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Path integrals and instantons in quantum gravity: Minisuperspace models

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While there does not at this time exist a complete canonical theory of full 3+1 quantum gravity, there does appear to be a satisfactory canonical quantization of minisuperspace models. The method requires no ''choice of time variable'' and preserves the systems' explicit reparametrization invariance. In the following study, this canonical formalism is used to derive a path integral for quantum minisuperspace models. As it comes from a well-defined canonical starting point, the measure and contours of integration are specified by this construction. The properties of the resulting path integral are analyzed, both exactly and in the semiclassical limit. Particular attention is paid to the role of the (unbounded) Euclidean action and Euclidean instantons are argued to contribute as $e^{-|S_E|/\hbar}$. [S0556-2821(96)04412-8]

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I. INTRODUCTION

Although a complete theory of 3+1 quantum gravity is not yet available, interesting arguments for the pair production of black holes [1–3], the instability of certain vacuum states [4], and even for a preferred ''ground state'' of the theory [5,6] can be made by analogy with field theories that are better understood. A common tool in such arguments is a path integral representation of a quantum gravity transition amplitude and/or a related semiclassical approximation. Our goal here will be to investigate this representation and the $\hbar \rightarrow 0$ limit by using an analogy with a different class of systems: the ''finite-dimensional reparametrization invariant models.''

While they are explicitly defined to have a finite number of degrees of freedom, such models possess many of the properties which distinguish Einstein-Hilbert gravity from the more common quantum mechanical systems or field theories. They are invariant under ''time reparametrization,'' a gauge transformation that mixes coordinates and momenta, and as a result they often possess constraints that are second order in momenta. Such ''Hamiltonian constraints'' are reminiscent of the ''Wheeler-DeWitt equation'' [7] of quantum gravity. In addition, they share with Einstein-Hilbert gravity the property that neither the Hamiltonian function nor the Euclidean action is bounded below.

Since a bounded Euclidean action is required for common arguments involving analytic continuation to Euclidean time, this property has raised concern about how a path integral for gravity might be defined and analyzed [8,9]. One proposal [8,10,11] is to ''rotate the contour of integration'' in the path integral until the Euclidean action becomes positive definite. We will study this question below and compare our results to what would follow from contour rotation.

An important and related point concerns the semiclassical approximation. Recall that the Einstein-Hilbert action takes the form

$$S=\int_{\mathcal{M}}\sqrt{-g}R+\text{boundary terms}, \tag{1.1}$$

where g is the determinant of some metric and R is its scalar curvature. One might, therefore, expect that quantum gravity path integrals can be treated as integrals of analytic functions and that the contour can be deformed from the original region of integration. Some arguments for the contribution of Euclidean instantons can be made in this way, by deforming Lorentzian metrics to Euclidean ones through the complex plane. However, once deformations into the complex plane are allowed, one must in principle include in the semiclassical analysis *any* stationary points which lie within the domain of analyticity of the integrand. Because of the branch cut introduced by the $\sqrt{g}$ factor in (1.1), the metric g effectively takes values on a Riemann surface and, at least for appropriate boundary conditions, the stationary points occur in pairs *with opposite signs of the action.* This point has been made many times [12–15] and a similar feature arises in our finite-dimensional reparametrization-invariant models. Which stationary phase points actually contribute to the result will depend on the particular contour of integration. This is, however, an issue that must be analyzed and one is led to wonder what determines this contour so that, for example, black hole pair creation calculations predict an exponentially suppressed rate for large mass and not one that is exponentially enhanced.

Our goal here is to investigate these issues in the finite-dimensional reparametrization invariant context by deriving our path integral from a canonical quantum formalism. The existence of a canonical formalism which can be applied to a large class of models and which does not require ''deparametrization'' or the imposition of gauge-fixing conditions is a fairly recent development [16–20] whose implications for path integral methods have not yet been explored. Such is our aim here, and we will find that the resulting path integral has two interesting properties. First, it can be written as an integral over both ''Lorentzian'' and ''Euclidean'' paths in which the contribution of Euclidean paths is always exponentially *suppressed* for small $\hbar$. Second, the Euclidean semiclassical approximation yields only exponentially damped contributions; in particular, Euclidean instantons always contribute with the weight $e^{-|S_E|/\hbar}$, where S_E is the Euclidean action of the instanton.

We begin by describing the aforementioned canonical formalism in Sec. II. This brief review is intended to provide a working understanding of the scheme without addressing all of the technical details or supplying all of the motivations. A discussion of these points can be found in the literature [16,17,19,20].

After describing the canonical formalism, we proceed in Sec. III to define our transition amplitude and to express it as a path integral. This transition amplitude is then evaluated in Sec. IV for two classes of exactly solvable models. In both, it is clear that ''Euclidean'' semiclassical contributions are exponentially suppressed for large $|S_E|$. Section V A rewrites the path integral in a more strongly convergent form which may be useful for numerical investigations. Section V B then addresses the semiclassical approximation. We close with a brief discussion in Sec. VI.

II. THE CANONICAL FORMALISM

We now describe the specific class of models to be addressed and review the canonical formalism of [16,17,19] on which our path integral will be based. The goal of this review is to provide a working understanding of the scheme and not to describe the technical subtleties in detail. For a more complete and rigorous presentation, see [16,19,20], and for a discussion of existence and uniqueness issues, see [20]. Essentially the same construction was introduced in [21,22] in slightly different contexts.

In this paper, we will study only finite-dimensional systems possessing a single constraint proportional to the system's Hamiltonian. We take the system to be expressed in canonical language in terms of a phase space Γ, which we shall assume to be $T^*\mathbf{R}^n$ and to be equipped with coordinates $x^i, p_i, i \in 0, \ldots, n-1$. Finally, we assume that the constraint is of the form

$$h = g^{ij}(x) p_i p_j + V(x). \tag{2.1}$$

As is well known, many such systems arise as ''minisuperspace models'' of gravitating systems [23–27] and so form a set of some interest. Note, however, that the method applies to more general models [16,17,19,20] and has been used to construct states of linearized gravity [21] as well as a Hilbert space of ''diffeomorphism-invariant'' states [19] in the loop representation approach to quantum gravity.

The quantization scheme to be followed here is known as the ''refined algebraic method'' (which is closely related to the ''Rieffel induction method'' of [16]) and may be thought of as an elaboration of the Dirac approach [28], in which the constraints are required to annihilate the so-called physical states. Specifically, the refined algebraic approach asks that we first quantize the system while completely ignoring the constraint. This provides an ''auxiliary'' Hilbert space $\mathcal{H}_{\text{aux}}$ in which to work. This space is called auxiliary because it contains much more than the physical states that satisfy the constraints. In our case, we will take this space to be $\mathcal{H}_{\text{aux}} = L^2(\mathbf{R}^n)$ with operators X^i (coordinates) and P_i (momenta) acting in the usual way. For simplicity in our expressions, we define our L^2 space using the measure $d^n x$. In this paper we follow the convention of [17] in denoting classical phase space functions by lower case letters while denoting quantum operators by capital letters. We use units in which $\hbar = 1$, except in Sec. V B which explicitly investigates the $\hbar \to 0$ limit.

The next step in the procedure is to ''quantize'' the constraint $h=0$. For our purposes, this simply means that we choose some self-adjoint operator H on $\mathcal{H}_{\text{aux}}$ which has the function h as its classical limit. The usual ambiguities are present at this level and we make no attempt to give a unique prescription. In fact, a somewhat greater ambiguity is present here than in quantizing the Hamiltonian of a nonrelativistic system. The point is that, classically, the constraint $h=0$ is equivalent to any constraint of the form $f(x)h=0$, although such a rescaling *can* affect our quantum prescription when $f(x)$ is not a constant.[1] Our viewpoint here is that this is just one more of the many ambiguities that arise when a classical system is quantized.

Now, if the spectrum of H were entirely discrete, the implementation of the Dirac prescription would be straightforward. Those eigenstates of H with eigenvalue zero would become the physical states of our theory and the ''physical Hilbert space'' could simply be the $H=0$ eigenspace of $\mathcal{H}_{\text{aux}}$. However, in typical cases H will also have a continuous spectrum at zero eigenvalue, for which the corresponding eigenstates will not be normalizable in the auxiliary Hilbert space but will instead be ''generalized eigenstates'' of H, a kind of distribution.

