Derivation of the Wheeler-DeWitt equation from a path integral for minisuperspace models

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(Received 29 March 1988)

We explore the relationship between path-integral and Dirac quantization for a simple class of reparametrization-invariant theories. The main object is to study minisuperspace models in quantum cosmology—models for quantum gravity in which one restricts attention to a finite number of degrees of freedom. Our starting point for the construction of the (Lorentzian) path integral is the very general and powerful method introduced by Batalin, Fradkin, and Vilkovisky. Particular attention is paid to the measure in the large, i.e., to the range of integration of the Lagrange multiplier. We show how to derive the Wheeler-DeWitt equation from our path-integral expression. The relationship between the choice of measure in the path integral and the operator ordering in the Wheeler-DeWitt equation is thus determined. The operator-ordering ambiguity in the Wheeler-DeWitt equation is completely fixed by demanding invariance under field redefinitions of both the three-metric and the lapse function. Our results are applied to two simple examples: the nonrelativistic point particle in parametrized form and the relativistic point particle. We also consider a simple minisuperspace example and discuss a difficulty that arises: namely, the problem of incorporating the fact that $\det h_{ij} > 0$ into the quantization procedure.

I. INTRODUCTION

Feynman's path-integral method provides a third formulation of quantum mechanics, very different, but complementary to the Schrödinger and Heisenberg canonical quantization methods.[1] The relationship between this method and the canonical quantization methods has been well explored for systems such as nonrelativistic quantum mechanics, which are described by a time-dependent Schrödinger equation; that is, there exists a derivation of the Schrödinger equation from the path integral. Most field theories of current interest, however, involve constraints reflecting gauge invariance, or reparametrization invariance. The canonical quantization method is then that of Dirac, in which the constraints become operators which annihilate physical states.[2] For these theories, the relationship between the Dirac quantization method and the path-integral method does not seem to have been very well explored.

One of the most interesting constrained systems is general relativity. In its Hamiltonian formulation, the theory is portrayed as the dynamics of three-surfaces.[3] There are four constraints, reflecting the invariance of the theory under four-dimensional diffeomorphisms. Three of the constraints, the momentum constraints, are linear in the momenta and generate diffeomorphisms within the three surfaces. This symmetry of the theory is very similar to that of an ordinary gauge theory. The fourth constraint, however, the Hamiltonian constraint, is quadratic in the momenta, and it is this that distinguishes general relativity from an ordinary gauge theory. The Hamiltonian constraint expresses the invariance of the theory under time reparametrizations, but it also generates the dynamics; thus the symmetry and dynamics of the theory are inextricably entangled. Because the quantization of ordinary gauge theories has been well studied, and because reparametrization invariance is a distinguishing feature of general relativity, it is of interest to those concerned with quantum gravity to study the quantization of simple models whose only symmetry is reparametrization invariance.

In this paper we will study in some detail the relationship between the Dirac and path-integral quantization methods for a class of reparametrization-invariant theories described by an action of the form

$$S=\int_{t'}^{t''} dt[p_\alpha \dot{q}^\alpha - NH(p_\alpha, q^\alpha)] \ . \tag{1.1}$$

Here N is a Lagrange multiplier which enforces the constraint $H=0$. The simplest examples of systems described by such an action are the nonrelativistic point particle in parametrized form and the relativistic point particle, although the main examples we will be concerned with are the minisuperspace models of quantum cosmology.[4] These are models for quantum gravity in which one freezes all but a finite number of degrees of freedom of the metric. This is often done, for example, by writing the four metric in the form

$$ds^2=-N^2(t)dt^2+h_{ij}dx^i dx^j \ , \tag{1.2}$$

where N is the lapse function, and an ansatz is made for the three metric h_{ij}, so that it is homogeneous and is described by a finite number of functions $q^\alpha(t)$. The q^α would typically be scale factors, anisotropy parameters, etc. With this ansatz, the momentum constraints of general relativity

$$\mathcal{H}^i=-2\pi^{ij}{}_{|j}=0 \tag{1.3}$$

are then vacuously satisfied, and the Hamiltonian constraint

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

reduces (after integration over the three-surface) to an expression of the form

$$H=\tfrac{1}{2}f^{\alpha\beta}(q)p_\alpha p_\beta+V(q)=0\ . \tag{1.5}$$

Here $f^{\alpha\beta}$ is the inverse of the metric on minisuperspace, $f_{\alpha\beta}$, and is of hyperbolic signature, $(-,+,+,+,\ldots)$. The system is therefore described by an action of the form (1.1).

In the Dirac quantization of this system, one introduces a wave function $\Psi(q)$, a function on minisuperspace. This function is annihilated by the operator version of the constraint (1.5):

$$\hat{H}\Psi(q)=0\ , \tag{1.6}$$

where in (1.6), the momenta have been replaced by the corresponding operators in the usual manner. There is an ambiguity in the canonical quantization procedure, because $f^{\alpha\beta}$ depends on q and one does not know how to distribute it between the momentum operators. This is the notorious operator-ordering problem. For gravitational systems (1.6) is known as the Wheeler-DeWitt equation.

In the path-integral quantization method the wave function is represented by an expression of the form

$$\Psi=\int \mathcal{D}p\,\mathcal{D}q\,\mathcal{D}N\exp\left[i\int dt(p_\alpha\dot{q}^\alpha-NH)\right]\ . \tag{1.7}$$

Since the action (1.1) is reparametrization invariant, it is necessary to include ghost and gauge-fixing terms in (1.7), to ensure that equivalent histories are counted only once. It is then normally asserted that expression (1.7) satisfies the Wheeler-DeWitt equation, (1.6), although this has never been demonstrated in detail.

The purpose of this paper is to construct the path integral (1.7), including all the ghost and gauge-fixing terms, and to define it explicitly, using a time-slicing procedure. We will then show, subject to certain assumptions, that it satisfies the Wheeler-DeWitt equation, and thus determine the relationship between the measure in (1.7) and the operator ordering in (1.6).

We begin in Sec. II by discussing the action, its reparametrization invariance, and gauge-fixing conditions which break it. The path integral for the propagation amplitude $G(q''\,|\,q')$ is constructed in Sec. III using the the method of Batalin, Fradkin, and Vilkovisky[5] (BFV). In Sec. IV a particular choice of gauge is made, and the integration over the ghost fields and Lagrange multipliers is performed. This yields a simple expression for the propagator, similar to the proper-time representation of Green's functions of the Klein-Gordon equation.[6] In Sec. IV the formalism is applied to the relativistic point particle and the nonrelativistic point particle in parametrized form. These examples clarify the range of integration of the Lagrange multiplier N (this is not fixed by the BFV procedure). In Sec. VI it is shown that the issue of driving the Wheeler-DeWitt equation reduces to a study of the derivation of the time-dependent Schrödinger equation in curved backgrounds. Previous work on this issue is described, and the relation between the path-integral measure and the operator ordering in the Wheeler-DeWitt equation thus determined. Invariance under field redefinitions of the three-metric restricts the Wheeler-DeWitt equation to be of the form

$$(-\tfrac{1}{2}\nabla^2+\xi R+V)\Psi=0\ , \tag{1.8}$$

where ∇^2 and R are the Laplacian and curvature in the minisuperspace metric, and ξ is an arbitrary constant. In Sec. VII we evaluate the path integral exactly for a simple model, and show that it satisfies the Wheeler-DeWitt equation. In Sec. VIII we discuss the invariance of the quantization procedure under field redefinitions of the lapse function. We show that for it to be invariant, one has to choose ξ in (1.8) in such a way that the operator $-\frac{1}{2}\nabla^2+\xi R$ is conformally covariant. The operator ordering is thus completely determined. In Sec. IX we discuss the problem of incorporating the fact that $\det h_{ij}>0$ into the path-integral quantization procedure, a problem noted in the minisuperspace example of Sec. VII. We summarize and conclude in Sec. X.

II. THE ACTION

We consider an action of the form

$$S=\int_{t'}^{t''}dt\,(p_\alpha\dot{q}^\alpha-NH)\ , \tag{2.1}$$

where α runs over D values and H is given by

$$H=\tfrac{1}{2}f^{\alpha\beta}(q)p_\alpha p_\beta+V(q)\ . \tag{2.2}$$

Much of what follows will depend only on the fact that H is quadratic in the momenta. p_α and N are free at the end points and the q^α are fixed and satisfy the boundary conditions

$$q^\alpha(t')=q^{\alpha'},\quad q^\alpha(t'')=q^{\alpha''}\ . \tag{2.3}$$

Variation with respect to p_α and q^α yields the field equations

$$\dot{q}^\alpha=N\{q^\alpha,H\},\quad \dot{p}_\alpha=N\{p_\alpha,H\}\ , \tag{2.4}$$

and variation with respect to N yields the constraint

$$H(p_\alpha,q^\alpha)=0\ . \tag{2.5}$$

The constraint reflects the most central feature of the action (2.1), which is that it is invariant under reparametrizations. More precisely, under the transformations

$$\delta q^\alpha=\epsilon(t)\{q^\alpha,H\},\quad \delta p_\alpha=\epsilon(t)\{p_\alpha,H\},\quad \delta N=\dot{\epsilon}(t)\ , \tag{2.6}$$

the action changes by an amount

$$\delta S=\left[\epsilon(t)\left[p^\alpha\frac{\partial H}{\partial p^\alpha}-H\right]\right]\Bigg|_{t'}^{t''}\ , \tag{2.7}$$

where $\epsilon(t)$ is an arbitrary parameter. Since, unlike the situation in gauge theories, the constraint H is quadratic in the momenta, (2.7) vanishes, if and only if,

$$\epsilon(t')=0=\epsilon(t'')\ . \tag{2.8}$$

The action is therefore invariant under reparametrizations (2.6) subject to the boundary conditions (2.8).

