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On the canonical approach to quantum gravity

Abhay Ashtekar
Department of Physics, Syracuse University, Syracuse, New York 13210 and Département de Physique, Université de Clermont-Fd., 63170 Aubière, France

Gary T. Horowitz
Institute for Advanced Study, Princeton, New Jersey 08540
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General relativity has the property that, under the natural projection mapping, the image of the constraint surface in the phase space is a *proper* subset of the configuration space. This feature is not shared by other field theories of direct physical interest such as the Yang-Mills theory, nor by constrained systems which have been modeled after general relativity and analyzed in detail. Therefore, to gain insight into this feature, a new example with a finite number of degrees of freedom is introduced and quantized. The analysis suggests that, in the canonical approach, the reduced phase-space method is likely to yield an incomplete description of quantum gravity. In particular, contrary to the indication provided by this method, quantum gravity may admit states with negative energies.

I. INTRODUCTION

Although the literature on the phase-space description of classical general relativity and the subsequent canonical approach to quantization is quite rich,[1] one aspect of the problem appears to have been overlooked, particularly in the context of quantization. This has to do with a peculiarity of the constraints of the classical theory. Certain parts of the configuration space are inaccessible to the physical states of the gravitational field. More precisely, as we shall see in Sec. II, the scalar constraint $C(q,p)=0$ depends quadratically on the momentum variables and in a complicated manner on the configuration variables with a consequence that the constraint surface $\overline{\Gamma}$ in the phase space Γ does not project down to all of the configuration space $\mathscr{C}$ but only to a *proper* subset $\overline{\mathscr{C}}$ thereof. While this feature plays no essential role in the classical theory—the arena for the Hamiltonian description is the phase space rather than the configuration space—it *is* significant for passage to quantum theory via canonical methods. For example, in the Schrödinger representation quantum states arise as functions on the configuration space so that the "size" of this space dictates the structure of the quantum Hilbert space.

The feature $\overline{\mathscr{C}}\neq\mathscr{C}$ can arise trivially if the constraint is independent of momenta (example: a particle restricted to move on the surface of a two-sphere in R^3). However, in this case, one can first get rid of the constraint, e.g., by noting that the reduced[2] phase space is, *naturally*, the cotangent bundle over $\overline{\mathscr{C}}$, and then base quantum theory directly on $\overline{\mathscr{C}}$.[3] In the case of general relativity, the natural cotangent-bundle structure fails to exist since the constraint function now depends on momenta as well. Had $C(q,p)$ been linear in momentum variables, the constraint would have led to no restriction on the configuration variables at all; $\overline{\mathscr{C}}$ would have been the same as $\mathscr{C}$. The constraint could be eliminated also in this case by simply redefining the configuration space since the reduced phase space would again admit a natural cotangent-bundle structure.[3] A familiar example where this situation occurs is the Yang-Mills theory, where the constraint $C(\vec{A},\vec{E})\equiv\mathrm{div}\vec{E}=0$ leads to no restriction on the configuration variables $\vec{A}$ and can be handled in a straightforward way both in the classical and the quantum theory. (The Yang-Mills constraint is analogous to the vector constraint in general relativity which is also well understood.) Do there exist simple systems with constraints which are quadratic in momenta? Two such examples are well known and have been studied in detail to gain insight into the situation in general relativity.[4] The first is the free relativistic particle where the constraint is $C(q,p)\equiv g^{ab}p_ap_b-\mu^2=0$, and the second is the so-called parametrized nonrelativistic particle, the constraint being

$$C(q,p)\equiv p_0+(1/2m)\vec{p}^{\,2}+V(\vec{q})=0\ .$$

These constraints *are* sufficiently complicated so as to prevent the reduced phase space from admitting a natural cotangent-bundle structure. However, in neither case does the constraint impose any restriction on the configuration variables; in both cases $\overline{\mathscr{C}}=\mathscr{C}$. Thus, although a number of constrained systems which mimic certain features of general relativity have been studied in the literature, apparently none of them has a constraint which restricts the configuration variables and, at the same time, obstructs the existence of a natural cotangent-bundle structure.