The strength of the refined algebraic quantization procedure is its ability to form a physical Hilbert space from such generalized states using an inner product that is, in a certain sense, induced from $\mathcal{H}_{\text{aux}}$. This has the advantage that any sufficiently ''nice'' operator A on $\mathcal{H}_{\text{aux}}$ which commutes with H induces a densely defined operator A_{phys} on the physical Hilbert space $\mathcal{H}_{\text{phys}}$. In addition, the map $A \mapsto A_{\text{phys}}$ is an ''*-algebra homomorphism,'' preserving multiplication, addition, and Hermitian conjugation of the operators. Since $\mathcal{H}_{\text{aux}}$ is a quantum version of the phase space Γ, it is through this induction process and the auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ that the *-algebraic properties of the observables on $\mathcal{H}_{\text{phys}}$ are connected to the reality properties of the classical phase space functions. This is in fact the important point, as the most ''physical'' requirement of an inner product is that it gives the proper adjointness relations to the quantum operators [32,33]. This construction is described below. The reader is encouraged to consult [17,19,20] for further details.

We shall in fact assume the spectrum of H to be *entirely* continuous at $H=0$. That this case is in some sense sufficient follows from the result [19,20] that the continuous and discrete eigenstates of H induce sectors of the physical Hilbert space which are *superselected* relative to each other. The presence of discrete eigenstates would, however, affect the formulation of the path integral in ways that we would prefer to ignore. We therefore content ourselves with the observation that many minisuperspace models can be formulated with a constraint having only a continuous spectrum at $H=0$ and restrict ourselves to this case; for details, see [17] and, in particular [18], for the case of the Bianchi type IX model.

In this situation and under a certain technical assumption concerning the operator H, the physical Hilbert space is

[1]In particular, the proposals of [29–31] are not compatible with our choice of inner product.

straightforward to construct. What we would really like is to ''project'' $\mathcal{H}_{\rm aux}$ onto the (generalized) states which are zero-eigenvalue eigenvectors of H. Of course, since none of these states are normalizable, this will not be a projection in the technical sense. Instead, it will correspond to an object which we will call $\delta(H)$, a Dirac delta ''function.'' Given the above mentioned assumption on H (see [20]), the object $\delta(H)$ can be shown to exist and to be uniquely defined. Technically speaking, however, it exists not as an operator in the Hilbert space $\mathcal{H}_{\rm aux}$, but as a map from a dense subspace $\mathcal{S}$ of $\mathcal{H}_{\rm aux}$ to the (for our purposes, topological) dual $\mathcal{S}'$ of $\mathcal{S}$. The space $\mathcal{S}$ may typically be thought of as a Schwarz space; that is, as the space of smooth rapidly decreasing functions on the configuration space. In this case, $\mathcal{S}'$ is the usual space of tempered distributions. Not surprisingly, this is reminiscent of the study of generalized eigenfunctions through Gel'fand's spectral theory [34] and $\mathcal{S}\subset\mathcal{H}_{\rm aux}\subset\mathcal{S}'$ forms a rigged Hilbert triple.

The key point is then as follows. While generalized eigenstates of H do not lie in $\mathcal{H}_{\rm aux}$, they can be related to normalizable states through the action of the ''operator'' $\delta(H)$. That is, generalized eigenstates $|\psi_{\rm phys}\rangle$ of H with eigenvalue 0 can always be expressed in the form $\delta(H)|\psi_0\rangle$, where $|\psi_0\rangle$ is a normalizable state in $\mathcal{S}\subset\mathcal{H}_{\rm aux}$. This choice of $|\psi_0\rangle$ is, of course, not unique and, in fact, we associate with the physical state $|\psi_{\rm phys}\rangle$ the entire *equivalence class* of normalizable states $|\psi\rangle\in\mathcal{S}$ satisfying

$$\delta(H)|\psi\rangle=|\psi_{\rm phys}\rangle. \qquad (2.2)$$

Each equivalence class of normalizable states will form a *single* state of the physical Hilbert space.

All that is left now is to ''induce'' the physical inner product from the auxiliary Hilbert space. Naively, the inner product of two physical states $|\phi_{\rm phys}\rangle$ and $|\psi_{\rm phys}\rangle$ may be written $\langle\phi|\delta(H)\delta(H)|\psi\rangle$, where $|\phi\rangle$ and $|\psi\rangle$ are normalizable states in the appropriate equivalence classes. This inner product is clearly divergent, as it contains $[\delta(H)]^2$. The resolution is simply to ''renormalize'' this inner product by defining the *physical* inner product to be

$$\langle\phi_{\rm phys}|\psi_{\rm phys}\rangle_{\rm phys}=\langle\phi|\delta(H)|\psi\rangle_{\rm aux}, \qquad (2.3)$$

where the subscripts ''phys'' and ''aux'' on the angular brackets indicate the two different inner products. Note that (2.3) does not depend on which particular states $|\phi\rangle,|\psi\rangle\in\mathcal{S}$ were chosen to represent the physical states $|\phi_{\rm phys}\rangle$ and $|\psi_{\rm phys}\rangle$. This construction parallels the case of a purely discrete spectrum as, if P_H were a projection onto normalizable zero-eigenvalue eigenstates of H, we would have $[P_H]^2=P_H$. Although $\delta(H)$ is not strictly speaking an operator, taking $|\phi\rangle$ and $|\psi\rangle$ to lie in $\mathcal{S}$ makes the above inner product well defined, as well as Hermitian. In the case of the free relativistic particle, this positive definite inner product corresponds to the Klein-Gordon inner product on the positive frequency states, but corresponds to *minus* the Klein-Gordon inner product on the negative frequency states. The positive and negative frequency subspaces are orthogonal as usual. A similar representation of the inner product holds in certain other cases [35].

Perhaps the most important feature of this approach is that it first defines the algebra of quantum observables (without requiring them to be found explicitly) and then provides an * representation of this algebra on the physical Hilbert space; that is, a representation on $\mathcal{H}_{\rm phys}$ in which the proper Hermitian conjugation relations hold. From the algebraic point of view, this is the fundamental goal of any quantization scheme, and it is this * representation that determines all physical predictions.

The representation is defined as follows. The observable algebra is defined by the * algebra of observables that commute with the constraint H and act ''nicely'' on the dense set $\mathcal{S}$ (see [19,20] for details). These are the analogues of the (smooth) gauge invariants of classical physics. Each such operator A then *induces* an operator $A_{\rm phys}$ on $\mathcal{H}_{\rm phys}$ through

$$A_{\rm phys}|\psi_{\rm phys}\rangle\equiv\delta(H)A|\psi\rangle, \qquad (2.4)$$

where again $|\psi\rangle$ is any state for which $|\psi_{\rm phys}\rangle=\delta(H)|\psi\rangle$. The operators $A_{\rm phys}$ then satisfy the same algebraic and Hermitian conjugation relations as the observables on $\mathcal{H}_{\rm aux}$, forming the desired * representation. The use of such operators and the physical inner product (2.3) has been shown to give physically reasonable results in interesting special cases [17,18] and in the semiclassical limit [36].

III. A PATH INTEGRAL FOR THE INNER PRODUCT

Having described how our models will be quantized, we now wish to derive a path integral formalism for these systems. To do so, we must first answer the question ''Just what quantity should we derive a path integral for?'' Path integrals are often used to represent the ''transition amplitudes'' that encode the time evolution of quantum systems. However, for the cases we consider, the Hamiltonian explicitly vanishes on the physical Hilbert space. Thus the operator e^{-iHt} is just the identity.

Nevertheless, we know that the physical states *do* contain information that we may call dynamical (see, for example [37–41], for general comments or [17,36] for a discussion in the context of this particular approach). Thus there should be some mathematical object which, more or less, encodes our idea of a ''transition amplitude.''

Apparently nontrivial path integral expressions for ''transition amplitudes'' have in fact been studied by a number of authors (e.g., [14,15,42]). In the minisuperspace context, all of these are transition amplitudes between two *configurations* x and x' (which are the analogues of the three-geometries of $3+1$ gravity), or perhaps their conjugate momenta. As a result, we will seek our transition amplitude in the auxiliary Hilbert space $\mathcal{H}_{\rm aux}$.

We take our transition amplitudes to be just the matrix elements of the operator $\delta(H)$ in $\mathcal{H}_{\rm aux}$. That is, we will compute $\langle x|\delta(H)|x'\rangle$ where $|x\rangle$ and $|x'\rangle$ are generalized eigenstates of the coordinate operators X^i. Our reasons for this are twofold. First, while expressed in terms of the auxiliary space, such matrix elements contain all of the information about $\mathcal{H}_{\rm phys}$ as they define the physical inner product. Second, when one of the coordinates (say, x^0) is considered to represent a ''clock'' and when this clock behaves semiclassically [36] this object does in a certain sense describe the amplitude for the ''evolution'' of the ''state'' x at ''time'' x^0 to the ''state'' x' at ''time'' $x^{0\prime}$. Here x represents the coordinates on a slice through the configuration space of constant x^0.

It is now straightforward to represent this object as a path integral. To do so, consider the path integral expression for the operator e^{-iNH} on $\mathcal{H}_{\rm aux}$, which we expect to exist and which can be derived in the usual way by skeletonization (see, for example, [43]) of paths between x at ''time'' zero and x' at ''time'' N. Note that by ''time'' we mean an additional parameter that we now introduce; *not* one of the coordinates x^i. We then integrate N from $-\infty$ to ∞ to turn e^{-iHN} into $\delta(H)$.