Before constructing a quantum theory based on the action (2.1), it is necessary to impose gauge-fixing conditions which break the reparametrization invariance (2.6). As discussed by Teitelboim,[7] the gauge-fixing condition must satisfy the following requirements: (i) it must fix the gauge completely, i.e., there must be no residual gauge freedom; (ii) using the transformations (2.6) it must be possible to bring any configuration, specified by p,q,N, into one satisfying the gauge condition.

These requirements are satisfied by a gauge-fixing condition of the form

$$\dot{N}=\chi(p,q,N) \ , \tag{2.9}$$

where χ is an arbitrary function of p, q, and N. This type of condition is analogous to the relativistic gauge-fixing condition used in ordinary gauge theories, $\partial^\mu A_\mu=0$ (A_0 plays the role of a Lagrange multiplier in the Hamiltonian formulation of gauge theories). An alternative possibility is to use the analogue of a canonical gauge (e.g., $\partial^i A_i=0$ or $A_3=0$), and this has been discussed by Hartle and Kuchar.[8] For parametrized theories, this involves singling out one of the dynamical variables, q^0 say, as a physical time coordinate. One then imposes a condition of the form $q^0=f(t)$, where f is an arbitrary monotonically increasing function of the time parameter t. The relationship between relativistic and canonical gauge-fixing conditions appears to be rather subtle for parametrized theories, and we hope to return to this issue in a future publication. The main difference is that the canonical condition restricts the paths to move forward in the direction of increasing q^0, whereas the condition (2.9) implies no such restriction. In this paper we will work only with condition (2.9).

The gauge condition (2.9) may be imposed at the level of the action using a Lagrange multiplier. One writes

$$S+S_{\rm gf}=\int_{t'}^{t''}dt\,[p_\alpha\dot{q}^\alpha-NH+\Pi(\dot{N}-\chi)] \ , \tag{2.10}$$

where $\Pi(t)$ is a Lagrange multiplier which, as we shall soon see, must vanish at the end points:

$$\Pi(t')=0=\Pi(t'') \ . \tag{2.11}$$

Let us check that (2.10) yields the correct field equations. Variation with respect to p_α and q^α yields

$$\dot{q}^\alpha=N\{q^\alpha,H\}+\Pi\{q^\alpha,\chi\} \ , \tag{2.12}$$

$$\dot{p}_\alpha=N\{p_\alpha,H\}+\Pi\{p_\alpha,\chi\} \ . \tag{2.13}$$

Variation with respect to Π yields the gauge condition (2.9), as intended, and variation with respect to N, subject to (2.11), yields the equation

$$\dot{\Pi}+H=0 \ . \tag{2.14}$$

Differentiating (2.14) with respect to t, and then using (2.12) and (2.13) one obtains the following equation for Π:

$$0=\ddot{\Pi}+\dot{H}=\ddot{\Pi}+\{\chi,H\}\Pi \ . \tag{2.15}$$

Since, however, Π is required to vanish at both end points, the unique solution to (2.15) is $\Pi(t)=0$ identically. The action (2.10) with the boundary conditions (2.11) thus yields the original field equations.

Finally, we note that the following exception to this conclusion exists. Equations (2.12) and (2.13) imply that $\{H,\chi\}$ is a constant, K say. If K just happened to take the value $n^2\pi^2/(t''-t')^2$, where n is an integer, then there would be nontrivial solutions to (2.15) satisfying the boundary conditions (2.11): namely, the eigenfunctions of the operator $-d^2/dt^2$, $\sin(n\pi[(t-t')/(t''-t')])$. However, we will eventually be working in the gauge $\chi=0$, for which this exceptional case cannot arise.

III. THE PATH INTEGRAL

Given the action (2.10), one might be tempted to proceed directly to a path-integral expression, since the action is now that of an unconstrained system. There is a good reason, however, why one cannot yet do this. This is that there is no guarantee that the resulting path-integral expression will be independent of our choice of gauge-fixing function χ; or in other words, we do not know what the measure is.

This problem is overcome by going to an extended phase space which includes ghost fields. Batalin, Fradkin, and Vilkovisky (BFV) have developed a very general method for doing this, based on Becchi-Rouet-Stora (BRS) invariance.[5] The basic idea is that one adds anticommuting ghost terms to the gauge-fixed action (2.10) in such a way that the resulting action is invariant under the global BRS symmetry. One then writes down a path integral in which the measure is taken to be the Liouville measure on the extended phase space (P,Q) consisting of the original bosonic variables plus the ghost fields. It is then possible to show, using a judiciously chosen BRS transformation on the variables (P,Q), that the path integral so constructed is independent of the choice of gauge-fixing function χ. This result is known as the Fradkin-Vilkovisky theorem.[5]

Rather than write down the ghost action straight away, we shall try and proceed in a more systematic fashion, although it is the nature of the subject that there are logical jumps which may only be totally justified retrospectively. BRS symmetry involves replacing the parameter $\epsilon(t)$ in (2.6) with $\Lambda c(t)$ where Λ is a constant anticommuting parameter and $c(t)$ is an anticommuting ghost field. Eventually, we wish to generate the BRS transformations using a Poisson bracket, so it is necessary to eliminate the time derivatives from the transformations. One therefore writes $\dot{c}=\rho$, and this is imposed in the action by adding a term $\bar{\rho}(\dot{c}-\rho)$, where ρ and $\bar{\rho}$ are (anticommuting) ghost field momenta. To make ρ dynamical, one then adds a term $\bar{c}\dot{\rho}$. The (provisional) ghost action is therefore given by

$$S_{\rm gh}=\int_{t'}^{t''}dt\,(\bar{\rho}\dot{c}+\bar{c}\dot{\rho}-\bar{\rho}\rho) \ . \tag{3.1}$$

With $\epsilon=\Lambda c$ and $\dot{c}=\rho$, Eq. (2.6) gives the BRS transformations

$$\delta p_\alpha=-\Lambda c\frac{\partial H}{\partial q^\alpha}, \quad \delta q^\alpha=\Lambda c\frac{\partial H}{\partial p_\alpha}, \quad \delta N=\Lambda\rho \ . \tag{3.2}$$

Under these transformations, the action (2.1) changes by

$$\delta S = \int_{t'}^{t''} dt \Lambda(\dot{c}-\rho)H + \left[\Lambda c(t) \left[p_\alpha \frac{\partial H}{\partial p_\alpha} - H \right] \right]_{t'}^{t''} . \tag{3.3}$$

Since ϵ satisfies (2.8), we will impose the boundary conditions

$$c(t') = 0 = c(t'') \tag{3.4}$$

and thus the second term in (3.3) vanishes. The first term is not zero, however, since $\dot{c} = \rho$ only on shell.

The idea now, is to find transformations of the remaining variables such that the total action is unchanged. The gauge-fixing term changes by

$$\delta S_{\text{gf}} = \int_{t'}^{t''} dt \left[\delta\Pi(\dot{N} - \chi) + \Pi \left[\Lambda\dot{\rho} - \Lambda c\{\chi, H\} - \Lambda\rho \frac{\partial \chi}{\partial N} \right] \right] \tag{3.5}$$

and the change in the ghost action is given by

$$\delta S_{\text{gh}} = \int dt \, [\delta\bar{\rho}(\dot{c}-\rho) + \delta\bar{c}\dot{\rho} + \bar{\rho}(\delta\dot{c} - \delta\rho) + \bar{c}\delta\dot{\rho}] . \tag{3.6}$$

If $\chi = 0$, it is easily seen that $\delta S + \delta S_{\text{gf}} + \delta S_{\text{gh}} = 0$, if one takes

$$\begin{aligned} &\delta\Pi = 0, \quad \delta c = 0, \quad \delta\rho = 0 , \\ &\delta\bar{c} = -\Lambda\Pi, \quad \delta\bar{\rho} = -\Lambda H . \end{aligned} \tag{3.7}$$

Moreover, for $\chi \neq 0$, it is not difficult to show that this is still the case if one adds the terms $c\{\chi, H\}\bar{c} + \rho(\partial\chi/\partial N)\bar{c}$ to the ghost action. The final form of the ghost action is, therefore,

$$S_{\text{gh}} = \int_{t'}^{t''} dt \left[\bar{\rho}\dot{c} + \bar{c}\dot{\rho} - \bar{\rho}\rho + c\{\chi, H\}\bar{c} + \rho \frac{\partial \chi}{\partial N}\bar{c} \right] . \tag{3.8}$$

The boundary conditions (3.4), supplemented with the conditions

$$\bar{c}(t') = 0 = \bar{c}(t'') \tag{3.9}$$

will ensure that the ghost fields vanish classically (ρ and $\bar{\rho}$ are free at the end points). To summarize, the total action is

$$S_T = S + S_{\text{gf}} + S_{\text{gh}} \tag{3.10}$$

and this is invariant under the BRS transformations (3.2) and (3.7), subject to the boundary conditions (3.4). The action yields the field equations (2.4) and (2.5) if one imposes the boundary conditions (2.3), (2.11), (3.4), and (3.9).

