,F\}, \quad \delta p_i=\epsilon\{p_i,F\} \tag{A2}$$

where ϵ is a constant parameter. Clearly, the measure is also unchanged by such a transformation. We will further suppose that the class of paths summed over is also invariant.

However, let us see what happens if we perform a change of variables of the form (A2) on (A1), but with ϵ taken to be a *functional* of the fields, $\epsilon=\epsilon[x^i(t),p_i(t)]$. We therefore go to new variables:

$$\tilde{x}^i(t)=x^i(t)+\epsilon\frac{\partial F}{\partial p_i}(x^i(t),p_i(t)) , \tag{A3}$$

$$\tilde{p}_i(t)=p_i(t)-\epsilon\frac{\partial F}{\partial x^i}(x^i(t),p_i(t)) . \tag{A4}$$

The action is still invariant under (A3) and (A4), because ϵ is a constant, but because ϵ is also a functional of the histories, the measure acquires a Jacobian factor J:

$$\mathcal{D}\tilde{x}^i\mathcal{D}\tilde{p}_i=\mathcal{D}x^i\mathcal{D}p_iJ \ , \tag{A5}$$

where

$$J=\det\left|\left|\frac{\delta\tilde{z}^A(t)}{\delta z^B(t')}\right|\right| . \tag{A6}$$

One has

$$\frac{\partial\tilde{x}^i(t)}{\partial x^j(t')}=\delta(t-t')\left[\delta^i_j+\epsilon\frac{\partial^2F}{\partial x^j\partial p_i}\right] + \frac{\delta\epsilon}{\delta x^j(t')}\frac{\partial F}{\partial p_i}(x^i(t),p_i(t)) \ , \tag{A7}$$

$$\frac{\partial\tilde{p}_j(t)}{\partial p_i(t')}=\delta(t-t')\left[\delta^i_j-\epsilon\frac{\partial^2F}{\partial p_i\partial x^j}\right] - \frac{\delta\epsilon}{\delta p_i(t')}\frac{\partial F}{\partial x^j}(x^i(t),p_i(t)) \ , \tag{A8}$$

and

$$\frac{\partial\tilde{p}_j(t)}{\partial x^i(t')}=O(\epsilon)=\frac{\partial\tilde{x}^i(t)}{\partial p_j(t')} . \tag{A9}$$

The matrix in (A6) is thus of the form $I+A$, where $A=O(\epsilon)$, and so $J=1+\mathrm{Tr}A$. The part of A coming from the usual canonical transformation (i.e., what one would have if ϵ was not a functional of the fields) is traceless, as expected, leaving

$$J=1+\int dt\left[\frac{\delta\epsilon}{\delta x^i(t)}\frac{\partial F}{\partial p_i}-\frac{\delta\epsilon}{\delta p_i(t)}\frac{\partial F}{\partial x^i}\right] . \tag{A10}$$

Because (A10) is of the form $1+O(\epsilon)$, we can write it as $\exp[O(\epsilon)]$. This means that the overall effect of the change of variables (A3) and (A4), with $\epsilon=\epsilon[x(t),p(t)]$, is to add to the action a term of the form

$$-i\int dt\left[\frac{\delta\epsilon}{\delta x^i(t)}\frac{\partial F}{\partial p_i}-\frac{\delta\epsilon}{\delta p_i(t)}\frac{\partial F}{\partial x^i}\right] . \tag{A11}$$

This is the main result.

Consider first the following case. Let

$$\epsilon[x^i(t),p_i(t)]=i\int dt\, E(x^i(t),p_i(t)) \ , \tag{A12}$$

where E is an arbitrary infinitesimal function of x^i and p_i. Then (A11) becomes

$$\int dt\left[\frac{\partial E}{\partial x^i}\frac{\partial F}{\partial p_i}-\frac{\partial E}{\partial p_i}\frac{\partial F}{\partial x^i}\right]=\int dt\{E,F\} . \tag{A13}$$

That is, a canonical transformation of an arbitrary function is effectively added to the Lagrangian. What this result implies is that any term of the form (A13) may be simply dropped from the path integral, because it can be got rid of by a change of variables.