The resulting path integral is then

$$\langle x|\delta(H)|x\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dN \int DxDp \exp\left(i\int_0^N dt[p\dot{x} - h(x(t),p(t))]\right) \tag{3.1}$$

where $\int_{-\infty}^{\infty} dN$ denotes an integral over the *single* variable N while $DxDp$ denotes the Liouville measure on the canonical path space [43]. Since the configuration variables are specified at the end points, there is ''one less'' set of integrations over the coordinates than over the momenta. The notation $h(x(t),p(t))$ stands for the ''symbol'' $\langle p=p(t)|H|x=x(t)\rangle_{\rm aux}/\langle p|x\rangle_{\rm aux}$ of the operator H, where $|p\rangle$ is an eigenstate of the momenta P_i.

In the usual way, gauge-fixing machinery and redundant integrations can now be introduced to write (3.1) in a form where its independence of ''gauge'' is more explicit. Halliwell [29] has performed this analysis in the reverse direction by starting with the Faddeev-Popov form and introducing the gauge-fixing condition $\dot{N}=0$. Since he arrives at just our result (3.1), his work allows us to express the physical inner product in the form

$$\langle x|\delta(H)|x\rangle = \frac{1}{2\pi}\int DNDxDp\,\delta(G)\Delta(G)\exp\left(i\int_0^1 dt[p\dot{x} - N(t)h(x(t),p(t))]\right) \tag{3.2}$$

where G is now any appropriate gauge-fixing function, $\Delta(G)$ is the associated Fadeev-Popov determinant, and the sum is over all paths $(x(t),p(t),N(t))$ in which $x^i(t)$, $p_i(t)$, and $N(t)$ are allowed to range over the entire real line. This is the path integral that we shall explore in Sec. V. For interested readers, the convergence properties of (3.1) and (3.2) are discussed in detail in Appendix A.

IV. EXACTLY SOLVABLE MODELS

Having derived a path integral for $\langle x|\delta(H)|x'\rangle$, the physical inner product, it is of interest to see what form this distribution takes in simple cases where an exact analytic expression can be obtained. As usual, the cases that we will study are the ''purely quadratic ones;'' the perturbed Bianchi type I model (or free relativistic particle) and the case of coupled harmonic oscillators.

A. Perturbed diagonal Bianchi type I

The Bianchi type I model is a minisuperspace describing spatially homogeneous spacetimes of the form $\mathcal{M}=T^3\times\mathbf{R}$ having a foliation by three-tori with flat Riemannian metrics (so that the tori form spacelike hypersurfaces of $\mathcal{M}$). In the diagonal version of this model the metric is such that, at each point $x\in\mathcal{M}$, three mutually orthogonal closed geodesics intersect at x and each encircles an arm of the torus once. This system may be formulated on the configuration space $\mathcal{Q}=\mathbf{R}^3$ with a constraint of the form

$$h_{BI} = -p_0^2 + p_1^2 + p_2^2. \tag{4.1}$$

In this case, the coordinate x^0 describes the volume of the three-torus while the coordinates x^1 and x^2 describe the ''anisotropies,'' the ratios of the lengths of minimal curves encircling the torus in different directions. We will consider a perturbed and slightly more general model on $\mathcal{Q}=\mathbf{R}^n$ for which the quantum constraint is

$$H = \frac{1}{2}\left(-P_0^2 + \sum_{i=1}^{n-1} P_iP_i + m^2\right) \tag{4.2}$$

for $m^2>0$. Note that without the perturbation (m^2), the action S would vanish on every classical solution and we would be unable to consider the semiclassical limit $|S|\gg 1$. The constant factor of $\frac{1}{2}$ affects none of the results, but conforms to the usual convention for the normalization of kinetic terms.

Such a system looks exactly like the free relativistic particle. However, we will intentionally avoid referring to this system by that name, as we feel that the *physics* of the two situations is quite distinct. This follows from the fact that the metric which defines the constraint's ''kinetic term'' has a different interpretation in each of the two cases. A free relativistic particle with $p_0<0$ is usually interpreted as ''traveling backwards in time,'' a process that we suppose to be physically disallowed. This leads to the usual preference for positive frequency states over negative frequency states. However, in the Bianchi type I model, a negative p_0 means only that the x^0 of the tori is decreasing with proper time—that is, that the universe is *collapsing*. This is not only a physically interesting process but a process which classically *must* occur in some minisuperspace models, such as Bianchi type IX [44]. Thus we are pleased to include the negative frequency states in our model.

We now proceed to compute the integral

$$\langle x|\delta(H)|x'\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dN\langle x|e^{-iHN}|x'\rangle = \frac{1}{\pi}\mathrm{Re}\left(\int_0^{\infty}\langle x|e^{-iHN}|x'\rangle\right), \tag{4.3}$$

where Re denotes the real part. The operator e^{-iHN} is just $e^{-im^2N/2}$ times a product of propagators for free nonrelativistic particles. As a result, its matrix elements are readily seen to be

$$\langle x|e^{-iHN}|x'\rangle = e^{(i\pi/2)(1-n/2)}(2\pi N)^{-n/2} \times \exp\left[-\frac{im^2}{2}\left(N-\frac{(x-x')^2}{m^2N}\right)\right] \quad (4.4)$$

for $N>0$. We can evaluate (4.3) using (3.471) of [45] to yield, for $(x-x')^2>0$,

$$\langle x|\delta(H)|x'\rangle = \frac{2}{\pi(2\pi)^{n/2}}\left[\frac{\sqrt{(x-x')^2}}{m}\right]^{(1-n/2)} \times K_{(n/2)-1}(m\sqrt{(x-x')^2}), \quad (4.5)$$

where $K_{(n/2)-1}$ is the modified Bessel function (of the second kind) of order $(n/2)-1$. Similarly, for $(x-x)^2<0$, we find

$$\langle x|\delta(H)|x'\rangle = \frac{1}{(2\pi)^{n/2}}\left[\frac{\sqrt{-(x-x')^2}}{m}\right]^{(1-n/2)} \times\left\{\cos\left[\pi\left(\frac{n-1}{2}\right)\right]J_{(n/2)-1}(m\sqrt{-(x-x')^2}) - \sin\left[\pi\left(\frac{n-1}{2}\right)\right]N_{(n/2)-1}(m\sqrt{-(x-x')^2})\right\}. \quad (4.6)$$

An intuitive feel for just why the answer is of this form may be obtained by noting that it describes a certain correlation function in free scalar field theory, or alternately by performing this integral in the semiclassical approximation. For the interested reader, the semiclassical analysis is carried out in Appendix B.

Note that, for $-(x-x')^2 \gg m^2$, the matrix elements are roughly $\sin[m\sqrt{-(x-x')^2}]$ or $\cos[m\sqrt{-(x-x')^2}]$ depending on the number of degrees of freedom. That is, they include equal contributions from what might be called the positive and negative frequency parts. Nevertheless, when $(x-x')^2 \gg m^2$, the matrix elements contain only the *decreasing* exponential $\exp[-m\sqrt{(x-x')^2}]$. This occurs even though the Euclidean action is unbounded below. Similar results hold for the case $m^2=-k^2<0$ for which the resulting physical inner product is obtained by replacing m with k and $(x-x')^2$ with $-(x-x')^2$ in (4.5) and (4.6). As might be expected, this is related to which points of the stationary phase contribute to $\langle x|\delta(x)|x'\rangle$ in the semiclassical approximation. We will return to this point in Sec. V and Appendix B.

It is interesting to compare the results (4.5) and (4.6) to what one might obtain by a ''contour rotation prescription'' of the sort suggested in [8]. The idea is to rotate the contour of the conformal mode (represented here by x^0) to imaginary values ($x^0 \to ix^0$) so that the Euclidean action becomes bounded below. We can certainly perform the integral (4.3) taking $-p_0^2$ to be replaced by p_0^2 in the Hamiltonian h. The result is just (4.5) above with $(x-x')^2$ replaced by $(x-x')^2_E \equiv \Sigma_{i=0}^n (x^i)^2$, since $(x-x')^2_E \geq 0$. The task is then to analytically continue back; $x^0 \to -ix^0$. For $(x-x')^2>0$, this clearly yields (4.5); the correct answer from our point of view. However, for $(x-x')^2<0$, the analytic continuation is ambiguous. Because of the branch cut that defines the square root, the answer will depend on which path is followed through the complex plane. As can be seen from (4.6), what we would call the ''right'' answer results from combining these two contributions with equal weights and with a phase that depends on n.