The BRS transformations may be concisely expressed by introducing the BRS charge $\Omega = cH + \rho\Pi$ and any BRS transformation is then of the form $\delta F = \{F, \Lambda\Omega\}$. The total action may now be written as

$$S_T = \int_{t'}^{t''} dt (p_\alpha \dot{q}^\alpha + \Pi\dot{N} + \bar{\rho}\dot{c} + \bar{c}\dot{\rho} - \{\bar{\rho}N + \bar{c}\chi, \Omega\}) . \tag{3.11}$$

The BRS invariance is now manifest. The "Hamiltonian" term is invariant by virtue of the Jacobi identity (and $\{\Omega, \Omega\} = 0$) and, since the BRS transformation is a canonical transformation on the extended phase space, the "$P\dot{Q}$" term changes by at most a boundary term, which vanishes as a consequence of the boundary conditions.

Given the gauge-fixed BRS-invariant action, we may now proceed to the path integral. Let

$$G_\chi(q^{\alpha''} \mid q^{\alpha'}) = \int \mathcal{D}\mu \exp(iS_T) , \tag{3.12}$$

where

$$\mathcal{D}\mu = \mathcal{D}p_\alpha \mathcal{D}q^\alpha \mathcal{D}\Pi \, \mathcal{D}N \, \mathcal{D}\rho \, \mathcal{D}\bar{c} \, \mathcal{D}\bar{\rho} \, \mathcal{D}c . \tag{3.13}$$

The integral may be defined by a time-slicing procedure and the measure (3.13) is then taken to be the Liouville measure $dP \wedge dQ$ on each time slice. The boundary conditions on the path integral are those discussed already: N, p_α, ρ, and $\bar{\rho}$ are integrated over on every slice, including the end-point slices; c, $\bar{c}$, and π are fixed and equal to zero at the end-point slices and q^α is fixed and satisfies (2.3) at the end points. More will be said later about the details of the skeletonization and the ranges of integration.

The key point of the BFV approach is that it is now possible to show that (3.12) is independent of the choice of gauge-fixing function χ. This is achieved by changing variables in the path integral (3.12) from the variables (P, Q) to a net set of canonical variables $(\tilde{P}, \tilde{Q})$ which are related to the old ones by a BRS transformation (3.2) and (3.7) with $\Lambda = -i \int dt \, \bar{c}(\tilde{\chi} - \chi)$. The action S_T is clearly invariant under this transformation, but since Λ is a functional of the fields, the measure acquires a Jacobian factor:

$$\mathcal{D}\mu = \mathcal{D}\tilde{\mu} \exp \left[i \int dt \{\bar{c}(\chi - \tilde{\chi}), \Omega\} \right] . \tag{3.14}$$

This factor has the effect of replacing χ by $\tilde{\chi}$ in (3.12). It follows that $G_\chi = G_{\tilde{\chi}}$, and thus the path integral is independent of χ, at least formally. This is the Fradkin-Vilkovisky theorem.

Certain qualifying remarks need to be made in relation to his result. First, the result is only formal in that it involves some kind of generalized canonical transformation on the variables of integration, but without referring to a particular definition of the path integral—by skeletonization, for example. It is very difficult to implement even genuine canonical transformations (i.e., those with $\Lambda = \text{const}$) in phase-space path integrals, let alone the more general class of transformations involved above.[9] It would be interesting to see if the above result can still be made to go through using a skeletonized definition of (3.12).

The second point is that one has to be careful about the boundary conditions and the domain of integration in (3.12). It is important that the domain of integration is preserved by the above change of variables. For the bosonic variables, this will be true if they are integrated over a fully infinite range. As we shall see, however, one may wish to allow N to take a half-infinite range, in which case the theorem may not work. We hope to return to this point in a future publication.

IV. THE GHOST AND LAGRANGE-MULTIPLIER INTEGRATIONS

Since the path integral is independent of χ, we may now make the gauge choice $\chi=0$. As a result of this choice, the ghosts decouple from the other variables and the ghost integration may be performed. We define this integration by splitting the time interval into $n+1$ equal intervals, $t''-t'=\epsilon(n+1)$. With a particular choice of skeletonization, the functional integral over the ghost fields is

$$\int \mathcal{D}\bar{\rho}\,\mathcal{D}c\,\mathcal{D}\rho\,\mathcal{D}\bar{c}\,\exp\left[i\int dt(\bar{\rho}\dot{c}+\bar{c}\dot{\rho}-\bar{\rho}\rho)\right]$$
$$=\int d\rho_{1/2}\cdots d\rho_{n+1/2}\int d\bar{\rho}_{1/2}\cdots d\bar{\rho}_{n+1/2}\int dc_1\cdots dc_n\int d\bar{c}_1\cdots d\bar{c}_n \times\exp\left[i\sum_{k=0}^{n}[\bar{\rho}_{k+1/2}(c_{k+1}-c_k)+\rho_{k+1/2}(\bar{c}_{k+1}-\bar{c}_k)-\epsilon\bar{\rho}_{k+1/2}\rho_{k+1/2}]\right], \tag{4.1}$$

where $c_0=0=c_{n+1}$ and $\bar{c}_0=0=\bar{c}_{n+1}$. In this and the following expressions it is implicit that the limit $\epsilon\to 0$ is taken, although some of the path integrals are so simple that this is not in fact necessary. Also, the particular choice of skeletonization is not important for the simple path integrals of this and the next section. The path integrals for which it is important are discussed in Sec. VI.

The integrations in (4.1) are carried out according to the usual rules of Berezin integration.[10] By shifting the variables of integration, the integration over the momenta may be performed, with the result

$$(i\epsilon)^{n+1}\int dc_1\cdots dc_n\int d\bar{c}_1\cdots d\bar{c}_n\exp\left[-\frac{i}{\epsilon}\sum_{k=0}^{n}(\bar{c}_{k+1}-\bar{c}_k)(c_{k+1}-c_k)\right]. \tag{4.2}$$

This in turn may be evaluated, to yield $(t''-t')$. This is what one would expect, for the following reason. The path integral (4.1) is very similar to that for the free nonrelativistic point particle, for which we know that the propagator is proportional to $(t''-t')^{-1/2}$. It differs, however, in that there are twice as many fields, and they are Grassmannian. One would therefore expect (4.1) to be proportional to the squared inverse of the propagator of the point particle, which is indeed the case. The ghost integration produces precisely the factor required to ensure that the final result is independent of t'' and t', as we shall see.

We may also carry out the integrations over Π and N. Since Π is fixed at the end points, while N is integrated over, it seems appropriate to skeletonize Π as a coordinate and N as a momentum. That is, we define the path integral over the gauge-fixing term to be

$$\int \mathcal{D}N\,\mathcal{D}\Pi\,\exp\left[i\int dt\,\Pi\dot{N}\right]=\int dN_{1/2}\cdots dN_{n+1/2}\frac{1}{(2\pi)^n}\int d\Pi_1\cdots d\Pi_n\exp\left[i\sum_{k=1}^{n}\Pi_k(N_{k+1/2}-N_{k-1/2})\right], \tag{4.3}$$

where $\Pi_0=0=\Pi_{n+1}$. This is equal to

$$\int dN_{1/2}\cdots dN_{n+1/2}\prod_{k=1}^{n}\delta(N_{k+1/2}-N_{k-1/2}). \tag{4.4}$$

We have n δ functions and $n+1$ integrations, and thus the functional integration over $N(t)$ collapses to a single ordinary integration over N ($=N_{1/2}$ say). With these simplifications, the path integral (3.12) reduces to

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\int dN(t''-t')\int \mathcal{D}p_\alpha\mathcal{D}q^\alpha\exp\left[i\int_{t'}^{t''}dt(p_\alpha\dot{q}^\alpha-NH)\right]. \tag{4.5}$$

This is the main expression we will be working with in the following sections. It is essentially the integral over all time separations of an ordinary quantum-mechanical propagator, and thus bears a close resemblance to the proper-time representation for Green's functions of the Klein-Gordon equation.[6]

V. THE NONRELATIVISTIC AND RELATIVISTIC POINT PARTICLES

We now show that the path-integral expression (4.5) reproduces the familiar and expected results in two simple examples. These examples will also help establish the range of N, since this is not fixed by the BFV procedure.