The generalization of this derivation to a phase-space path integral including anticommuting variables is straightforward, although we will not go into the details (see, for example, Ref. 10). The Fradkin-Vilkovisky theorem—that the path integral is independent of the gauge-fixing function χ—follows from applying this generalized result to the path integral (3.17), with F taken to be the generator of BRST transformations. However, to prove the desired transformation properties of the path integral below, it turns out that we need to be able to drop not only terms of the form (A13), but also terms involving time derivatives of the fields. For this reason it is necessary to consider the following more general case, not obviously covered by the original works.

Let

$$\epsilon[x^i(t),p_i(t)]=i\int dt\, E(x^i(t),\dot{x}^i(t),p_i(t),\dot{p}_i(t)) \ , \tag{A14}$$

where E now depends on the derivatives of the fields, as well as on the fields themselves. One thus has

$$\frac{\delta\epsilon}{\delta x^i(t)}=\frac{\partial E}{\partial x^i}-\frac{d}{dt}\left[\frac{\partial E}{\partial\dot{x}^i}\right] , \tag{A15}$$

$$\frac{\delta\epsilon}{\delta p_i(t)}=\frac{\partial E}{\partial p_i}-\frac{d}{dt}\left[\frac{\partial E}{\partial\dot{p}_i}\right] . \tag{A16}$$

Equation (A11) now becomes

$$\int dt\left[\frac{\partial E}{\partial x^i}\frac{\partial F}{\partial p_i}-\frac{\partial E}{\partial p_i}\frac{\partial F}{\partial x^i}+\frac{\partial E}{\partial\dot{x}^i}\frac{d}{dt}\left[\frac{\partial F}{\partial p_i}\right] - \frac{\partial E}{\partial\dot{p}_i}\frac{d}{dt}\left[\frac{\partial F}{\partial x^i}\right]\right] \tag{A17}$$

(after integrating by parts and assuming that the boundary terms vanish). Now note, however, that under the transformation generated by F, one has

$$\delta x^i=\frac{\partial F}{\partial p_i},\quad \delta p_i=-\frac{\partial F}{\partial x^i} ,$$

(with $\epsilon=1$). Equation (A17) may therefore be written

$$\int dt\left[\frac{\partial E}{\partial x^i}\delta x^i+\frac{\partial E}{\partial\dot{x}^i}\delta\dot{x}^i+\frac{\partial E}{\partial p_i}\delta p_i+\frac{\partial E}{\partial\dot{p}_i}\delta\dot{p}_i\right] =\delta\int dt\, E . \tag{A18}$$

This is the final result and the most general one we will need.

What the above result means is that the value of the path integral is unchanged by the addition to the action of a term of the form

$$\delta\int dt\, E(x^i,p_i,\dot{x}^i,\dot{p}_i) \ , \tag{A19}$$

where δ is a canonical transformation under which the action is invariant, and E is an arbitrary function of not only x^i,p_i, but also $\dot{x}^i,\dot{p}_i$. One would again expect this result to generalize to the case of interest, namely, that of an extended phase space with the canonical transformation a BRST transformation. Of course, we have not have actually proved this generalized version, but merely indicated how the proof would go. However, we expect the result to be true and we will use it in Appendix B. It is reassuring to note that a detailed proof has been given using the antibracket-antifield formalism.[37]

APPENDIX B: TRANSFORMATION OF THE BFV PATH INTEGRAL

In this appendix we will demonstrate explicitly that the gauge-fixing machinery transforms according to our assumptions.

For convenience we begin by recording the relevant formulas. The original action is

$$S_0=\int_{t'}^{t''}dt(p_i\dot{q}^i-H_0-\lambda^\alpha T_\alpha)\ , \tag{B1}$$

where T_α and H_0 obey the Poisson-brackets relations

$$\{T_\alpha,T_\beta\}=U^\gamma_{\alpha\beta}T_\gamma,\quad \{H_0,T_\alpha\}=V^\beta_\alpha T_\beta\ . \tag{B2}$$

The structure coefficients obey the following Jacobi identities:

$$U^\sigma_{\alpha\beta}U^\mu_{\gamma\sigma}-\{U^\mu_{\alpha\beta},T_\gamma\}+(\text{antisymmetrization on }\alpha\beta\gamma)=0\ , \tag{B3}$$

$$\{H_0,U^\gamma_{\alpha\beta}\}+\{T_\beta,V^\gamma_\alpha\}-\{T_\alpha,V^\gamma_\beta\}+U^\sigma_{\alpha\beta}V^\gamma_\sigma+V^\sigma_\alpha U^\gamma_{\beta\sigma}-V^\sigma_\beta U^\gamma_{\alpha\sigma}=0\ . \tag{B4}$$

The action is invariant under the transformation

$$\delta_\epsilon q^i=\epsilon^\alpha\{q^i,T_\alpha\},\quad \delta_\epsilon p_i=\epsilon^\alpha\{p_i,T_\alpha\}\ , \tag{B5}$$

$$\delta_\epsilon\lambda^\alpha=\dot{\epsilon}^\alpha-U^\alpha_{\beta\gamma}\lambda^\beta\epsilon^\gamma-V^\alpha_\beta\epsilon^\beta\ , \tag{B6}$$

with suitable boundary conditions on ϵ^α.