B. Coupled harmonic oscillators

In order to more thoroughly explore the properties of exactly solvable models, we now study the case of coupled harmonic oscillators. However, to fit with the general character of minisuperspace models, we will take one of the oscillators to have negative energy. That is, we will again take our system to be defined on the phase space $\Gamma = T^*\mathbf{R}^n$, with the constraint

$$0 = h = \frac{1}{2}\left(-p_0^2-(x^0)^2\omega^2+\sum_{i=1}^{n-1}[p_i^2+(x^i)^2\omega^2]\right) \equiv \frac{1}{2}[p^2+\omega^2x^2] \quad (4.7)$$

for $\omega^2>0$. We could, in principle, also study the case where one or more of the harmonic oscillators is inverted [with Hamiltonian $\frac{1}{2}(p^2-\omega^2x^2)$], but we will not do so here. For simplicity, we assume n to be even. Models of the form (4.7) do arise as minisuperspace models of gravity interacting with scalar fields [46] and many of their aspects have been studied in the literature [46–48].

Strictly speaking, however, this model does *not* fall into the class allowed by Sec. II. Since it is a sum of harmonic oscillator Hamiltonians, instead of the constraint H having a purely continuous spectrum at zero [when quantized in the usual way on $L^2(\mathbf{R}^n)$], its spectrum is purely *discrete*—not just at zero, but everywhere. This creates a number of subtleties, such as the fact that there are rather few zero-eigenvalue eigenstates of the constraint unless all of the oscillators have commensurate frequencies. Furthermore, unless an appropriate constant is added to H, it will in general have *no* eigenstates with eigenvalue zero. Thus a better way to quantize this model might be to rewrite the constraint (see, for example, [17,18,36]) in such a way that the spectrum is purely continuous.[2] Unfortunately, this necessarily destroys the purely quadratic form of the action and thus the exact solvability of the model.

Our purpose in studying this model is not to examine the detailed predictions of the cosmological scenario of [46], but rather to investigate the general mathematical properties of the expressions (3.1) and (3.2) for the physical inner product. Thus we will quantize this model using the constraint operator

$$H = \frac{1}{2}\left[-P_0^2-(X^0)^2\omega^2+\sum_{i=1}^{n-1}[P_i^2+(X^i)^2\omega^2]\right]+\left[1-\frac{n}{2}\right]\omega. \quad (4.8)$$

[2]This continuous spectrum form of the constraint is in fact in better accord with the global properties of the original gravitational model of [46].

The frequencies and constants in (4.8) are specifically chosen so that there seem to be a sufficient number of zero-eigenvalue eigenvectors. We shall not concern ourselves with whether or not such choices are ''natural.''

However, if we are to proceed in this way, expressions (3.1) and (3.2) must be modified. This is because their aim was to calculate the operator $\delta(H)$ and, now that the spectrum of H is discrete, this object is highly divergent: when acting on a normalizable state $|\psi\rangle$ for which $H|\psi\rangle=0$, $\delta(H)$ cannot possibly be defined.

As stated in Sec. II, the analogous object for the case of a discrete spectrum is the projection $P_{H=0}$ onto the zero-eigenvalue subspace for the operator H. An expression for $\langle x|P_{H=0}|x'\rangle$ analogous to (3.1) and (3.2) can be found by realizing that the ''evolution operator'' e^{-iNH} is, in this case, periodic in N with period $2\pi/\omega$. This, of course, is the source of the would-be divergence in $\delta(H)=(1/2\pi)\int_{-\infty}^{\infty}dNe^{-iNH}$, but it also allows us to express the projection $P_{H=0}$ as the integral over a single cycle of N:

$$P_{H=0}=\frac{\omega}{2\pi}\int_{-\pi/\omega}^{\pi/\omega}dNe^{-iNH}=\frac{\omega}{\pi}\int_{0}^{\pi/\omega}dN(e^{-iNH}+e^{iNH}). \tag{4.9}$$

Similarly, the analogues of (3.1) and (3.2) are given by taking N to exist on a periodic interval of length $2\pi/\omega$.

As in the perturbed Bianchi type I model, the operator e^{-iHN} is a product of evolution operators for nonrelativistic particles which can be evaluated exactly; perhaps most easily by using the semiclassical approximation (which is exact for quadratic Hamiltonians). For $\pi/\omega>N>0$, the result is

$$\langle x|e^{-iHN}|x'\rangle=\left(\frac{\omega}{2\pi\sin\omega N}\right)^{n/2}e^{i(\pi/2)(1-n/2)}e^{iS_{\rm cl}(x,x';N)} \tag{4.10}$$

where

$$S_{\rm cl}(x,x';N)=\frac{\omega}{2}\,\frac{(x^2+x'^2)\cos\omega N-2x\cdot x'}{\sin\omega N} \tag{4.11}$$

is the action of the least action path between x and x' traversed in the *given* time N. Note that this path is unique for $N\neq 0,\ \pi/\omega$. Here, $x\cdot x'$ denotes $-x^0x^{0\prime}+\Sigma_{i=1}^{n-1}x^ix^{i\prime}$.

All that remains is to evaluate the integral over N in (4.9). For the case $n=2$, we may refer to [49,50]. More generally, if we define $a=-\omega(x^2+x'^2)/2$ and $b=\omega x\cdot x'$ then the result may be expressed as

$$\langle x|P_{H=0}|x'\rangle=2\omega{\rm Re}\left\{(2\pi)^{-(n/2)}ie^{i(\pi/2)(1-n/2)}\times\left(i\frac{\partial}{\partial b}\right)^{(n/2)-1}H_0^{(1)}(\sqrt{b^2-a^2})\right\}, \tag{4.12}$$

using (6.677) from [45]. Here, $H_0^{(1)}$ is the usual Hankel function of the first kind and the square root is defined by $\sqrt{re^{i\theta}}=r^{1/2}e^{i\theta/2}$ for $0\leqslant\theta\leqslant\pi$. Thus, when $a^2>b^2$, (4.12) takes the form

$$\langle x|P_{H=0}|x'\rangle=\frac{4\omega}{\pi}(2\pi)^{-n/2}\left(\frac{\partial}{\partial b}\right)^{(n/2)-1}K_0(\sqrt{a^2-b^2}). \tag{4.13}$$

The results (4.12) and (4.13) may in turn be written as a sum of Hankel functions of orders $0<\nu<n/2-1$ by using the usual Bessel function recurrence relations.

The matrix elements (4.12) have the same general structure as those of (4.5) and (4.6). That is, they are a Bessel function of order $n/2-1$ of the square root of a function of x and x'. Recall that in the case of perturbed Bianchi type I, the behavior of this Bessel function was determined by the sign of $(x-x')^2$; that is, by whether the points x and x' could be connected by a ''Lorentzian'' classical solution (with real lapse N) or by a ''Euclidean'' solution with imaginary lapse. A similar phenomenon occurs for our coupled oscillator model. Pairs of configurations (x,x') may be separated into three distinct classes: those for which $-a/b>1$, those for which $1>-a/b>-1$, and those for which $-1>-1/b$. Only for the first category ($-a/b>1$) does a ''Euclidean'' classical solution (with imaginary lapse) exist. Such solutions come in pairs with Euclidean actions $S_E=\pm\sqrt{a^2-b^2}$. Similarly, a ''Lorentzian'' solution (with real lapse) exists only for the second case, $1>-a/b>-1$. These solutions also come in pairs, with actions $S=\pm\sqrt{b^2-a^2}$. For the third case ($-a/b<-1$), the configurations x and x' may be connected by *complex* classical solutions with Re$N=\pi/\omega$ (but no such solutions exist for the first two classes of pairs). The Euclidean action is also real for this last case, and is again given by $S_E=\pm\sqrt{a^2-b^2}$.

The semiclassical approximation is valid (in our units) when $|S|=\sqrt{|b^2-a^2|}\gg 1$ so that, once again, when x and x' are connected by a Lorentzian solution, this approximation contains contributions of both forms e^{iS} and e^{-iS} which are equally weighted up to a phase. However, when the connecting solution is Euclidean (or complex with real Euclidean action), only the exponentially *decreasing* solution contributes and the leading semiclassical term is $e^{-|S_E|}$. We follow the usual convention of $iS=-S_E$ so that this exponentially decreasing factor corresponds to the stationary point with positive Euclidean action.

This seems to indicate a general property of the semiclassical approximation (and perhaps of the entire expression) for (3.1) and (3.2) which we shall investigate further in Sec. V. Note that this case is more subtle than that of the perturbed Bianchi type I model since that model had the property that (for $m^2>0$) the Euclidean action of a Euclidean solution is always positive when the ''Euclidean lapse'' iN is positive. In contrast, for coupled harmonic oscillators, a Euclidean solution with positive Euclidean lapse can have a Euclidean action with either sign. This, therefore, is much closer to the generic case.