A. The parametrized nonrelativistic point particle

The first example is the nonrelativistic point particle in parametrized form. The usual action for the point particle is

$$S=\int_{t'}^{t''} dt \left[p_i \frac{dq^i}{dt} - h(p_i,q^i) \right] , \tag{5.1}$$

where t is the preferred Newtonian time parameter and $i=1,2,3$. The theory is put into parametrized form by introducing an arbitrary time parameter τ and then raising t to the status of a dynamical variable $t=q^0(\tau)$, with conjugate momentum $p_0(\tau)$ constrained to be equal to $-h(p_i,q^i)$. One thus adopts the action

$$S=\int_{\tau'}^{\tau''} dt \left[p_\alpha \frac{dq^\alpha}{d\tau} - N[p_0+h(p_i,q^i)] \right] , \tag{5.2}$$

where N is a Lagrange multiplier. This action is clearly of the form (2.1) with $\alpha=0,1,2,3$ and

$$H(p_\alpha,q^\alpha)=p_0+h(p_i,q^i) . \tag{5.3}$$

The path integral (4.5) for the system may be written

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\int dN(\tau''-\tau')\int \mathcal{D}p_i\mathcal{D}q^i\exp\left[i\int d\tau \left[p_i\frac{dq^i}{d\tau}-Nh(p_i,q^i)\right]\right]\int \mathcal{D}p_0\mathcal{D}q^0\exp\left[i\int d\tau \left[p_0\frac{dq^0}{d\tau}-Np_0\right]\right] . \tag{5.4}$$

The functional integral over p_i,q^i has the form of an ordinary quantum-mechanical propagator with time parameter $N\tau$:

$$\int \mathcal{D}p_i\mathcal{D}q^i\exp\left[i\int d\tau \left[p_i\frac{dq^i}{d\tau}-Nh(p_i,q^i)\right]\right]=\langle q^{i''},N\tau''\,|\,q^{i'},N\tau'\rangle . \tag{5.5}$$

A natural choice of skeletonization for the functional integral over p_0,q^0 is

$$\int \mathcal{D}p_0\mathcal{D}q^0\exp\left[i\int d\tau \left[p_0\frac{dq^0}{d\tau}-Np_0\right]\right]=\int \frac{d(p_0)_{1/2}}{2\pi}\cdots\frac{d(p_0)_{n+1/2}}{2\pi}\int dq_1^0\cdots dq_n^0 \times\exp\left[i\sum_{k=0}^{n}(p_0)_{k+1/2}(q_{n+1}^0-q_n^0-\epsilon N)\right] , \tag{5.6}$$

where $\epsilon=(\tau''-\tau')/(n+1)$. The p_0 integrations yield

$$\int dq_1^0\cdots dq_n^0\prod_{k=0}^{n}\delta(q_{k+1}^0-q_k^0-\epsilon N)=\delta(t''-t'-N(\tau''-\tau')) \tag{5.7}$$

and our final expression for (5.4) is

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\int dN(\tau''-\tau')\delta(t''-t'-N(\tau''-\tau'))\langle q^{i''},N(\tau''-\tau')\,|\,q^{i'},0\rangle . \tag{5.8}$$

Without loss of generality, let $(\tau''-\tau')>0$. Now consider the range of integration for N. Let us first suppose it is from $-\infty$ to $+\infty$. Then (5.8) yields

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\langle q^{i''},t''\,|\,q^{i'},t'\rangle \tag{5.9}$$

so G is a solution to the Schrödinger equation:

$$\left[i\frac{\partial}{\partial t''}-\hat{h}''\right] G(q^{\alpha''}\,|\,q^{\alpha'})=0 , \tag{5.10}$$

where $\hat{h}''$ is the operator corresponding to h at $q^{i''}$. But now let the range of integration be 0 to $+\infty$. Then the δ function in (5.8) contributes only if $t''-t'>0$. It follows that

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\theta(t''-t')\langle q^{i''},t''\,|\,q^{i'},t'\rangle , \tag{5.11}$$

so G is a Green's function of the Schrödinger operator. That is,

$$\left[i\frac{\partial}{\partial t''}-\hat{h}''\right] G(q^{\alpha''}\,|\,q^{\alpha'})=i\delta(t''-t')\delta^{(3)}(q^{i''}-q^{i'}) . \tag{5.12}$$

B. The relativistic point particle

Our next example is the relativistic point particle, which is described by the action (2.1) with

$$H=\eta^{\mu\nu}p_\mu p_\nu+m^2\ , \tag{5.13}$$

where $\mu=0,1,2,3$ and $\eta^{\mu\nu}$ is the usual Minkowski metric, with signature $(-\ +\ +\ +)$. With a particular choice of skeletonization, Eq. (4.5) is

$$G(q^{\mu''}\,|\,q^{\mu'})=\int dN(\tau''-\tau')\int d^4q_1\cdots d^4q_n\int\frac{d^4p_{1/2}}{(2\pi)^4}\cdots\int\frac{d^4p_{n+1/2}}{(2\pi)^4}\times\exp\left[i\sum_{k=0}^{n}[p_{k+1/2}\cdot(q_{k+1}-q_k)-\epsilon N(p_{k+1/2}\cdot p_{k+1/2}+m^2)]\right]\ , \tag{5.14}$$

where $q_0=q'$ and $q_{n+1}=q''$. The q integrations may be performed to yield n δ functions, each of the form $\delta^{(4)}(p_{k+1/2}-p_{k-1/2})$, and then all but one of the p integrations may be performed, with the result

$$G(q^{\mu''}\,|\,q^{\mu'})=\int\frac{d^4p}{(2\pi)^4}\int dT\exp(i[p\cdot(q''-q')-T(p\cdot p+m^2)])\ , \tag{5.15}$$

where $T=(\tau''-\tau')N$.

If the range of N is $-\infty$ to $+\infty$, then the T integration may be performed, to yield

$$G(q^{\mu''}\,|\,q^{\mu'})=\int\frac{d^4p}{(2\pi)^3}\delta(p\cdot p+m^2)e^{ip\cdot(q''-q')}\ . \tag{5.16}$$

Clearly,

$$(-\Box''+m^2)G(q^{\mu''}\,|\,q^{\mu'})=0\ , \tag{5.17}$$

so G is a solution to the Klein-Gordon equation. If, on the other hand, the range of N is 0 to $+\infty$, then

$$G(q^{\mu''}\,|\,q^{\mu'})=-i\int\frac{d^4p}{(2\pi)^4}\frac{e^{ip\cdot(q''-q')}}{(p\cdot p+m^2-i\epsilon)}\ , \tag{5.18}$$

where the $i\epsilon$ factor has been added to ensure convergence at the upper end of the T integration. This factor obliges one to integrate (5.18) along the contour in the p_0 plane corresponding to the Feynman Green's function. G therefore satisfies

$$(-\Box''+m^2)G(q^{\mu''}\,|\,q^{\mu'})=-i\delta^{(4)}(q^{\mu''}-q^{\mu'})\ . \tag{5.19}$$

Both of these examples have been discussed from a somewhat different perspective, using a canonical gauge, by Hartle and Kuchar.[8]

VI. QUANTUM MECHANICS IN CURVED BACKGROUNDS

The results of the preceding section concerning the range of N are quite general, as we now show. From there, we can complete the derivation of the Wheeler-DeWitt equation. The functional integral part of (4.5) has the form of an ordinary quantum-mechanical propagator with time Nt:

$$\int\mathcal{D}p_\alpha\mathcal{D}q^\alpha\exp\left[i\int_{t'}^{t''}dt(p_\alpha\dot q^\alpha-NH)\right]=\langle q^{\alpha''},Nt''\,|\,q^{\alpha'},Nt'\rangle\ . \tag{6.1}$$

Thus, introducing $T=N(t''-t')$, Eq. (4.5) becomes

$$G(q^{\alpha''}\,|\,q^{\alpha'})=\int dT\langle q^{\alpha''},T\,|\,q^{\alpha'},0\rangle\ . \tag{6.2}$$

Let us first take the range of T to be 0 to ∞. The propagator (6.1) will satisfy a time-dependent Schrödinger equation, so operating on (6.2) with $\hat H''$, the Hamiltonian operator at q'', one obtains

$$\begin{aligned}\hat H''G(q^{\alpha''}\,|\,q^{\alpha'})&=\int_0^\infty dTi\frac{\partial}{\partial T}\langle q^{\alpha''},T\,|\,q^{\alpha'},0\rangle\\&=i[\langle q^{\alpha''},T\,|\,q^{\alpha'},0\rangle]_0^\infty\\&=-i\langle q^{\alpha''},0\,|\,q^{\alpha'},0\rangle\\&=-i\delta(q^{\alpha''}\,|\,q^{\alpha'})\ .\end{aligned} \tag{6.3}$$

Equation (6.2) is therefore a Green's function of the Wheeler-DeWitt operator. Similarly, one may see that if T is integrated from $-\infty$ to $+\infty$, one obtains a solution to the Wheeler-DeWitt equation.