The gauge-fixing and ghost actions are given, respectively, by (3.7) and (3.8). The content of the Fradkin-Vilkovisky theorem, as we outlined in Appendix A, is that the path integral constructed from these actions is independent of the gauge-fixing function χ. In deriving the transformation properties of the gauge-fixing machinery below, we will be performing a transformation of the form (B5) and (B6) on the gauge-fixing and ghost actions. This will generate, among other terms, terms of the form $\delta_\epsilon\chi$. By the above theorem, the appearance of such terms does not change the value of the path integral, and so they may be dropped. However, because we are working in a so-called "relativistic" gauge, the gauge-fixing action also involves the term $\Pi_\alpha\dot{\lambda}^\alpha$, which under the transformation (B6) leads to a term of the form $\Pi_\alpha\delta_\epsilon\dot{\lambda}^\alpha$ in the gauge-fixing action and to corresponding terms in the ghost action. These extra terms *cannot* be absorbed into the definition of χ. It is for this reason that we need the generalization of the Fradkin-Vilkovisky theorem described in Appendix A.

In anticipation of the extra terms generated, we will add to the total action the term $-\delta_{\rm BRS}(\dot{\bar{c}}_\alpha\psi^\alpha)$, where $\psi^\alpha(q^i,\lambda^\alpha)$ is an arbitrary (commuting) function, depending only on q^i and λ^α, and $\delta_{\rm BRS}$ is a BRST transformation under which the action is invariant. The theorem of Appendix A guarantees that addition of this term will not change the value of the integral. One has

$$-\delta_{\rm BRS}(\dot{\bar{c}}_\alpha\psi)=-\dot{\Pi}_\alpha\psi^\alpha-\dot{\bar{c}}_\alpha\{\psi^\alpha,T_\beta\}c^\beta-\dot{\bar{c}}_\alpha\frac{\partial\psi^\alpha}{\partial\lambda^\beta}\rho^\beta \tag{B7}$$

(restricting to the case in which the $U^\alpha_{\beta\gamma}$ are independent of the p_i). The gauge-fixing and ghost actions are now therefore not just (3.7) and (3.8), but are given by

$$S_{\rm GF}=\int_{t'}^{t''}dt\,\Pi_\alpha(\dot{\lambda}^\alpha+\dot{\psi}^\alpha(q^i,\lambda^\alpha)-\chi^\alpha(p_i,q^i,\lambda^\alpha))\ , \tag{B8}$$

and

$$S_{\rm ghost}=\int_{t'}^{t''}dt\left[\bar{\rho}_\alpha\dot{c}^\alpha+\rho^\alpha\dot{\bar{c}}_\alpha-\bar{\rho}_\alpha\rho^\alpha-\bar{c}_\alpha\{\chi^\alpha,T_\beta\}c^\beta-\bar{c}_\alpha\frac{\partial\chi^\alpha}{\partial\lambda^\beta}\rho^\beta\right.$$
$$\left.-\bar{\rho}_\alpha V^\alpha_\beta c^\beta-\bar{\rho}_\alpha U^\alpha_{\beta\gamma}\lambda^\beta c^\gamma-\frac{1}{2}\bar{c}_\alpha c^\gamma\{\chi^\alpha,U^\beta_{\gamma\sigma}\}\bar{\rho}_\beta c^\sigma-\dot{\bar{c}}_\alpha\{\psi^\alpha,T_\beta\}c^\beta-\dot{\bar{c}}_\alpha\frac{\partial\psi^\alpha}{\partial\lambda^\beta}\rho^\beta\right]\ . \tag{B9}$$

The Fradkin-Vilkovisky theorem is now that the path integral constructed from the actions (B1), (B8), and (B9) is independent of the choice of χ^α and ψ^α. Note that, strictly speaking, the canonical Hamiltonian structure is lost as a result of the appearance of the $\dot{\psi}^\alpha$ term, because the kinetic term in the total action is no longer of the form $P_\alpha\dot{Q}^\alpha$. If one wished to proceed to quantize with a gauge-fixing action of the form (B8), it would be necessary to perform various field redefinitions to recover the original form.[37] This will not be necessary here, however, because we are only introducing ψ^α to see what sort of terms arising in the transformation of the original gauge-fixing and ghost actions (3.7) and (3.8) may be removed by the change of variables described in Appendix A.