As in the perturbed Bianchi type I model, we briefly compare (4.12) with a contour rotation scheme where x^0 is rotated to ix^0. Again, this gives just the right result in the ''Euclidean sector'' ($a^2>b^2$), but the branch cut of the square root creates an ambiguity when analytically continuing back to the ''Lorentzian sector'' $a^2<b^2$. Our result (4.12) includes both possible outcomes, equally weighted up to an n-dependent phase.

V. THE GENERAL CASE

In Secs. IV A and IV B, we discoverd several interesting properties of the exact results (4.5), (4.6), and (4.12). We will now argue that these properties should hold in general. Specifically, we first show in Sec. V A that the inner product may be expressed as a path integral over both Lorentzian *and* Euclidean paths (and combinations thereof) in which the contribution of the Euclidean paths is exponentially suppressed for small $\hbar$. Such an expression is more convergent than (3.1) and (3.2) and may be of use for numerical investigations. A representation of this form also indicates that Lorentzian instantons (with either sign of the action) and Euclidean instantons with positive Euclidean action will contribute to our transition amplitude in the semiclassical limit. We then argue in Sec. V B that, in addition, Euclidean instantons with negative action do *not* contribute to the semiclassical limit.

A. A simplified expression

Our general strategy will be to simplify the path integral by performing the integrals in (3.2) over the momenta *and* over the lapse; thus we assume that we may change the order of integration. The result will (almost) be a configuration space path integral in which, in effect, the constraint equation

$$g_{ij}(x)\frac{\dot{x}^i\dot{x}^j}{N^2}+V(x)=0 \tag{5.1}$$

has been solved for the lapse N. That is, we will obtain a path integral based on a Baierlein-Sharp-Wheeler-like [51] form

$$S=\int dt\sqrt{g_{ij}\dot{x}^i\dot{x}^jV(x)} \tag{5.2}$$

of the classical action.

We begin with the expression (3.2) for the matrix elements $\langle x|\delta(H)|x'\rangle$. Having written the integral in a form where Faddeev-Popov technology applies, we are now free to use any gauge-fixing condition we wish. Because we would like to integrate out the momenta, we will use a gauge condition of the form $G(x)=0$ where G is a function of the coordinate variables *only* (see [52] for a discussion of canonical gauges in this context). In addition, we assume $\nabla G\cdot\nabla G>0$; that is, that ∇G is spacelike. Unfortunately, $G=0$ is not really a ''good'' gauge condition [53] as there will always exist points in phase space at which the Poisson brackets $\{G,H\}=p\cdot\nabla G$ of G with H vanish (such as where all momenta vanish). Nevertheless, such a condition is often ''good'' on all but a set of measure zero. Having admitted our treatment to be heuristic, we assume that we may use such a gauge condition below.

Now, since there is only a single constraint, the Faddeev-Popov determinant takes the particularly simple form of a product over times t:

$$\Delta(\{G,H\})=\prod_t|\{G,H\}(t)|=\prod_t|\nabla G(t)\cdot_t p(t)| \tag{5.3}$$

where the inner product $\cdot_t$ denotes a contraction through the (co)metric $g^{ij}(x(t))$.

For common factor orderings of the quantum constraint H, the symbol $h(x,p)$ will be quadratic in the momenta p. We shall assume that it takes the form

$$h(x,p)=g^{ij}(x)p_ip_j+V_q(x) \tag{5.4}$$

where the subscript q on V indicates that the potential may receive quantum corrections such as terms proportional to the curvature of g_{ij} [54,55]. In order to be explicit, we shall assume the signature of g to be everywhere $(1,n-1)$.

Most of the the momentum integrals are of the form $\int_{-\infty}^{\infty}dp e^{i(p\dot{x}-\lambda p^2)}$ and can be performed exactly using stationary phase methods. However, the presence of the absolute value $|\nabla G\cdot p|$ means that, for each value of t, there will be one momentum integral which cannot be performed in this way. It will be sufficient for our purposes to leave this integral undone, and to simply perform the others. The component of p in the direction of $\nabla G(x(t))$ will be denoted $p_\parallel$. Similarly, $n_\parallel(x(t))$ will be the unit vector in the direction of $\nabla G(x(t))$. Performing these momentum integrals yields the expression

$$\begin{aligned}\langle x|\delta(H)|x'\rangle=\int DNDxDp_\parallel\exp\Bigg[i\frac{1}{2}\int_0^1dtg^\perp_{ij}\frac{\dot{x}^i\dot{x}^j}{N}\\ -N(V_q(x)+p_\parallel^2)\Bigg]\\ \times\prod_t\exp\left[i\frac{\pi\mathrm{sgn}(N)}{2}\left(\frac{n-3}{2}\right)\right]\\ \times|N(t)|^{(1-n)/2}\sqrt{-\det g^\perp}\,\delta[G(x(t))]\\ \times|\nabla G(x(t))||p_\parallel|\end{aligned} \tag{5.5}$$

where the usual product of normalization factors at each time has been dropped (they may be absorbed into the definition of the measure). Here $g^\perp_{ij}$ is the induced metric on surfaces of constant $G(x)$.

Finally, we wish to perform the integrals over N. As in the explicitly soluble models discussed in Sec. IV, these integrals may be expressed in terms of Bessel functions. Note that each such integral is of the form

$$\begin{aligned}I=\int_{-\infty}^{\infty}dN\exp\left[i\frac{\pi\mathrm{sgn}(N)}{2}\left(\frac{n-3}{2}\right)\right]|N(t)|^{(1-n)/2}\\ \times\exp\left(i\left[\frac{1}{2}g_{ij}\frac{\dot{x}^i\dot{x}^j}{N}-N(V_q(x)+p_\parallel^2)\right]\right).\end{aligned} \tag{5.6}$$

This is essentially the same integral with which we were faced in Sec. IV A. Introducing $v\equiv V+n_\parallel^2p_\parallel^2$, $k\equiv g_{ij}\dot{x}^i\dot{x}^j$, and dropping constant normalization factors, the integral yields

$$I=(k/v)^{(3-n)/4}K_{(n-3)/2}(\sqrt{kv}) \tag{5.7}$$

when $kv>0$ and

$$I=\pi\mathrm{Re}\{(-k/v)^{(3-n)/4}e^{i\pi(n-2)/2}H^{(1)}_{(n-3)/2}(\sqrt{-kv})\} \tag{5.8}$$

when $kv<0$.

As a result, the physical inner product may be written

$$\langle x|\delta(H)|x'\rangle = \int DxDp_{\parallel}\prod_t I(k,v)\,\delta(G)|\nabla G||p_{\parallel}|\sqrt{-\det g^{\perp}}. \tag{5.9}$$

The connection to the Baierlein-Sharp-Wheeler-like (5.2) should be clear: since Bessel functions are exponentials at large arguments, if the momenta $p_{\parallel}$ were replaced by their semiclassical values $\dot{x}\cdot\nabla G\sqrt{v/k}$ then (5.9) would be a path integral based on the action (5.2), although with a rather complicated measure.

This expression may be thought of as a sum over both Lorentzian and Euclidean bits of path at each time. Here, we say that a segment of path is Lorentzian when $kv>0$, so that a real lapse N would be associated with this segment by solving the constraint

$$\frac{k}{N^2}+v=0. \tag{5.10}$$

Similarly, a bit of path with $k/v<0$ is Euclidean as the corresponding lapse is imaginary. Note that this occurs despite the original expression (3.1) being an integral only over a real classical lapse N. As in our exactly solvable models, the Lorentzian bits contribute with both signs of the action but the Euclidean path bits are always exponentially *suppressed* when the corresponding $|S_E|$ is large. A similar result is obtained if other momentum integrals are left undone as well, so long as the momenta at each time are integrated over at least one two-plane with signature $(-,+)$.

The argument of every Bessel function is now manifestly positive. As a result, the fact that neither the Lorentzian nor the Euclidean action is positive definite has disappeared from sight. If we define a slightly modified function I_ϵ by $I_\epsilon(k,v)=I(k,v)$ for $kv>0$ and

$$I_\epsilon(k,v)\equiv \mathrm{Re}\{(-k/v)^{(3-n)/4}e^{i\pi(n-2/2)} \times H^{(1)}_{(n-3)/2}([1-i|\epsilon|]\sqrt{-kv})\} \tag{5.11}$$

for $kv<0$, then $I_\epsilon(k,v)$ vanishes in the limit of large kv (for $\epsilon\neq 0$). Our matrix elements may therefore be expressed in the form

$$\langle x|\delta(H)|x'\rangle = \lim_{\epsilon\to 0}\int DxDp_{\parallel}\prod_t I_\epsilon(k(t),v(t)) \times\delta(G(x(t)))|\nabla G(x(t))||p_{\parallel}|\sqrt{-\det g^{\perp}} \tag{5.12}$$

for which the integrand is exponentially decreasing. As it converges more strongly than (3.1), we may hope that (5.12) will be of use in numerical computations.