Clearly certain assumptions are being made here concerning the behavior of the propagator (6.1) as $T\to\pm\infty$. If (6.1) is to be regarded as an ordinary function, then clearly it must go to zero as $T\to\pm\infty$ for (6.2) to converge. Typical examples of quantum-mechanical propagators behave like an inverse power or T multiplied by an oscillatory function, so do indeed have the desirable behavior. It could be, however, that (6.2) converges in a distributional sense, in which case the validity of the steps in (6.3), at least for the case $-\infty<T<\infty$, is more subtle. For the case $0<T<\infty$, a Wick rotation to Euclidean time is possible, and the propagator (6.1) goes to zero exponentially fast as the Euclidean time approaches

∞. For the gravity case, the Wick rotation must also be accompanied by the conformal rotation in order to make the Hamiltonian positive.[11] Note that it does not seem to be possible to construct a Euclidean path integral if N has a fully infinite range.

We have now almost completed the derivation of the Wheeler-DeWitt equation. We have not, however, given a definition of the path integral in (6.1); nor have we given an explicit expression for the Hamiltonian operator $\hat{H}''$. The whole issue of deriving the Wheeler-DeWitt equation reduces, therefore, to that of constructing a skeletonized version of the path-integral expression (6.1), and then determining the associated operator $\hat{H}''$ in the time-dependent Schrödinger equation

$$\left[i\frac{\partial}{\partial T} - \hat{H}'' \right] \langle q^{\alpha''}, T \mid q^{\alpha'}, 0 \rangle = 0 \ . \tag{6.4}$$

We are thus led to study quantum mechanics in curved backgrounds, a subject that has been well studied over many years by numerous authors, including DeWitt,[12] Pauli,[13] DeWitt-Morette, Elworthy, Nelson, and Sammelman,[14] Hartle and Hawking,[15] Cheng,[16] Parker,[17] and most recently by Kuchar.[18] Much of what follows constitutes a description of the work of the above authors, so will be presented only in outline. The most comprehensive treatment is that of Kuchar,[18] and it is his that we will follow most closely.

In the usual canonical quantization procedure there arises an operator-ordering ambiguity when one replaces the momenta p_α by the corresponding operators in (2.2). This is partially alleviated by demanding that the resulting Schrödinger equation exhibit covariance under coordinate transformations of the q^α. One is then obliged to replace $f^{\alpha\beta}p_\alpha p_\beta$ with $-\hbar^2\nabla^2$ in (2.2), where ∇^2 is the Laplacian in the metric $f^{\alpha\beta}$. However, the correct classical limit is still obtained, and covariance is still respected if one adds a curvature term $\hbar^2 R$, the scalar curvature in the metric $f^{\alpha\beta}$. The most general form for $\hat{H}$ is, therefore,

$$\hat{H} = -\frac{\hbar^2}{2}\nabla^2 + \xi\hbar^2 R + V(q) \ , \tag{6.5}$$

where ξ is an arbitrary constant *whose value is not determined by the canonical quantization procedure alone.* Particular values of ξ may be preferred if there exist additional symmetries, such as conformal invariance or supersymmetry,[19] but in general this arbitrariness remains and the quantum theory is not unique. With this in mind, let us turn to the path-integral description.

Historically, the path-integral formulation of quantum mechanics in curved backgrounds began with configuration-space path integrals,[12–17] in which one considers an expression of the form

$$\int \mathcal{D}q \, \exp(iS[q(t)]) \ , \tag{6.6}$$

where $S[q(t)]$ is the configuration-space form of (2.1) (with $N=1$):

$$S[q(t)] = \int_{t'}^{t''} dt [\tfrac{1}{2} f_{\alpha\beta}\dot{q}^\alpha \dot{q}^\beta - V(q)] \ . \tag{6.7}$$

The expression (6.6) is normally defined by a time-slicing procedure. The variables q,t are represented by discrete variables q_k, t_k, where $k=0,1,\ldots(n+1)$ and $t_0=t'$, $t_{n+1}=t''$, $q_0=q'$, and $q_{n+1}=q''$. Proper meaning is then given to (6.1) only after one has specified, in terms of these discrete variables, (i) a covariant skeletonization of the action $S[q(t)]$ and (ii) a covariant measure.

There is a natural choice for the first requirement: one uses the Hamilton-Jacobi function $S(q'',t'' \mid q',t')$. This is equal to the action of the classical path connecting (q',t') to (q'',t''). The Hamilton-Jacobi function is a scalar in both of its arguments, and thus covariance is easy to maintain using the following skeletonized approximation to the action:

$$S[q(t)] = \sum_{k=0}^{n} S(q_{k+1}, t_{k+1} \mid q_k, t_k) \ . \tag{6.8}$$

Adjacent vertebral points of the skeletonized path are therefore connected by classical paths.

For the measure, on the other hand, there is no unique natural choice. In fact there is a whole family of acceptable measures. Parker, for example, used the following definition of the measure:[17]

$$\mathcal{D}q = \frac{1}{(2\pi i\epsilon)^{D(n+1)/2}} \prod_{j=1}^{n} d^D q_j [f(q_j)]^{1/2} \times \prod_{k=0}^{n} [\Delta(q_{k+1}, q_k)]^p \ , \tag{6.9}$$

where

$$\Delta(q_{k+1}, q_k) = [f(q_{k+1})]^{-1/2} \det \left[-\frac{\partial^2 S}{\partial q_{k+1}\partial q_k} \right] \times [f(q_k)]^{-1/2} \tag{6.10}$$

is the Morette-Van Vleck determinant and $f=\det f_{\alpha\beta}$. This measure is covariant for all values of the arbitrary parameter p. It may be shown that the corresponding Schrödinger equation involves a Hamiltonian operator of the form (6.5) with $\xi = \frac{1}{3}(1-p)$. We therefore see that the operator-ordering problem in the canonical quantization procedure appears in a configuration-space path integral as an ambiguity in the choice of covariant measure.

It is sometimes claimed that such ambiguities in the measure can be resolved by going to a path integral in phase space, for which there is a privileged measure, namely, the Liouville measure. This misconception was finally laid to rest by Kuchar,[18] who studied the covariant skeletonization of phase-space path integrals, for systems on curved backgrounds. Let us consider therefore, an expression of the form

$$\int \mathcal{D}p_\alpha \mathcal{D}q^\alpha \exp\left[i\int dt (p_\alpha \dot{q}^\alpha - H) \right] \ . \tag{6.11}$$

Once again the path integral is defined by a time-slicing procedure. The discrete representation of the q's is as above. For the p's, one introduces $n+2$ discrete variables p_k, $k=0,1,\ldots n+1$. Only $n+1$ of them are integrated over, because it always turns out that, as a result of the skeletonization, the integrand is independent of either p_0 or p_{n+1}. (Alternatively, one can introduce $n+1$

variables $p_{k+1/2}$, $k=0,1,\ldots n$ and integrate over all of them, but we shall use the former method, in order to follow Kuchar.) Once again one needs to specify both (i) and (ii). But now the difficulties are reversed. In phase space, there is indeed a privileged measure, the Liouville measure,

$$\mathcal{D}p_\alpha \mathcal{D}q^\alpha = d(p_\alpha)_0 \prod_{k=1}^{n} d(p_\alpha) k^d q_k^\alpha \tag{6.12}$$

and this ensures covariance under point transformations (the extra p integration means that the propagator is a scalar density at the initial end point). Kuchar observed, however, that there is no natural analogue of the Hamilton-Jacobi function. There is no function $S(q'',p'',t''\mid q',p',t')$ equal to the action of a classical path with given q and p at both end points, since clearly such a path does not in general exist. Consequently, there is no unique natural skeletonization of the action.

Nevertheless, Kuchar[18] showed how to skeletonize the action in a covariant manner by introducing a function $S(q'',t''\mid q',p',t')$, defined as follows. The idea is that one first calculates the classical path $q(t)$ from (q',t') to (q'',t''). An arbitrary initial momentum p' is then chosen (independently of $\dot{q}$), and this is extended to a function $p(t)$ by transporting it along the path $q(t)$ using a certain differential equation (e.g., the parallel transport equation and the geodesic deviation equation). The function $S(q'',t''\mid q',p',t')$ is then defined to be

$$S(q'',t''\mid q',p',t') = \int_{t'}^{t''} dt[p_\alpha(t)\dot{q}^\alpha(t) - H(p_\alpha(t),q^\alpha(t))] \ . \tag{6.13}$$

This function turns out to have all the properties one needs, in particular, it transforms covariantly under point canonical transformations, and we can now write down the covariant phase-space path integral:

$$\int d(p_\alpha)_0 \prod_{k=1}^{n} d(p_\alpha)_k dq_k^\alpha \times \exp\left[i \sum_{k=0}^{n} S(q_{k+1},t_{k+1}\mid q_k,p_k,t_k) \right] . \tag{6.14}$$

The point is, however, that there is a whole class of functions $S(q'',t''\mid q',p',t')$ that do the job. In fact, loosely speaking, there is a one-parameter family. This ambiguity comes partly from the freedom to choose the differential equation with which to transport the momentum, but also from the freedom to make certain modifications to (6.13) while preserving covariance. On performing the momentum integration in (6.14), one reproduces the one-parameter family of covariant measures (6.9), to which correspond the one-parameter family of Hamiltonian operators (6.5). The arbitrariness in the quantum theory expressed through the parameter ξ thus permeates the configuration-space and phase-space path-integral formulations, as well as the canonical quantization procedure. It is not fixed solely by covariance.