With these preliminaries out of the way, we may now proceed to the proof of assumption (4). We will begin by considering the path integral with the gauge conditions

$$C^\alpha(p_i,q^i,\lambda^\alpha)=\dot{\lambda}^\alpha-\chi^\alpha(p_i,q^i,\lambda^\alpha)\ , \tag{B10}$$

and ask how it transforms. Under the transformation (B5) and (B6), the gauge condition is shifted by an amount

$$\delta_\epsilon C^\alpha=\delta_\epsilon\dot{\lambda}^\alpha-\delta_\epsilon\chi^\alpha\ . \tag{B11}$$

This corresponds, in the gauge-fixing action (B8), to going from gauge-fixing functions $\psi^\alpha=0$, χ^α to $\psi^\alpha=\delta_\epsilon\lambda^\alpha$ and $\chi+\delta_\epsilon\chi$. The gauge-fixing weight factor is of the form

$$\Delta_C=\int\mathcal{D}c^\alpha\mathcal{D}\bar{\rho}_\alpha\mathcal{D}\bar{c}_\alpha\mathcal{D}\rho^\alpha\exp(iS_{\rm ghost})\ . \tag{B12}$$

To prove assumption (4), our goal is therefore to prove that under the transformation (B5) and (B6) the change in the quantity $\mathcal{D}z^A\Delta_C$ consists solely of replacing χ by $\chi+\delta_\epsilon\chi$, and $\psi^\alpha=0$ by $\psi^\alpha=\delta_\epsilon\lambda^\alpha$, in the action (B9).

The proof has four steps: (i) We apply the transformation (B5) and (B6) to (B12); (ii) we perform a certain change of variables of the ghosts in the path integral (B12); (iii) we show that the total change in the ghost action in (B12) is precisely the change of the gauge-fixing functions ψ,χ described above; (iv) we show that the change in the measure in the path integral (B12) is precisely canceled by the change in the measure $\mathcal{D}z^A$.

We have not been able to carry out the proof in the case of general relativity for all gauge choices of the form (B10), but only for the case $\chi^\alpha=0$. We have, however, been able to treat the case of arbitrary χ^α for ordinary gauge theories. We therefore treat each of these two cases separately.

1. General relativity in the gauge $\dot\lambda^\alpha=0$

For general relativity, one has $H_0=0$, $V^\beta_\alpha=0$, and the structure coefficients $U^\alpha_{\beta\gamma}$ depend only on the q^i. In the gauge $\dot\lambda^\alpha=0$, the ghost action is

$$S_{\text{ghost}}=\int_{t'}^{t''}dt(\bar\rho_\alpha\dot c^\alpha+\rho^\alpha\dot{\bar c}_\alpha-\bar\rho_\alpha\rho^\alpha-\bar\rho_\alpha U^\alpha_{\beta\gamma}\lambda^\beta c^\gamma)\ . \tag{B13}$$

Step (i). Under the transformation (B5) and (B6), the only change in Δ_C comes from the ghost action. It is

$$\delta_\epsilon S_{\text{ghost}}=\int_{t'}^{t''}dt(-\bar\rho_\alpha c^\gamma\epsilon^\sigma\{U^\alpha_{\beta\gamma},T_\sigma\}\lambda^\beta-\bar\rho_\alpha c^\gamma U^\alpha_{\beta\gamma}\dot\epsilon^\beta+\bar\rho_\alpha c^\gamma U^\alpha_{\beta\gamma}U^\beta_{\mu\nu}\lambda^\mu\epsilon^\nu)\ . \tag{B14}$$