The presence of such a constraint in general relativity raises a key question: Will the permissible wave functions $\Psi(q)$ of quantum gravity be forced to have support in $\overline{\mathscr{C}}$, or can they also have support in the classically forbidden region $\mathscr{C}-\overline{\mathscr{C}}$? Note that any approach that requires one to first go to the reduced phase space[2] $\hat{\Gamma}$ and then quantize, e.g., by introducing *some* cotangent-bundle structure—or, more generally, *some* polarization—on $\hat{\Gamma}$, would *a priori* exclude the possibility of wave functions with support on the classically forbidden region. By construction, $\hat{\Gamma}$ has no knowledge of $\mathscr{C}-\overline{\mathscr{C}}$. Yet the tunneling effects of this sort are so characteristic of quantum mechanics that one is tempted to think that $\Psi(q)$ *should* be allowed to penetrate in the classically forbidden region unless infinite barriers present themselves. Note that such a quantum tunneling would have consequences of direct physical significance. An example—perhaps the most striking one—is provided by the issue of ground-state energy of quantum gravity. In the classical theory, the restriction of the Hamiltonian to the constraint surface $\overline{\Gamma}$ is a function E^{ADM}, the Arnowitt-Deser-Misner (ADM) energy, which depends only on the configuration variable q; $E^{\text{ADM}}\equiv E^{\text{ADM}}(q)$. Furthermore, thanks to recent powerful theorems,[5] one now knows that E^{ADM} is a non-negative function on $\overline{\Gamma}$, vanishing only at those points (q,p) which correspond to Minkowski space. Hence, at first thought, one may expect that the Hamiltonian of quantum gravity would also be non-negative. However, there also exist[6] semiclassical calculations which indicate that the Gaussian wave function peaked at the flat three-geometry—the perturbative ground state—would be unstable in full quantum gravity. This suggests that the true ground state of the full theory may have negative energy. (Note that, unlike in other physical theories, the "zero of energy" cannot be shifted in the gravitational case so that the value of the ground-state energy is absolute.) Since the calculations are only semiclassical, however, *a priori* it is not clear if the results reflect the basic features of the full theory or if they are only quirks of the approximation schemes adopted. The framework of canonical quantization provides an ideal platform from where one can evaluate this situation. How does the situation look from this platform? As we shall see, the key question here is whether or not physically permissible wave functions tunnel into the classically forbidden region. If they do not, i.e., if their support is restricted to $\overline{\mathscr{C}}$, one expects the energy to be non-negative also in the quantum theory since E^{ADM} depends only on the configuration variables and is non-negative on $\overline{\mathscr{C}}$. If, on the other hand, the wave functions $\Psi(q)$ do penetrate into the classically forbidden region $\mathscr{C}-\overline{\mathscr{C}}$, *where the classical energy can be negative,* one may have quantum states with negative energies.

The purpose of this paper is to shed some light on these issues using a model-constrained system.

Section II summarizes the Hamiltonian description of asymptotically flat gravitational fields in general relativity and explains, in particular, how the feature under discussion arises. We have devoted an entire section to this description for the following reason. Whereas asymptotic flatness is crucial to the issues which we wish to discuss here, this is precisely the context which appears not to have drawn sufficient attention. In the literature on canonical quantization, the focus is on spatially compact universes.[7] In the spatially compact context, the Hamiltonian of general relativity is equal to the scalar constraint function and vanishes identically. A great deal of effort has been devoted to the understanding of the significance of this feature and the resulting conceptual problems have been the central themes of the work on canonical quantization in recent years. In the asymptotically flat context, on the other hand, the Hamiltonian does *not* vanish. On the constraint surface, it reduces precisely to the ADM energy function $E^{\text{ADM}}(q)$. Consequently, in this context, the overall scenario changes substantially.