So we have described the relation between the skeletonized version of the path integral in (6.1) and the Hamiltonian operator (6.5), and our derivation of the Wheeler-DeWitt equation is complete. To summarize, with the skeletonizations described in Secs. IV and VI the path-integral expression (3.12) satisfies the equation

$$\hat{H}''G(q^{\alpha''}\mid q^{\alpha'}) = \begin{cases} -i\delta(q^{\alpha''}\mid q^{\alpha'}) & \text{if } 0<N<\infty \ , \\ 0 & \text{if } -\infty<N<\infty \ , \end{cases} \tag{6.15}$$

where $\hat{H}''$ is of the form (6.5).

Finally, although the coefficient ξ does not appear to be fixed by covariance in the time-dependent Schrödinger equation, as we have gone to some effort to emphasize, we shall argue in Sec. VIII that it *is* fixed in the Wheeler-DeWitt equation, by demanding invariance under field redefinitions involving the lapse function.

VII. A MINISUPERSPACE EXAMPLE

We now consider a simple minisuperspace example. Consider a Robertson-Walker model described by the metric

$$ds^2 = \frac{-N^2(t)}{q(t)} dt^2 + q(t) d\Omega_3^2 \ , \tag{7.1}$$

where $d\Omega_3^2$ is the metric on the unit three-sphere. We will take the action to be the Einstein-Hilbert action, with a cosmological term. It is easily shown that the Hamiltonian then is[20]

$$H = \tfrac{1}{2}(-4p^2 + \lambda q - 1) \ . \tag{7.2}$$

The path-integral expression (4.5) for the propagation amplitude may therefore be written

$$G(q''\mid q') = \int dT\, e^{-iT/2} \int \mathcal{D}p\, \mathcal{D}q \exp\left[i\int_0^T dt[p\dot{q} - \tfrac{1}{2}(-4p^2 + \lambda q)] \right] . \tag{7.3}$$

One could proceed by first evaluating the functional integration over p and q, since this is a standard result—it is just the ordinary quantum-mechanical propagator for a system with a linear potential. However, the resulting T integration is rather difficult, and it turns out to be easier to perform the integrations in a different order.

Since the system is so simple it is not necessary to resort to the sophistication of Sec. VI to skeletonize the path integral. We will define the functional integral over p and q in (7.3) to be the limit as $\epsilon \to 0$ of the expression

$$(2\pi)^{-n} \int dp_{1/2} \cdots dp_{n+1/2} \int dq_1 \cdots dq_n \exp\left[i \sum_{k=0}^{n} \left[p_{k+1/2}(q_{k+1} - q_k) - \frac{\epsilon}{2}(-4p_{k+1/2}^2 + \lambda q_k) \right] \right] , \tag{7.4}$$

where as usual, $\epsilon = T/(n+1)$ and $q_0 = q'$, $q_{n+1} = q''$. The q integrations are easily performed, with the result

$$(2\pi)^{-n}\int dp_{1/2}\cdots dp_{n+1/2}\prod_{k=1}^{n}\delta\left[p_{k-1/2}-p_{k+1/2}-\frac{\epsilon\lambda}{2}\right]\exp\left[i\left[2\epsilon\sum_{k=0}^{n}p_{k+1/2}^2+p_{n+1/2}q''-p_{1/2}q'+O(\epsilon)\right]\right] . \quad (7.5)$$

The n δ functions imply that $p_{k+1/2} = p_{1/2} - k\epsilon\lambda/2$. All but one of the p integrations may then be performed, to yield

$$\int dp \exp\left[i\left[2\epsilon\sum_{k=0}^{n}\left[p-\frac{\epsilon\lambda}{2}k\right]^2+\left[p-\frac{\epsilon\lambda}{2}n\right]q''-pq'+O(\epsilon)\right]\right] . \quad (7.6)$$

Carrying out the sums over k, inserting the result in (7.3), and setting $\epsilon\to 0$, one obtains

$$G(q''\,|\,q') = \int dT \int dp \exp\left[i\left[\left[2p^2+\frac{1-\lambda q''}{2}\right]T-\lambda p T^2+\frac{\lambda^2T^3}{6}+p(q''-q')\right]\right] . \quad (7.7)$$

If desired, one could now carry out the p integration to yield the standard result for the propagator with a linear potential. However, as already stated, it turns out to be easier to integrate T first. Let us take the range of T to be $-\infty$ to $+\infty$. Then one may write $T=\tilde{T}+2p/\lambda$ and, after some algebra, one obtains

$$G(q''\,|\,q') = \int_{-\infty}^{\infty} d\tilde{T}\int_{-\infty}^{\infty} dp \exp\left[\frac{i\lambda^2}{6}\tilde{T}^3+\frac{i(1-\lambda q'')}{2}\tilde{T}\right]\exp\left[\frac{i4p^3}{3\lambda}+\frac{ip(1-\lambda q')}{\lambda}\right] . \quad (7.8)$$

G is therefore a product of two Airy functions[21]

$$G(q''\,|\,q') = \frac{2\pi^2}{(4\lambda)^{1/3}}\mathrm{Ai}\left[\frac{1-\lambda q''}{(2\lambda)^{2/3}}\right]\mathrm{Ai}\left[\frac{1-\lambda q'}{(2\lambda)^{2/3}}\right] . \quad (7.9)$$

Since the curvature vanishes in one dimension, there is no operator ordering ambiguity, and the Wheeler-DeWitt equation is

$$\hat{H}G = \tfrac{1}{2}\left[4\frac{d^2}{dq^2}+\lambda q-1\right]G=0 . \quad (7.10)$$

It is easy to verify that (7.9) is a solution to (7.10), as expected.

However, we know that there is a second solution to (7.10). How do we generate it from the path integral? One way is to observe that the Wheeler-DeWitt equation (7.10) is unchanged by the transformation $(1-\lambda q)\to e^{2\pi i/3}(1-\lambda q)$. It follows that applying this transformation to the above solution will yield a second solution. It is

$$\mathrm{Ai}(e^{2\pi i/3}z) = \tfrac{1}{2}e^{\pi i/3}[\mathrm{Ai}(z) - i\,\mathrm{Bi}(z)] , \quad (7.11)$$

where $z=(1-\lambda q)(2\lambda)^{-2/3}$. This second solution is clearly linearly independent of the first. Another way of generating a second solution is to integrate along a different contour in (7.8). For example, the contour running from $-\infty$ to 0 and then from 0 to $-i\infty$ yields (7.11). We have thus seen that we can use the path integral to generate a complete set of solutions to (7.10).

In performing the above calculation, however, there is an important restriction that we have failed to recognize. This is that q, being a scale factor in (7.1), is positive. Strictly speaking therefore, the problem should be treated using the formulation of quantum mechanics appropriate to restricted intervals, which is actually rather difficult. Part of the problem is that in writing down the skeletonization (7.4), it is implicitly assumed that both p and q are integrated from $-\infty$ to $+\infty$. We will defer further discussion of this point until later.

For the moment, however, we note that the fact that $q>0$ is not a problem if, as we have been doing here, one is simply using the path integral to generate solutions to the Wheeler-DeWitt equation. The point is that there is no mathematical inconsistency in allowing q to take a fully infinite range—one can evaluate the path integral, and solve the Wheeler-DeWitt equation. The fact that the physically relevant range of q is $q>0$ means only that one is required to find solutions satisfying prescribed boundary conditions at the end points of the physically relevant range—i.e., at $q=0$ and $q=\infty$. But since we have generated a complete set of solutions, this can clearly be achieved.

If one is just using the path integral to generate solutions, therefore, the fact that the physically relevant range of q is $q>0$ presents no problem. The difficulties arise, however, when one tries to incorporate the positivity of q into the path integral from the very beginning. This will be discussed in the Sec. IX. Before that, however, we reconsider the result (6.15) in the light of the example of this section.

VIII. INVARIANCE UNDER FIELD REDEFINITIONS

A reasonable property to demand of any quantum theory is that it be insensitive to the way we choose to define the fields involved; that is, it should be invariant under field redefinitions. The construction of Sec. VI guarantees that this is the case for redefinitions of the three-metric, represented by the q's. More precisely, if one chose to perform the calculation with a different set of variables $\bar{q}(q)$, then the answer would be the same as that obtained by performing the calculation in terms of q and then substituting for $\bar{q}$ at the end. At the level of the Wheeler-DeWitt equation, this has been achieved by demanding that all quantities constructed from the metric $f_{\alpha\beta}$ are covariant.