Step (ii). Now we perform a change of variables, which we denote $\tilde\delta$, on the ghosts in the path integral (B12):

$$\tilde\delta c^\alpha=U^\alpha_{\beta\gamma}\epsilon^\beta c^\gamma,\quad \tilde\delta\bar\rho_\alpha=-U^\gamma_{\beta\alpha}\epsilon^\beta\bar\rho_\gamma\ , \tag{B15}$$

$$\tilde\delta\rho^\alpha=U^\alpha_{\beta\gamma}\epsilon^\beta\rho^\gamma,\quad \tilde\delta\bar c_\alpha=0\ . \tag{B16}$$

The resulting change in the ghost action is

$$\tilde\delta S_{\text{ghost}}=\int_{t'}^{t''}dt(U^\alpha_{\beta\gamma}\epsilon^\beta\rho^\gamma\dot{\bar c}_\alpha+\bar\rho_\alpha U^\alpha_{\beta\gamma}\dot\epsilon^\beta c^\gamma+\bar\rho_\alpha\dot U^\alpha_{\beta\gamma}\epsilon^\beta c^\gamma+\bar\rho_\nu c^\gamma U^\alpha_{\beta\gamma}U^\nu_{\sigma\alpha}\lambda^\beta\epsilon^\sigma-\bar\rho_\alpha c^\nu U^\alpha_{\beta\gamma}U^\gamma_{\sigma\nu}\lambda^\beta\epsilon^\sigma)\ . \tag{B17}$$

Step (iii). Combining (B17) and (B14), the terms involving $\dot\epsilon^\alpha$ cancel, and the total change in the ghost action is

$$\begin{aligned}\delta_\epsilon S_{\text{ghost}}+\tilde\delta S_{\text{ghost}}=\int_{t'}^{t''}dt[&-\bar\rho_\alpha c^\gamma\epsilon^\sigma\{U^\alpha_{\beta\gamma},T_\sigma\}\lambda^\beta+U^\alpha_{\beta\gamma}\epsilon^\beta\rho^\gamma\dot{\bar c}_\alpha+\bar\rho_\alpha\dot U^\alpha_{\beta\gamma}\epsilon^\beta c^\gamma\\ &+\bar\rho_\alpha c^\gamma\epsilon^\sigma\lambda^\beta(U^\mu_{\sigma\beta}U^\alpha_{\gamma\mu}+U^\mu_{\beta\gamma}U^\alpha_{\sigma\mu}+U^\mu_{\gamma\sigma}U^\alpha_{\beta\mu})]\ .\end{aligned} \tag{B18}$$

Now consider the first term in (B18) and the three terms which involve two structure coefficients. We may use the Jacobi identity (B3) on these four terms, and (B18) simplifies to

$$\delta_\epsilon S_{\text{ghost}}+\tilde\delta S_{\text{ghost}}=\int_{t'}^{t''}dt[\bar\rho_\alpha\epsilon^\beta c^\gamma(\dot U^\alpha_{\beta\gamma}-\{U^\alpha_{\beta\gamma},\lambda^\sigma T_\sigma\})+\dot{\bar c}_\alpha U^\alpha_{\gamma\beta}\rho^\gamma\epsilon^\beta-\bar\rho_\alpha c^\sigma\{U^\alpha_{\beta\gamma},T_\sigma\}\lambda^\beta\epsilon^\gamma]\ . \tag{B19}$$

As we discussed in Sec. IV, we are allowed to use the field equations obtained by extremizing the action with respect to the momenta (i.e., the relationship between momenta and velocities). In particular, we may use the equations

$$\dot U^\alpha_{\beta\gamma}=\{U^\alpha_{\beta\gamma},\lambda^\sigma T_\sigma\},\quad \dot{\bar c}_\alpha=-\bar\rho_\alpha\ . \tag{B20}$$

Equation (B19) therefore becomes

$$\delta_\epsilon S_{\text{ghost}}+\tilde\delta S_{\text{ghost}}=\int_{t'}^{t''}dt(\dot{\bar c}_\alpha U^\alpha_{\gamma\beta}\rho^\gamma\epsilon^\beta+\dot{\bar c}_\alpha c^\sigma\{U^\alpha_{\beta\gamma},T_\sigma\}\lambda^\beta\epsilon^\gamma)\ . \tag{B21}$$

Equation (B21) is precisely of the form

$$\int_{t'}^{t''}dt\left[-\dot{\bar c}_\alpha\frac{\partial\psi^\alpha}{\partial\lambda^\beta}\rho^\beta-\dot{\bar c}_\alpha\{\psi^\alpha,T_\beta\}c^\beta\right]\ , \tag{B22}$$

with $\psi^\alpha=\delta_\epsilon\lambda^\alpha$. This therefore completes step (iii).