B. Instantons and the semiclassical approximation

The expression (5.9) for our transition amplitude includes an explicit sum over both Lorentzian and Euclidean paths, as well as arbitrary combinations of the two. In the semiclassical approximation, this result indicates that both Lorentzian and Euclidean stationary points contribute to the physical inner product, so long as the latter have positive Euclidean action. In fact, since the contribution of Euclidean path bits is exponentially suppressed in (5.9) for small $\hbar$, it appears that stationary points with negative Euclidean action *never* contribute, as was suggested by the examples of Sec. IV. However, we have not yet shown this carefully. In particular, it is possible that a stationary point of the action, while not actually on the contour over which the integration is performed, might contribute to the semiclassical approximation.[3] In general, in fact, we *do* expect such stationary points to contribute, as the contour of integration could easily be deformed to reach a complex stationary point lying just off the real axis. If the contour, say, for the variable k in (5.9) can be deformed far enough, it could wrap around the branch point at $k=0$ to reach a stationary point on the ''second sheet'' of the Riemann surface on which k exists. Such a stationary point would then contribute as $e^{+|S_E|}$ to the inner product $\langle x|\delta(H)|x'\rangle$. We will now argue that this does not occur. Because we study the semiclassical approximation, the factors of $\hbar$ will be restored below.

Let us first note that, if the semiclassical approximation is to hold, our matrix elements must be of the form

$$\langle x|\delta(H)|x'\rangle = e^{iS(x,x')/\hbar}C(x,x') \tag{5.13}$$

where $C(x,x')$ is slowly varying in comparison with $e^{iS(x,x')/\hbar}$. In particular, since $S(x,x')$ is continuous on regions $\mathcal{R}$ of $\mathbf{R}^n\times\mathbf{R}^n$ where the number n of connecting paths in constant, $C(x,x')$ must be continuous there as well.

In general, we expect the union of the boundaries of such regions $\mathcal{R}$ to have measure zero so that the union U of the interiors has measure 1. We therefore *assume* that this is so and consider only the open subset U on which $\langle x|\delta(H)|x'\rangle$ is continuous.

If the matrix element $\langle x_0|\delta(H)|x_0'\rangle$ takes the form $e^{+|S_E(x_0,x_0')|/\hbar}$ (to leading semiclassical order[4]) at some pair $(x_0,x_0')\in U$, it must in fact take this form on some open rectangular region $V_\hbar\times W_\hbar$ ($V_\hbar\subset\mathbf{R}^n$, $W_\hbar\subset\mathbf{R}^n$) containing (x_0,x_0'). If the diameters of $V_\hbar$ and $W_\hbar$ are much less than $\hbar[|\partial S_E/\partial x|]^{-1}$ and $\hbar[|\partial S_E/\partial x'|]^{-1}$, respectively, then $S(x,x')/\hbar$ is essentially constant on $V_\hbar\times W_\hbar$. As a result, $\langle x|\delta(x)|x'\rangle$ is essentially real on $V_\hbar\times W_\hbar$ and satisfies $\langle x|\delta(H)|x'\rangle\geq e^{\lambda/\hbar}$ where (say) $\lambda=\frac{1}{2}|S_E(x,x')|$.

We now choose two states $|\phi\rangle$ and $|\psi\rangle$ in $\mathcal{S}$ whose representations $\langle x|\phi\rangle=f([x-x_0]/\hbar)$ and $\langle x|\psi\rangle=g([x-x_0]/\hbar)$ are positive real, supported in $V_\hbar$ and $W_\hbar$, respectively, and have $f(y)$ and $g(y)$ independent of $\hbar$. Let us define

[3]We have already seen an example of such behavior as the Euclidean paths that are explicitly included in (5.12) correspond to stationary points of the N integrals at imaginary lapse (and therefore off the original *real* contour).

[4]The fact that a Euclidean path dominates does not necessarily require the matrix elements to be real and positive; there may in fact be an overall phase that we have neglected. The point is that this phase is both independent of $\hbar$ (for small $\hbar$) and slowly varying with x and x'.

$$a_\phi = \hbar^{-n}\int_{\mathbf{R}^n}\langle x|\phi\rangle d^n x = \int_{\mathbf{R}^n} f(y) d^n y,$$

$$a_\psi = \hbar^{-n}\int_{\mathbf{R}^n}\langle x|\psi\rangle d^n x = \int_{\mathbf{R}^n} g(y) d^n y, \tag{5.14}$$

$$b_\phi = \hbar^{-n}\int_{\mathbf{R}^n}|\langle x|\phi\rangle|^2 d^n x, \quad b_\psi = \hbar^{-n}\int_{\mathbf{R}^n}|\langle x|\psi\rangle|^2 d^n x.$$

It follows that a_ϕ, a_ψ, b_ϕ, and b_ψ are real, positive, and independent of $\hbar$. Note that the physical inner product of our two states satisfies

$$\langle \phi_\hbar|\delta(H)|\psi_\hbar\rangle \geq \hbar^{2n} a_\phi a_\psi e^{\lambda/\hbar} \tag{5.15}$$

to leading semiclassical order and that the expression on the right diverges as $\hbar \to 0$.

We will now derive a contradiction. To do so, we return to our original expression for the inner product,

$$\langle \phi_\hbar|\delta(H)|\psi_\hbar\rangle = \int_{-\infty}^{+\infty}\langle \phi_\hbar|e^{-iHN/\hbar}|\psi_\hbar\rangle. \tag{5.16}$$

Recall that, for $|\phi_\hbar\rangle, |\psi_\hbar\rangle \in \mathcal{S}$, this integral *converges* at large N. Effectively, this is because the states $|\phi_\hbar\rangle$ and $|\psi_\hbar\rangle$ are characterized (to accuracy ϵ) by some minimal energy scale[5] $E_\hbar$ and the integration over the region $|N| > T_\hbar \approx \hbar/E_\hbar$ yields a negligible contribution. Note, however, that since $|\phi_\hbar\rangle$ and $|\psi_\hbar\rangle$ have norms $\sqrt{\hbar^n b_\phi}$ and $\sqrt{\hbar^n b_\psi}$ and since the operator $e^{-iHt/\hbar}$ is unitary, we have the bounds

$$\langle \phi_\hbar|e^{-iHN/\hbar}|\psi_\hbar\rangle \leq \hbar^n \sqrt{b_\phi b_\psi} \tag{5.17}$$

and

$$\langle \phi_\hbar|\delta(H)|\psi_\hbar\rangle \leq \hbar^{n+1} C \sqrt{b_\phi b_\psi}/E_\hbar \tag{5.18}$$

where C is some constant independent of $\hbar$. In order to compare this bound with the semiclassical expression (5.15), we estimate $E_\hbar$ as follows.

Recall that $h = g^{ij}(x)p_i p_j + V(x)$. The states $|\phi_\hbar\rangle$ and $|\psi_\hbar\rangle$ are characterized by coordinates x_0 and x_0' (which are independent of $\hbar$) and by momentum scales

$$p_\hbar = \frac{\hbar}{\mathrm{diam}(V_\hbar)} = \left[\frac{\partial S_E}{\partial x}\right], \quad p_\hbar' = \frac{\hbar}{\mathrm{diam}(W_\hbar)} = \left[\frac{\partial S_E}{\partial x'}\right] \tag{5.19}$$

which are also independent of $\hbar$. As a result, $E_\hbar \approx g(x_0)p_\hbar^2 + V(x_0)$ is independent of $\hbar$ and the bound (5.18) *vanishes* as $\hbar \to 0$, in contradiction with (5.15). Here, $g(x_0)$ is some bound on the components of the $g^{ij}(x)$ at $x = x_0$. We thus conclude that, at least for minisuperspace models, Euclidean instantons always contribute to our transition amplitude as $e^{-|S_E|/\hbar}$. Similarly, complex instantons must contribute as $e^{i\mathrm{Re}S/\hbar}e^{-|\mathrm{Im}S/\hbar|}$, where Im denotes the imaginary part.

[5] This is the energy at which $|\langle \phi_\hbar|\delta(H)|\psi_\hbar\rangle - \langle \phi_\hbar|\delta(H-E_\hbar)|\psi_\hbar\rangle| < \epsilon$. As a result, it is related to a sort of continuity [20] of the spectral representations of $|\phi_\hbar\rangle$ and $|\psi_\hbar\rangle$. $E_\hbar$ depends on the functions f and g as well as on $\hbar$ and the accuracy ϵ. In particular, it is not a property of the Hamiltonian H alone and in no way corresponds to a mass gap for the system.