As it stands, however, the formalism is not invariant under field redefinitions involving the lapse function N. Since any reference to N is absent in (6.15), this is not so obvious, but it may be seen by considering a simple example. Consider the minisuperspace example of the previous section, for the case $\lambda=0$, with N defined by the metric (7.1). It is described by the action

$$S=\int dt\left[p\dot{q}-\frac{N}{2}(-4p^2-1)\right] . \quad (8.1)$$

The Wheeler-DeWitt equation is

$$\left[4\frac{d^2}{dq^2}-1\right]\Psi(q)=0 \quad (8.2)$$

with solutions $\Psi(q)=e^{\pm q/2}$. Suppose however, one uses a new lapse function $\tilde{N}$, defined by $\tilde{N}=q^{-1}N$. The four-metric is now given by

$$ds^2=q(t)[-\tilde{N}^2(t)dt^2+d\Omega_3^2] \quad (8.3)$$

and the action is

$$S=\int dt\left[p\dot{q}-\frac{\tilde{N}}{2}(-4qp^2-q)\right] . \quad (8.4)$$

Classically, this action is just as good as (8.1). In each, N and $\tilde{N}$ are regarded as independent of q. The Wheeler-DeWitt corresponding to (8.4), however, is

$$\left[4q^{1/2}\frac{d}{dq}q^{1/2}\frac{d}{dq}-q\right]\tilde{\Psi}(q)=0 , \quad (8.5)$$

where in accordance with the formalism developed so far, we replaced $-qp^2$ with the Laplacian. The operator in (8.5) is clearly not equivalent to that in (8.2) since it differs by first-derivative terms. Indeed, the solutions to (8.5) are given in terms of modified Bessel functions:[21] $\tilde{\Psi}(q)=q^{1/4}I_{1/4}(q/2)$ and $\tilde{\Psi}(q)=q^{1/4}K_{1/4}(q/2)$. There is no obvious exact relationship between these solutions and the solutions to (8.2), although the dominant terms in $\tilde{\Psi}(q)$ are of the form $e^{\pm q/2}$ for large q, so they do at least agree semiclassically, as one would expect. The point is that the Wheeler-DeWitt equations describe different quantum theories, so the procedure is not invariant under field redefinitions involving the lapse function.

More generally, the problem may be presented as follows. We showed that the action

$$S=\int dt\{{}_{\alpha}\dot{q}^{\alpha}-N[\tfrac{1}{2}f^{\alpha\beta}p_{\alpha}p_{\beta}+V(q)]\} \quad (8.6)$$

corresponds to the Wheeler-DeWitt equation

$$H\Psi=[-\tfrac{1}{2}\nabla^2+\xi R+V(q)]\Psi(q)=0 . \quad (8.7)$$

Suppose, however, one defines a new lapse function $\tilde{N}$, given by $N=\Omega^{-2}\tilde{N}$, where Ω is an arbitrary function of q. Ω may be absorbed into the Hamiltonian by defining $\tilde{f}^{\alpha\beta}=\Omega^{-2}f^{\alpha\beta}$ and $\tilde{V}(q)=\Omega^{-2}V(q)$. The action is then given by

$$S=\int dt\{p_{\alpha}\dot{q}^{\alpha}-\tilde{N}[\tfrac{1}{2}\tilde{f}^{\alpha\beta}p_{\alpha}p_{\beta}+\tilde{V}(q)]\} . \quad (8.8)$$

This is completely equivalent to (8.6) at the classical level, and there is no obvious reason why it should not be used as a starting point for quantization. The corresponding Wheeler-DeWitt equation is

$$\tilde{H}\tilde{\Psi}=[-\tfrac{1}{2}\tilde{\nabla}^2+\xi\tilde{R}+\tilde{V}(q)]\tilde{\Psi}(q)=0 , \quad (8.9)$$

where $\tilde{\nabla}^2$ and $\tilde{R}$ are, respectively, the Laplacian and scalar curvature in the metric $\tilde{f}_{\alpha\beta}$.

For (8.7) and (8.9) to describe the same quantum theory, one would need $\tilde{H}\tilde{\Psi}$ to be proportional to $H\Psi$ [so that (8.9) implies (8.7), and vice versa], where $\tilde{\Psi}$ and Ψ are related in a simple way. This will not in general be true. Nevertheless, let us look for a relationship between $\tilde{\Psi}$ and Ψ of the form $\tilde{\Psi}(q)=\Omega^{\gamma}\Psi(q)$, for some constant γ. Then a standard calculation shows that

$$\begin{aligned}\tilde{H}\tilde{\Psi}=\Omega^{\gamma-2}H\Psi-\tfrac{1}{2}(2\gamma+D-2)\Omega^{\gamma-3}\nabla\Omega\cdot\nabla\Psi\\ +\Omega^{\gamma-2}[A\,\Omega^{-1}\nabla^2\Omega+B\,\Omega^{-2}(\nabla\Omega)^2]\Psi ,\end{aligned} \quad (8.10)$$

where the dot product is with respect to the metric $f^{\alpha\beta}$ and

$$\begin{aligned}A&=-\frac{\gamma}{2}+2(D-1)\xi ,\\ B&=-\tfrac{1}{2}[\gamma(\gamma-1)+\gamma(D-2)]+\xi(D-1)(D-4) .\end{aligned} \quad (8.11)$$

D, recall, is the dimension of the minisuperspace. Equation (8.10) shows that (8.7) and (8.9) are not in general equivalent for arbitrary γ and ξ. However, if we choose $\gamma=(2-D)/2$, then the coefficient of $\nabla\Omega\cdot\nabla\Psi$ vanishes, and (8.7) and (8.9) differ only in their potentials. Moreover, with this choice the coefficients A and B are then both proportional to $(D-2)+8(D-1)\xi$. The main point now, is that ξ is totally arbitrary—it is not fixed by demanding covariance in the q's, as we went to some length to emphasize in Sec. VI. We are therefore free to make the choice

$$\xi=-\frac{D-2}{8(D-1)} , \quad (8.12)$$

which implies that $A=B=0$, and thus $\tilde{H}\tilde{\Psi}=\Omega^{\gamma-2}H\Psi$. This means that (8.7) and (8.9) are equivalent, so the quantization procedure *can* be made invariant under field redefinitions of N, providing ξ is chosen to take the value (8.12) (Ref. 22).

Equation (8.12) is of course the value for which the operator $-\frac{1}{2}\nabla^2+\xi R$ is conformally covariant, and the above calculation showing that this is the case is very standard. Equation (8.10) is written out explicitly, so that one can see that the case $D=1$ is exceptional. Although we motivated the discussion by a one-dimensional example, the above procedure does not work for $D=1$. In one dimension, there is no curvature, so the terms proportional to ξ are absent from (8.10) and (8.11). One can then either choose $\gamma=0$ so that $A=B=0$, or one can choose $\gamma=\frac{1}{2}$, so that the coefficient of $\nabla\Omega\cdot\nabla\Psi$ vanishes.

But one way or another, extra terms still remain and it does not seem to be possible to achieve invariance under field redefinitions of N for $D=1$, at least by this approach.

In conclusion, the operator-ordering ambiguity in the Wheeler-DeWitt equation for $D>1$ is completely fixed by demanding invariance under field redefinitions of both the three metric and the lapse function. Note, however, that we have pursued the issue of invariance under rescalings of N only at the level of the canonical quantization procedure, not at the path-integral level, although this is presumably not too difficult.

IX. QUANTUM MECHANICS ON A HALF-INFINITE RANGE

In Sec. VII we encountered the problem of doing quantum mechanics in terms of the variable q whose physical range was the positive real line. This problem is not in any way an artifact of the particular model under consideration, but is a manifestation of the fact that the three-metric h_{ij} satisfies the condition $\det h_{ij}>0$. It is therefore important to face up to this issue from the very beginning.

In the canonical quantization of gravity, this sort of difficulty was recognized a long time ago by Klauder.[23] To see the problems that arise, consider a simple one-dimensional system with coordinate q restricted to lie on the positive real line R^+. The first problem one discovers is that the momentum operator is not Hermitian. To see that this is the case, consider the operator obtained by exponentiating the momentum operator (times i). If the momentum operator were Hermitian, one would obtain the unitary translation operator, with which one could translate into the region $q<0$. The momentum operator cannot therefore, be Hermitian. Hermiticity of the Hamiltonian can be preserved, however, by imposing the boundary conditions $\psi'(0)+\alpha\psi(0)=0$ at $q=0$, where α is an arbitrary parameter. Normally one envisages a physical situation in which the conditions at $q=0$ are known, and thus the value of α is given.

Quantum-mechanical propagators may be constructed using an eigenfunction expansion. One finds the eigenfunctions $u_n(q)$ of the Hamiltonian subject to the above boundary conditions, and subject to the usual fall-off conditions at infinity. The propagator is then given in terms of these functions by an expression of the form

$$\langle q'',t''|q',t'\rangle=\sum_n e^{-iE_n(t''-t')}u_n^*(q'')u_n(q') . \quad (9.1)$$

The above boundary conditions will then be incorporated into the propagator.