Step (iv). Finally, we consider the transformation of the measure in (B12) and the measure $\mathcal{D}z^A$. Consider first

$$\mathcal{D}z^A=\mathcal{D}q^i\mathcal{D}p_i\mathcal{D}\lambda^\alpha\ . \tag{B23}$$

The transformation (B5) is canonical on the pair q^i,p_i, and so the measure $\mathcal{D}q^i\mathcal{D}p_i$ is invariant, and we need only worry about the measure $\mathcal{D}\lambda^\alpha$. Now consider the measure in (B12):

$$\mathcal{D}c^\alpha\mathcal{D}\bar\rho_\alpha\mathcal{D}\bar c_\alpha\mathcal{D}\rho^\alpha\ . \tag{B24}$$

The transformation (B15) is canonical, and so the part of the measure $\mathcal{D}c^\alpha\mathcal{D}\bar\rho_\alpha$ is invariant. The remaining part of the measure (B24) is not, however, invariant under (B16).

So it remains for us to consider how the remaining part of measure

$$\mathcal{D}\rho^\alpha\mathcal{D}\lambda^\alpha \tag{B25}$$

transforms under the change of variables (B6) and (B16), which we rewrite

$$\delta_\epsilon \lambda^\alpha = U^\alpha_{\beta\gamma}\epsilon^\beta\lambda^\gamma + \dot{\epsilon}^\alpha , \tag{B26}$$

$$\tilde{\delta}\rho^\alpha = U^\alpha_{\beta\gamma}\epsilon^\beta\rho^\gamma . \tag{B27}$$

Providing the range of integration of the λ^α integrals is taken to be infinite, the essentially constant shift $\dot{\epsilon}^\alpha$ may be absorbed, and the transformations (B26) and (B27) on λ^α and ρ^α are then identical. The Jacobian factor arising from the change in the measure for each thus involves an expression of the form $(1+U^\alpha_{\alpha\beta}\epsilon^\beta)$, which does not vanish. However, because ρ^α is anticommuting, the Jacobian arising in the transformation of its measure is precisely the *inverse* of that arising from the transformation of $\mathcal{D}\lambda^\alpha$. The two Jacobians therefore cancel and (B25) is invariant. This completes the proof of assumption (4).

2. Gauge theories in the gauge $\dot{\lambda}^\alpha = \chi^\alpha$

For gauge theories one has $H_0 \neq 0$ and $U^\alpha_{\beta\gamma}=\text{const}$. We will also allow the V^β_α to be nonzero constants, although they vanish for most cases of interest. Rather than go through the whole proof again, we will just consider the extra terms that arise as a result of including χ^α and V^β_α and show that they cancel.

Consider first the extra terms arising due to χ^α. In step (i) the extra terms contributing to $\delta_\epsilon S_{\text{ghost}}$ are

$$\int_{t'}^{t''} dt \left[-\bar{c}_\alpha\{\delta_\epsilon\chi^\alpha, T_\beta\}c^\beta - \bar{c}_\alpha \frac{\partial}{\partial\lambda^\beta}(\delta_\epsilon\chi^\alpha)\rho^\beta \right. \\ -\bar{c}_\alpha\{\chi^\alpha, T_\sigma\}U^\sigma_{\beta\gamma}\epsilon^\gamma c^\beta \\ \left. -\bar{c}_\alpha\frac{\partial\chi^\alpha}{\partial\lambda^\gamma}U^\gamma_{\beta\sigma}\epsilon^\sigma\rho^\beta \right] , \tag{B28}$$

where we have used the fact that

$$\delta_\epsilon\left[\frac{\partial\chi^\alpha}{\partial\lambda^\beta}\right] = \frac{\partial}{\partial\lambda^\beta}(\delta_\epsilon\chi^\alpha) - \frac{\partial\chi^\alpha}{\partial\lambda^\gamma}\frac{\partial}{\partial\lambda^\beta}(\delta_\epsilon\lambda^\gamma) . \tag{B29}$$

In step (ii) the extra terms contributing to $\tilde{\delta}S_{\text{ghost}}$ are

$$\int_{t'}^{t''} dt \left[-\bar{c}_\alpha\{\chi^\alpha, T_\sigma\}U^\sigma_{\gamma\beta}\epsilon^\gamma c^\beta - \bar{c}_\alpha\frac{\partial\chi^\alpha}{\partial\lambda^\gamma}U^\gamma_{\sigma\beta}\epsilon^\sigma\rho^\beta \right] . \tag{B30}$$

Equation (B30) precisely cancels with the third and fourth terms in (B28), showing that the overall change is just a change of gauge-fixing function, $\chi^\alpha \to \chi^\alpha + \delta_\epsilon\chi^\alpha$, which is the desired result.