VI. DISCUSSION

The goal of this work was to use a canonical formalism (the refined algebraic or Rieffel induction method) to represent a minisuperspace transition amplitude as a path integral and to investigate this expression both exactly and in the semiclassical limit. We have seen that the path integral may be written in the form (5.12) which explicitly sums over both Lorentzian path bits (which appear with both signs of the action) and Euclidean path bits which are exponentially suppressed. As a result, we conclude that any Lorentzian or positive action Euclidean stationary point may contribute to our transition amplitude in the semiclassical limit. We also argued in Sec. V B that Euclidean instantons with *negative* Euclidean action (which would be exponentially enhanced) do *not* contribute in the semiclassical limit.

It seems reasonable to assume that similar results hold in full $3+1$ gravity, Kaluza-Klein theory, dilaton gravity, or any other diffeomorphism-invariant theory of gravity with indefinite Euclidean action. However, it should be noted that the most interesting instantons in quantum gravity (e.g., [1–6,13–15,56–58]) are rather far from our minisuperspace models. In particular, they involve processes in which the spatial topology of the initial state differs from the spatial topology of the final state; an effect which appears to be ruled out by construction in our context (see, however, [14,15]). An argument could certainly be made that such instantons are qualitatively different and that our results have no bearing on their interpretation. On the other hand, we note that the arguments of Sec. V B did not rely on the details of our model, but followed from the unitarity of e^{-iHN} and the existence of an appropriate subspace $\mathcal{S} \subset \mathcal{H}_{\mathrm{aux}}$. One would expect such arguments to generalize readily if refined algebraic or Rieffel induction methods are applicable at all. At the very least, our arguments are suggestive, and it is worthwhile to briefly discuss below the hypothesis that our results do generalize to such cases.

Many instanton calculations, such as the pair creation calculations of [1–3], implicitly assume that the relevant stationary point is the one with positive Euclidean *lapse*. So long as the corresponding Euclidean action is positive (as it is in all of the pair creation examples [1–3]), this is just the conclusion that would follow from Sec. V B. We will therefore concentrate on situations where the Euclidean action is *negative*. Perhaps the most interesting use of such instantons was seen in the arguments of Baum [56], Hawking [57], and Coleman [58] that the cosmological constant Λ should vanish. They supposed that, in some way, the quantum state of the universe provides a probability distribution for Λ and proceeded to estimate this distribution through instanton calculations. The large negative action of four-sphere instantons for small positive Λ was used to argue that this distribution is exponentially large (or even larger [58]) for Λ near zero.

While we have been interested in the transition amplitude and not in a particular quantum state, we note that *every* physical state $|\psi_{\rm phys}\rangle$ in our scheme may be expressed in the form

$$\langle x|\psi_{\rm phys}\rangle = \int dx' \langle x|\delta(H)|x'\rangle\langle x|\psi\rangle \tag{6.1}$$

for some $|\psi\rangle \in \mathcal{S}$. As a result, the arguments of Sec. V B imply that no physical state has a ''wave function'' $\langle x|\psi_{\rm phys}\rangle$ which behaves as $e^{|S_E(x)|}$ in any region of superspace. This suggests that the instantons of [56–58] would not, in fact, contribute to the desired distribution. Following a similar line of reasoning, [9,59] arrive at this same conclusion. Other arguments against and comments on the Baum-Coleman-Hawking mechanism include [60–64].

Another point to be addressed is the argument of [13] that only stationary points with $\mathrm{Re}\sqrt{g_E} \geqslant 0$ (where g_E is the Euclidean metric) should contribute to the path integral. In our notation this restriction would be $\mathrm{Re}(iN) \geqslant 0$; i.e., positive Euclidean lapse. The argument of [13] was based on considering the normalizability of an induced quantum state for the matter (nongravitational) fields. The issue concerned whether this state is an exponentially growing or decaying function of these fields; that is, it had to do with the state functional at large values of the matter fields. While we have argued that stationary points with $\mathrm{Re}(iN) < 0$ may contribute, the fact that the Euclidean action of matter fields is positive for $\mathrm{Re}(iN) > 0$ means that for large values of the matter fields our condition of positive Euclidean action is equivalent to the condition $\mathrm{Re}(iN) > 0$ of [13]. This is as one would expect since exponentially increasing functions do not define generalized eigenstates of the constraint. As a result, we see that our arguments are consistent with the general requirements of [13] for reproducing quantum field theory in curved spacetime.

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APPENDIX A: CONVERGENCE OF THE PATH INTEGRAL REPRESENTATIONS

In this appendix we discuss in detail the convergence properties of the path integrals (3.1) and (3.2) for the physical inner product. These expressions do in fact converge, so long as all integrations are appropriately interpreted.

Let us begin by noting that $\langle \phi|e^{-iHN}|\psi\rangle$ is well defined for all $|\phi\rangle, |\psi\rangle \in \mathcal{H}_{\rm aux}$, and, in particular, for all $|\phi\rangle, |\psi\rangle \in \mathcal{S}$. This follows from the fact that e^{iHN} is a unitary (and therefore bounded) operator on $\mathcal{H}_{\rm aux}$. As a result, $\langle x|e^{-iHN}|x'\rangle$ is a well-defined distribution on $\mathcal{S}\times\mathcal{S}$; that is, $\langle x|e^{-iHN}|x'\rangle$ is a member of the dual space $\mathcal{S}'\times\mathcal{S}'$.

Note that this holds for *all* real N, even though the expression for $\langle x|e^{-iHN}|x'\rangle$ (for the case $H = -P_0^2 + P_1^2 = m^2$, for example) as a function of N, x, and x' may have an essential singularity at $N=0$ (see, e.g., [14,15]). This is nothing more than the fact that the distribution $\delta(x-x')$ cannot be represented by a smooth function. In fact, $\langle x|e^{-iHN}|x'\rangle$ is a *continuous* function of N in the topology of $\mathcal{S}'\times\mathcal{S}'$, even at $N=0$. There is thus no difficulty with the N integral at any finite value of N.

We expect the result of this integral to be $\langle x|\delta(H)|x'\rangle$. Our technical assumptions guarantee that the limit

$$\lim_{\substack{a\to-\infty \\ b\to+\infty}} \int_a^b dN \langle x|e^{-iHN}|x'\rangle \tag{A1}$$

does in fact converge to $\langle x|\delta(H)|x'\rangle$ (in the topology of $\mathcal{S}'\times\mathcal{S}'$), and does so independently of how the limits of a and b are taken [20]. Any lack of convergence of (3.1) must therefore arise from the path integral representation of $\langle x|e^{-iHN}|x'\rangle$. It is to this expression that we now turn.

Our assumptions (from [20]) guarantee that $(1-iHt)$ maps $\mathcal{S}$ into $\mathcal{S}$ so that the operator $(1-iHN/k)^k$ is also a member of $\mathcal{S}'\times\mathcal{S}'$. It follows that the integrations in the k-skeletonized path integral

$$I_k = \int \frac{dp_0}{2\pi}\prod_{i=1}^{k}\frac{dp(t_i)dq(t_i)}{2\pi}e^{ip(t_i)[q(t_i)-q(t_{i-1})]} \times\left(1 - i\frac{N}{k}h(p(t_i),q(t_i))\right) \tag{A2}$$

must converge in the sense of defining elements of $\mathcal{S}'\times\mathcal{S}'$.

In addition, for fixed states $|\phi\rangle \in \mathcal{S}$ and $|\psi\rangle \in \mathcal{S}$, we have

$$\langle \phi|e^{-iHt}|\psi\rangle - \langle \phi|(1-iHt)|\psi\rangle \leqslant Ct^2 \tag{A3}$$

for small t and some (state-dependent) constant C. Thus the $k\to\infty$ limit of the k-skeletonized path integral converges (as a sequence in $\mathcal{S}'\times\mathcal{S}'$) to $\langle x|e^{-iHN}|x'\rangle$. We conclude that, when appropriately interpreted, the expression (3.1) does, in fact, converge, despite the oscillatory nature of the exponential and the fact that the ''Euclidean action'' is unbounded below. Since (3.2) is designed to exactly reproduce (3.1), we have established the convergence of this expression as well.

APPENDIX B: STATIONARY POINTS AND ANALYTICITY OF THE MEASURE

We now show how the the analytic structure of the measure in (4.3) determines the overall form of the results (4.5) and (4.6) by evaluating this result in the semiclassical approximation. The structure of the results (4.12) and (5.9) is determined in essentially the same way.

Consider the integral (4.3):

$$\langle x|\delta(H)|x'\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dN \frac{\exp\left[i\frac{\pi}{2}\left(1-\frac{n}{2}\right)\mathrm{sgn}(N)\right]}{(2\pi|N|)^{n/2}} \times \exp\left(-i\frac{m^2}{2}\left[N-\frac{(x-x')^2}{m^2N}\right]\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dN \frac{e^{-i\pi n/4}}{(2\pi N)^{n/2}} e^{(i\pi/2)\mathrm{sgn}(N)} \times \exp\left(-i\frac{m^2}{2}\left[N-\frac{(x-x')^2}{m^2N}\right]\right) \qquad \text{(B1)}$$

where the function $N^{n/2}$ is $(\sqrt{N})^n$ and $\sqrt{N}$ is defined to have a branch cut along the *positive* imaginary axis. Note that $\mathrm{sgn}(N)$ may be interpreted as an analytic function which is constant on the left and right half planes with a cut along the entire imaginary axis.