In the path-integral approach, the problems with the restriction to $q>0$ appear as difficulties with the skeletonization procedure. An essential property of a skeletonized path integral is that it yields the correct WKB approximation to the propagator at short time separations. The configuration-space path integral described in Sec. VI with the measure (6.9) will generally have this property. Recall, however, that this construction involves the action of the classical path connecting adjacent vertebral points of the lattice. It is implicitly assumed that this classical path is unique. The problem is that this will not be true in the presence of a boundary at $q=0$. For then, there will be two classical paths—the direct path and a second path which is reflected off $q=0$. This means that the WKB approximation to the propagator is not a single expression of the form e^{iS} but a sum of two such terms. The path-integral construction of Sec. VI will not, therefore, reduce to the WKB approximation to the propagator at short time separations, because it involves only one factor of the form e^{iS} on each time slice. In general, it does not seem to be possible to construct a path-integral representation of the propagator using the usual skeletonization procedure but with q integrated from 0 to ∞ on each slice.

These problems do not mean that a skeletonized definition of the path integral consistent with the restriction $q>0$ is not possible. Such skeletonizations are possible, although they are rather complicated and will not be pursued here.[23] We merely point out that the standard skeletonization used for the case $-\infty<q<\infty$ cannot be naively applied to the case $q>0$.

At this point one might think that the above difficulties could be alleviated by a change of variables. One could write $q=e^x$, for example, for then x takes a fully infinite range. However, this does not work. The point is that the difficulty is not so much that $q>0$, but rather, the fact that there exists more than one classical path connecting any two points. If, in terms of q, there are two classical paths, a direct and a reflected path, then the same will be true of x. In terms of x there will be, in addition to the direct path, a second classical path which goes to $x=-\infty$ and back in a finite period of time; thus once again there will be two terms of the form e^{iS} in the WKB approximation to the propagator.

This example illustrates that even if the variables that one is working with have a fully infinite range, one has to do a careful analysis of the classical solutions before using the path integral to construct the propagator. Or to put it another way, one cannot escape global problems by a change of coordinates.

In the case of gravity, it has been suggested that one should work not with the three-metric h_{ij}, but with the dreibein e_i^a, where $h_{ij}=e_i^a e_j^b\delta_{ab}$, $a,b=1,2,3$ for then the inequality constraint $\det h_{ij}>0$ is automatically satisfied without any restrictions on the range of the dreibein.[24] In the example of the preceding section this corresponds to writing $q=a^2$ and letting a take an infinite range. Once again, however, the problems still arise, because there still exist reflected paths, so there is no easy way round the difficulty in the path-integral approach. Nevertheless, these changes of variables are still useful in the canonical quantization procedure since the momentum conjugate to a variable taking an infinite range may be represented by a Hermitian operator.

These issues simply mean that it is difficult to incorporate the fact that $q>0$ into the path integral from the beginning. They do not prevent one from making good use of the path integral, as indeed we did in the Sec. VII. For example, one can calculate the quantum-mechanical propagator when $q>0$ using the method of images. First, one extends the potential into the region $q<0$ in such a way that $V(q)=V(-q)$. One then uses the path integral to calculate the propagator $\langle q'',t\mid q',0\rangle$ letting the q's take a fully infinite range. This propagator will be a solution to the Schrödinger equation, and will be a δ function at $t=0$. By the symmetry of the potential, a second such solution is given by $\langle q'',t\mid -q',0\rangle$ and these two solutions may be superposed to satisfy prescribed boundary conditions at $q=0$. The propagator in the region $q>0$ is thus obtained.

Finally, it is appropriate to remark on the validity of the skeletonization of the lapse function integral in Sec. IV because there we allowed N to be integrated over a half-infinite range. As mentioned above, the skeletonization procedure involves considering the classical path between two points of the lattice, and this was problematic for q because of the existence of reflected paths. For N, however, the "classical field equation" is just the gauge condition, $\dot{N}=0$; thus there can be only one path connecting N_k to N_{k+1}. There are no reflected paths, so the above problems do not arise, at least for the gauge choice we have been using.

X. SUMMARY AND DISCUSSION

We have discussed the relationship between the Dirac and path-integral quantization schemes for a simple class of reparametrization-invariant systems, with a particular emphasis on the minisuperspace models of quantum cosmology. We showed how to construct the gauge-fixed path integral with the correct measure using the method of Batalin, Fradkin, and Vilkovisky. Our path-integral expressions were all defined explicitly using a time-slicing procedure. We showed that the path-integral expression was either Green's function of the Wheeler-DeWitt operator or a solution to the Wheeler-DeWitt equation, depending on the range of the lapse function N. Our main result is that the Wheeler-DeWitt operator (and thus the path-integral measure) is uniquely fixed by demanding that the quantization procedure is invariant under field redefinitions of both the three-metric h_{ij} and the lapse function N. It is

$$\hat{H}=-\tfrac{1}{2}\nabla^2-\frac{D-2}{8(D-1)}R+V \tag{10.1}$$

for $D>1$. We also discussed the problems involved in respecting the constraint $\det h_{ij}>0$.

Throughout this paper, a number of remarks have been made concerning the range of the lapse function N. It is perhaps useful to draw these together. The BFV procedure described in Sec. III does not explicitly fix the domains of integration. In Secs. V and VI, therefore, we investigated the consequences of choosing either infinite or half-infinite ranges for N. We found that the path integral then generated, respectively, either a solution to the Wheeler-DeWitt equation or a Green's function of the Wheeler-DeWitt operator. It was also pointed out that one appears to be obliged to take the range $0<N<\infty$ if one wishes to construct a Euclidean functional integral. We argued in Sec. IX that the skeletonization of N was not problematic, in the gauge $\dot{N}=0$, although in general half-infinite ranges do suffer from difficulties.

We suggested at the end of Sec. III that the Fradkin-Vilkovisky theorem may not work if the range of N is $N>0$. In fact an example may now be given which appears to show this explicitly. Consider the example of Sec. VII (the problems with the half-infinite range for q are not relevant here). Originally we worked in the gauge $\dot{N}=0$. Suppose, however, we work in the gauge $\dot{N}=\alpha p$, where α is an arbitrary constant, and for simplicity we let $\lambda=0$. The Fradkin-Vilkovisky theorem implies that the path integral ought to be independent of α. Once again the ghosts decouple and the path integral may be evaluated exactly. The result is of the form (7.7), with $\lambda=0$, but with T replaced by $T+\alpha(t''-t')p/2$. Clearly if N (and, hence, T) has an infinite range, then the α dependence may be absorbed by a shift of T and the final result is independent of α, as intended. If, however, T has a half-infinite range then the result will depend on α explicitly. This could be related to the fact that the argument given in Sec. IX for the validity of the skeletonization of N no longer applies.

Finally, we mention the related papers of Teitelboim[7] and Barvinsky and Ponomariov.[25] Teitelboim[7] discussed many of the issues involved in the construction of the path integral for quantum gravity, but his manipulations remain formal throughout. Barvinsky and Ponomariov[25] also gave a path-integral construction, and claim to derive the Wheeler-DeWitt equation from it, although once again, the manipulations are purely formal. By contrast, in this work, by concentrating on the special case of minisuperspace models we have been able to give the path-integral expressions precise meaning by a time-slicing procedure, thereby establishing the precise relationship between the path-integral measure and the operator ordering.

There are many more issues which are yet to be addressed, such as the construction of a Euclidean path integral and the implementation of the boundary conditions proposal of Hartle and Hawking.[26] It is also of interest to consider the much more difficult question of the derivation of the Wheeler-DeWitt equation for the full theory, with nontrivial momentum constraints and an infinite number of degrees of freedom. A formal Euclidean path integral for the full theory, using the BFV method, has been given by Schleich,[27] although a derivation of the Wheeler-DeWitt equation was not given. These and other issues will be discussed in future publications.

Note added. After completion of this work, I received a paper by Moss[28] who also realized that the coefficient of the curvature term should be (8.12). A further point of interest in this connection is that the probability measure proposed by Hawking and Page,[29] namely, $|\Psi|^2(-f)^{1/2}$, is not invariant under the rescalings described in Sec. VIII. However, the probability measure constructed from the conserved current $J^\alpha=if^{\alpha\beta}(\Psi\nabla_\beta\Psi^*-\Psi^*\nabla_\beta\Psi)$ is invariant; thus it appears that any interpretation of the wave function must involve the conserved current, with its associated difficulties with negative probabilities. This point was also noted by Moss.[30]

ACKNOWLEDGMENTS

I am very grateful to Arley Anderson, Jim Hartle, Jorma Louko, Kristin Schleich, and Bernard Whiting for useful conversations. This research was supported in part by the National Science Foundation under Grant No. PHY82-17853, supplemented by funds from the National Aeronautics and Space Administration, at the University of California at Santa Barbara.

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