Now consider the extra terms arising due to V^β_α. In step (i) an extra term arises in $\delta_\epsilon S_{\text{ghost}}$ through the transformation of λ^α [Eq. (B6)]. It is

$$\int_{t'}^{t''} dt\, \bar{\rho}_\gamma U^\gamma_{\alpha\sigma}V^\alpha_\beta\epsilon^\beta c^\sigma . \tag{B31}$$

In step (ii) the presence of the term $\bar{\rho}_\alpha V^\alpha_\beta c^\beta$ leads, in $\tilde{\delta}S_{\text{ghost}}$, to the terms

$$\int_{t'}^{t''} dt\, \bar{\rho}_\gamma\epsilon^\beta c^\sigma(U^\gamma_{\beta\alpha}V^\alpha_\sigma - V^\gamma_\alpha U^\alpha_{\beta\sigma}) . \tag{B32}$$

However, it is readily seen that the sum of (B31) and (B32) vanishes, by virtue of the Jacobi identity (B4). This completes the proof of assumption (4) for gauge theories.

For the most general case, the presence of the four-ghost term, absent in the two cases above, severely complicates matters, and we have not been able to carry out the calculation explicitly.

APPENDIX C: FADDEEV-POPOV ARGUMENT

Faddeev and Popov have given an elegant and direct formal argument for arriving at the gauge-fixed form of (2.15) of a sum over histories for gauge theories whose gauge group is a semisimple Lie group.[26] The result of this argument that Δ_C—the Faddeev-Popov invariant determinant—and the measure are separately invariant under transformations of the form (2.12). To appreciate why the ostensibly more complicated (or at least more lengthy) arguments for the invariance of the combination $\mathcal{D}z_A\Delta_C$ are necessary for gravitational theories or for gauge theories based on nonsemisimple Lie groups, it is instructive to understand how the Faddeev-Popov construction does not apply to these cases. Since our discussion is probably well known to some (indeed we learned much of it from Teitelboim), we shall be brief.

The Faddeev-Popov argument runs like this: Consider a gauge field $A(x)$ (group and spacetime indices suppressed) whose action is invariant under g: $A \to {}^gA$, where g is an element of a group G. For a gauge-fixing condition $C(A)=0$, define a partition of unity by

$$1 = \Delta_C[A]\int d\mu_R(g)\delta[C({}^gA)] , \tag{C1}$$

where $d\mu_R(g)$ is the *right* invariant measure on G. Equation (C1) is taken to define Δ_C. It is a direct consequence of the right invariance of $d\mu_R(g)$ that Δ_C so defined is invariant under gauge transformations:

$$\Delta_C[{}^gA] = \Delta_C[A] . \tag{C2}$$

Insert (C1) into any sum over gauge fields defined by a gauge-invariant measure and a gauge-invariant integrand [e.g., exp (iS)]. A translation of the integration variable factors the integral into an invariant gauge-fixed form involving the combination $\Delta_C[A]\delta[C(A)]$ times an integral over the gauge group. This latter integral contributes an overall multiplicative factor of the group volume. This is the Faddeev-Popov result.

An integral analogous to that in (C1) over the *left* invariant group measure is easily evaluated as a determinant:

$$\int d\mu_L(g)\delta[C({}^gA)] = \det M_C(A) , \tag{C3}$$

where M_C is the response of C to an infinitesimal group action away from that value s for which the gauge condition is satisfied. That is, if $C[{}^sA]=0$ and $g=s+\xi$,

$$\delta_\xi C = C[{}^{s+\xi}A] - C[{}^sA] \equiv M_C(A)\xi . \tag{C4}$$

The integral in (C3) becomes explicit when written out in terms of coordinates on the group manifold. The infinitesimal elements ξ define vectors with components

ξ^a at the element s. A left translation of the integration in (C3), $\xi \rightarrow r\xi$, $r \epsilon G$, can be chosen so the transformed eigenvectors of M_C coincide with the coordinate directions. Equation (C3) follows directly. Since a left translation is involved, it is the left invariant measure which is relevant in (C3).