Now, for large N (and $m^2>0$), the exponential factor decays in the lower half plane but grows in the upper half plane. As a result, the contour may be closed in the lower half plane. Note that, because of the cut corresponding to $\mathrm{sgn}(N)$, the integrations along the negative imaginary axis do not cancel, but instead give equal contributions and add together. Since, for $(x-x')^2>0$, the integrand vanishes as N approaches zero from the lower half plane, the essential singularity at $N=0$ does not contribute in the semiclassical limit. This limit is therefore dominated by the stationary point in the lower half plane, for which the integrand in Eq. (B1) is exponentially suppressed by a factor of $e^{-m\sqrt{(x-x')^2}}$ in agreement with the leading behavior of (4.5).

[1] G. W. Gibbons, in *Fields and Geometry*, Proceedings of the 22nd Karpacz Winter School of Theoretical Physics: Fields and Geometry, Karpacz, Poland, edited by A. Jadczyk (World Scientific, Singapore, 1986).

[2] D. Garfinkle and A. Strominger, Phys. Lett. B **256**, 146 (1992).

[3] F. Dowker, J. Gauntlett, G. Gibbons, and G. Horowitz, Phys. Rev. D **52**, 6929 (1995); F. Dowker, J. Gauntlett, S. Giddings, and G. Horowitz, *ibid.* **50**, 2662 (1994).

[4] E. Witten, Nucl. Phys. **B195**, 481 (1982).

[5] S. W. Hawking, in *Astrophysical Cosmology*, edited by H. A. Brück *et al.* (Pontifica Academia Scientarium, Vatican City, 1982).

[6] J. B. Hartle and S. W. Hawking, Phys. Rev. D **28**, 2960 (1983); S. W. Hawking, Nucl. Phys. **B239**, 257 (1984).

[7] B. DeWitt, Phys. Rev. **160**, 1113 (1967).

[8] G. W. Gibbons, S. W. Hawking, and M. J. Perry, Nucl. Phys. **B138**, 141 (1978).

[9] S. B. Giddings, Int. J. Mod. Phys. A **5**, 3811 (1989).

[10] J. B. Hartle and K. Schleich, in *Quantum Field Theory and Quantum Statistics*, edited by T. A. Batalin *et al.* (Hilger, Bristol, 1987).

[11] K. Schleich, Phys. Rev. D **39**, 2192 (1989).

[12] J. B. Hartle, J. Math. Phys. **30**, 452 (1989).

[13] J. J. Halliwell and J. B. Hartle, Phys. Rev. D **41**, 1815 (1990).

[14] J. J. Halliwell and J. Louko, Phys. Rev. D **39**, 2206 (1989).

[15] J. J. Halliwell and J. Louko, Phys. Rev. D **42**, 3997 (1990).

[16] N. P. Landsman, J. Geom. Phys. **15**, 285 (1995).

[17] D. Marolf, Class. Quantum. Grav. **12**, 1199 (1994).

[18] D. Marolf, Class. Quantum. Grav. **12**, 1441 (1995).

[19] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourão, and T. Thiemann, J. Math. Phys. **36**, 6456 (1995).

[20] D. Marolf, in *Proceedings of the Symposium on Differential Geometry and Mathematical Physics*, edited by W. Kondracki (Banach Center Publications, Warsaw, in press).

[21] A. Higuchi, Class. Quantum. Grav. **8**, 1961 (1991); **8**, 1983 (1991); **8**, 2005 (1991); **8**, 2023 (1991).

[22] M. Henneaux and C. Teitelboim, Ann. Phys. (N.Y.) **143**, 127 (1982).

[23] C. Misner, in *Magic Without Magic*, edited by J. R. Klauder (W.H. Freeman, San Francisco, 1972).

[24] C. Misner, K. Thorne, and J. Wheeler, *Gravitation* (W. H. Freeman, New York, 1973), p. 805.

[25] R. Jantzen, Commun. Math. Phys. **64**, 211 (1979); in *Cosmology of the Early Universe*, edited by L. Fang and R. Ruffini (World Scientific, Singapore, 1984).

[26] M. Ryan and L. Shepley, *Homogeneous Relativistic Cosmologies* (Princeton University Press, Princeton, NJ, 1975).

[27] A. Ashtekar, R. Tate, and C. Uggla, Int. J. Mod. Phys. D **2**, 15 (1993).

[28] P. A. M. Dirac, *Lectures on Quantum Mechanics* (Yeshiva University, New York, 1964).

[29] J. J. Halliwell, Phys. Rev. D **38**, 2468 (1988).

[30] P. Hájíček and K. Kuchař, Phys. Rev. D **41**, 1091 (1990).

[31] I. Moss, Ann. Inst. Henri Poincaré, **49**, 341 (1988).

[32] A. Ashtekar, *Lectures on Non-Perturbative Canonical Gravity* (World Scientific, Singapore, 1991).

[33] A. Rendall, Class. Quantum Grav. **10**, 605 (1993); in *Canonical Gravity: From Classical to Quantum*, edited by J. Ehlers and H. Friedrichs (Springer, Berlin, 1994).

[34] I. M. Gel'fand and N. Ya. Vilenkin, *Generalized Functions, Vol. 4, Applications of Harmonic Analysis* (Academic, New York, 1964).

[35] J. Hartle and D. Marolf (in preparation).

[36] D. Marolf, Class. Quantum. Grav. **12**, 2469 (1995).

[37] B. DeWitt, in *Gravitation: An Introduction to Current Research*, edited by L. Witten (Wiley, New York, 1962).

[38] C. Rovelli, in *Conceptual Problems of Quantum Gravity*, edited by A. Ashtekar and J. Stachel (Birkhäuser, Boston, 1991), p. 141.

[39] C. Rovelli, Phys. Rev. D **42**, 2638 (1990).

[40] C. Rovelli, Phys. Rev. D **43**, 442 (1991).

[41] C. Rovelli, Class. Quantum Grav. **8**, 297 (1991).

[42] J. B. Hartle, in *Gravitation and Quantizations*, Proceedings of the Les Houches Summer School, Les Houches, France, 1992, edited by J. Zinn-Justin and B. Julia, Les Houches Summer School Proceedings Vol. 57 (North-Holland, Amsterdam, 1995); Report No. gr-qc/9304006 (unpublished).

[43] M. Henneaux and C. Teitelboim, *Quantization of Gauge Systems* (Princeton University Press, Princeton, NJ, 1992), Sec. 15.1.

[44] X. Lin and R. Wald, Phys. Rev. D **41**, 244 (1990).
[45] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic, New York, 1980).
[46] D. N. Page, J. Math. Phys. **32**, 3427 (1991).
[47] A. Ashtekar and R. S. Tate, J. Math. Phys. **35**, 6434 (1994).
[48] J. Louko, Phys. Rev. D **48**, 2708 (1993).
[49] J. Louko and R. Laflamme, Phys. Rev. D **43**, 2730 (1991).
[50] C. Kiefer, Ann. Phys. (N.Y.) **207**, 53 (1991).
[51] R. F. Baierlein, D. H. Sharp, and J. A. Wheeler, Phys. Rev. **126**, 1864 (1962).
[52] M. Henneaux, C. Teitelboim, and J. D. Vergara, Nucl. Phys. **B387**, 391 (1992).
[53] M. Henneaux and C. Teitelboim, *Quantization of Gauge Systems* [43], Sec. 1.4.
[54] B. DeWitt, Rev. Mod. Phys. **29**, 377 (1957).
[55] K. Kuchař, J. Math. Phys. **24**, 2122 (1983).
[56] E. Baum, Phys. Lett. **133B**, 183 (1983).
[57] S. W. Hawking, Phys. Lett. **134B**, 403 (1984).
[58] S. Coleman, Nucl. Phys. **B310**, 643 (1988).
[59] S. Giddings, in *Modern Quantum Field Theory*, Proceedings of the International Colloquium on Modern Field Theory, Tata Institute, Bombay, India, 1990, edited by S. Das *et al.* (World Scientific, Singapore, 1991).
[60] J. Polchinski, Phys. Lett. B **219**, 251 (1988).
[61] A. Strominger, Nucl. Phys. **B319**, 722 (1989).
[62] W. Fischler and I. Klebanov, Nucl Phys. **B327**, 157 (1989).
[63] W. Fischler and L. Susskind, Phys. Lett. B **217**, 48 (1989).
[64] M. Duncan and L. Jensen, Nucl. Phys. **B336**, 100 (1990).