For groups where the left and right invariant measures coincide, Δ_C and $\det M_C$ are related by

$$\Delta_C[A] = [\det M_C(A)]^{-1} . \tag{C5}$$

This will be the case, for example, for semisimple Lie groups.[38] The identity (C5) allows Δ_C to be expressed as an integral over ghost fields in a familiar way.

When left and right invariant measure coincide, it follows from (C5) and (C2) that $\det M_C(A)$ is invariant under gauge transformation. When they do not coincide, it is not invariant, but its transformation properties may be computed from (C3). Let T_a be the infinitesimal generators of G satisfying $[T_a, T_b] = C^c_{ab} T_c$. Then in "canonical" coordinates $\Lambda^a(g)$, such that $g = \exp(\Lambda^a T_a)$, we have[39]

$$d\mu_L(g) = d\mu_R(g) \exp[\omega(g)] , \tag{C6}$$

where

$$\omega(g) = \Lambda^c(g) C^a_{ca} . \tag{C7}$$

Then, using the invariance the integrals in (C1), it is easy to compute that

$$\delta_\xi [\det M_C(A)]^{-1} = (1 + \delta_\xi \Lambda^c C^a_{ca})(\det M_C)^{-1} . \tag{C8}$$

Thus only when the trace of the structure constants vanishes will $\det M_C$ be invariant under gauge transformations. The trace vanishes for semisimple groups.[38]

The Faddeev-Popov construction of a gauge-fixed sum over histories involving a gauge-invariant determinant thus works directly only for theories whose symmetries are based on group [so that Eq. (C1) is meaningful] and further a group whose left and right invariant measures coincide [so that Eq. (C5) follows]. Invariant sums over histories constructed for gravitational theories in their Hamiltonian form do not fall in this class. Most importantly, as stressed by many,[10,13] the infinitesimal symmetries of the Hamiltonian action do not exponentiate to form a group. The structure functions $U^\alpha_{\beta\gamma}$ are *functions* of the canonical coordinates, not structure *constants*. It is for this reason that the more general BFV construction, whose invariance can be explicitly demonstrated, is needed.

As the above arguments show, even if the BFV construction is used to *define* a sum over histories in the Faddeev-Popov form by integrating out the ghost fields, we cannot expect the individual parts of the resulting integrand to have the transformation properties of the Faddeev-Popov case. In such a construction Δ_C would be *defined* by the integral of the ghost action over the ghost fields as in (4.12). Where the ghost action is not quadratic, it will not define a determinant. Even when it does so, it may not be invariant under gauge transformations because of (C8). The transformation properties of Δ_C were the subject of the previous appendix. Indeed, the transformation law (C8) may be explicitly verified by the techniques described there. What Appendix B does show is that, although Δ_C may not be a determinant, and although it may not be invariant, the combination $\mathcal{D}z_A \Delta_C$ transforms in such a way as to define an invariant path integral in the sense of Sec. II.

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[36]More specifically, the sum over histories in (5.14) can be thought of as a sum over $(X^\mu(x),\gamma_{ij}(x),\phi(x))$ *in between* the constant τ planes followed by a sum over the values *on* all planes except the last where the values must coincide with the argument of ψ. A small value of ϵ does not necessarily guarantee that the sum in between lattice planes will be dominated by the classical history. The action is *invariant* under the reparametrizations of τ, so that there is no fixed meaning to a small ϵ. However, the integral over histories (5.14) is carried out in the presence of gauge-fixing conditions which dictate a fixed relationship between the general coordinates x^α and the special fields $X^\mu(x)$. Two slices which differ by a small amount of $T(x)$ everywhere differ by a small amount of proper time [cf. (5.2)], and in the presence of such gauge conditions the action becomes large as ϵ becomes small. The sum in between the slices becomes dominated by the classical history, and we obtain a skeletonized path integral of the form to which Feynman's derivation can be applied.

[37]J. M. L. Fisch and M. Henneaux, Phys. Lett. B **226**, 80 (1989).

[38]See, e.g., M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison-Wesley, Reading, MA, 1962), p. 309ff.

[39]This was explained to us by Claudio Teitelboim. For an application of this difference in other circumstances, see C. Teitelboim, J. Math. Phys. **25**, 1093 (1984).