Using this scenario as a guide, we introduce, in Sec. III, a model system with a finite number of degrees of freedom. The model mimics general relativity in several ways: it has a constraint, quadratic in momenta, with the property that, under the natural projection, the image $\overline{\mathscr{C}}$ of the constraint surface is a proper subset of the configuration space $\mathscr{C}$; the constraint is preserved under time evolution; and a positive-energy theorem is satisfied classically. Since the system has only a finite number of degrees of freedom, one can quantize it in a straightforward manner. Following Dirac,[8] the constraint is carried over to quantum theory by imposing the condition $\underline{C}(q,p)\cdot\Psi(q)=0$ on the physical states $\Psi(q)$, where $\underline{C}(q,p)$ is the quantum operator corresponding to the classical constraint function $C(q,p)$. (There are no factor-ordering problems.) We find that physical states *can* have support on the classically forbidden region $\mathscr{C}-\overline{\mathscr{C}}$. Furthermore, the physical subspace admits states for which the expectation value of the Hamiltonian is negative. Thus, because of tunneling, the classical positive-energy theorem fails to go over to the quantum theory. Finally, we compare this quantum description with the one obtained using the reduced phase space and explicitly show that the latter contains only a part of the states of the former; the reduced-phase-space method yields an incomplete quantum theory.

In Sec. IV, we discuss the possible significance of these results to quantum gravity.

II. HAMILTONIAN DESCRIPTION OF THE ASYMPTOTICALLY FLAT GRAVITATIONAL FIELD

We first give a summary of the phase-space formulation of classical general relativity in the asymptotically flat context and then discuss briefly the problems associated with quantization.

Fix a C^∞ manifold Σ, diffeomorphic to R^3 (Ref. 9). Denote by $\mathscr{C}$ the space of positive-definite three-metrics q_{ab} on Σ with respect to which Σ is complete and which are asymptotically flat at spatial infinity in the sense of Ref. 10. Denote by Γ the cotangent bundle of $\mathscr{C}$. Thus, elements of Γ are pairs (q_{ab},p^{ab}), where $p^{ab}=p^{(ab)}$ are tensor densities of weight 1. The action of the cotangent vectors p^{ab} on the tangent vectors δq_{ab} is given by

$$p\cdot\delta q=\int_\Sigma p^{ab}\delta q_{ab}\ . \tag{2.1}$$

The integral on the right-hand side is independent of the choice of a volume element since the integrand is a scalar density of weight 1 and converges because of the fall-off conditions of Ref. 10. $\mathscr{C}$ represents the configuration space, and Γ the phase space. Consider the surface $\overline{\Gamma}$ in Γ defined by the pairs (q,p) satisfying the constraint equations

$$C^a\equiv D_b p^{ab}=0, \tag{2.2}$$

$$C\equiv p_{ab}p^{ab}-\tfrac{1}{2}p^a{}_a p^b{}_b-(\det q)R=0\ , \tag{2.3}$$

where D and R are the derivative operator and the scalar curvature of q_{ab}, respectively, and where the indices are raised and lowered by q_{ab}. $\overline{\Gamma}$ will be referred to as the *constraint surface*. Every point (q,p) of $\overline{\Gamma}$ provides an initial datum for Einstein's vacuum equation, where q_{ab} is the intrinsic three-metric and $\pi^{ab}\equiv(\det q)^{-1/2}(p^{ab}-\tfrac{1}{2}p^m{}_m q^{ab})$ is the extrinsic curvature. Furthermore, thanks to the main result of Ref. 10, one now knows that the resulting space-time is asymptotically flat at spatial infinity (i^0) in the sense of [the definition (3.1) of] Ref. 11.

Had Γ been finite dimensional, say n, a surface $\overline{\Gamma}$ of dimension m in Γ could have been specified (locally) by $n-m$ equations of the type $C_i(x^\alpha)=0$, where i runs from 1 to $n-m$ and α from 1 to n, x^α being a chart on Γ. One can ensure that none of the equations is redundant (e.g., C_2 is *not* just $C_1^{1/2}$ or C_1^2) by requiring that C_i be differentiable everywhere on $\overline{\Gamma}$ and that the $(n-m)$ covector fields $\partial C_i/\partial x^\alpha$ be linearly independent at each point. These conditions ensure that C_i can themselves be used as the $n-m$ coordinates of Γ which vanish on $\overline{\Gamma}$. In the actual case under discussion, we can obtain analogous equations by multiplying C^a and C of Eqs. (2.2) and (2.3) by suitable test fields, integrating over Σ, and setting the result equal to zero:

$$C_{N^a}\equiv\int_\Sigma N_a C^a=\int_\Sigma N_a D_b p^{ab}=0\ , \tag{2.4}$$

$$\begin{aligned}C_N&\equiv\int_\Sigma NC(\det q)^{-1/2}\\&=\int_\Sigma N[p^{ab}p_{ab}-\tfrac{1}{2}p^2\\&\qquad-(\det q)R](\det q)^{-1/2}\\&=0\ .\end{aligned} \tag{2.5}$$

(Note that, unlike C_{N^a} and C_N, C^a and C are not *functions* on Γ. Hence, to obtain the analogs of C_i of the finite-dimensional case, it is necessary to introduce the test fields N^a and N.) What conditions should N^a and N satisfy? One can show that *C_{N^a} and C_N are not differentiable unless N and N^a tend to zero at spatial infinity.*[12] This is a general feature and does not depend sensitively on the technicalities involved in the choice of function spaces. Hence, from now on, we assume that the fields N^a and N which enter in the expressions of C_{N^a} and C_N satisfy this fall-off property. The constraint surface $\overline{\Gamma}$ is now determined by Eqs. (2.4) and (2.5).

What are the canonical transformations generated by C_{N^a} and C_N? As is well known,[1] the action of C_{N^a} is the same as the induced action on Γ of the spatial diffeomorphism group generated by N^a on Σ ($q_{ab}\to q_{ab}+\epsilon\mathscr{L}_N q_{ab}$ and $p^{ab}\to p^{ab}+\epsilon\mathscr{L}_N p^{ab}$ in the infinitesimal form), and the action of C_N corresponds to diffeomorphisms in the timelike direction generated by Nt^a in the four-dimensional solution of Einstein's equation obtained from each (q,p) in $\overline{\Gamma}$, t^a being the unit normal to Σ (regarded as a submanifold in the solution). It is important to note that, since N^a and N are required to go to zero at infinity, the diffeomorphisms are all identity there; in terms of i^0, they induce the identity transformation of the asymptotic Poincaré group.[11] To obtain asymptotic translations, one must allow N^a and N to go to nonzero constant fields at infinity. However, when this is done, C_{N^a} and C_N are no longer differentiable functions on Γ, and, consequently, fail to generate *any* canonical transformation. *This is in fact the main reason behind the asymptotic conditions on N^a and N imposed above.* To summarize, then, the canonical transformations generated by the constraint functions correspond to diffeomorphisms which are asymptotically identity. These do *not* include the diffeomorphisms which feature in the asymptotic Poincaré group. In particular, the translations are excluded.

What are the generators of translations? One can show[12] that these are

$$H_{T^a}\equiv\frac{-1}{8\pi}\int_\Sigma T_aC^a+\frac{1}{8\pi}\oint_S T^aP_{ab}dS^b\ , \qquad (2.6)$$

$$H_T\equiv\frac{1}{16\pi}\int_\Sigma TC(\det q)^{-1/2} + \frac{1}{16\pi}\oint_S T(\partial_a q_{bc}-\partial_b q_{ac})e^{ac}dS^b\ , \qquad (2.7)$$

where T^a is a vector field on Σ which is asymptotically a space translation, T a scalar field on Σ which is asymptotically a constant, e^{ab} a fixed flat metric on Σ,[10] ∂ the covariant derivative compatible with e^{ab}, and where S is the two-sphere at infinity of Σ. Even though T^a and T fail to vanish asymptotically, the presence of the surface terms makes H_{T^a} and H_T differentiable on Γ. H_{T^a} is the spatial momentum and H_T is the energy. Note that, even on the constraint surface $\overline{\Gamma}$, H_{T^a} and H_T do not vanish identically. In fact, on $\overline{\Gamma}$,

$$H_T(q,p)=\frac{1}{16\pi}\oint_S T(\partial_a q_{bc}-\partial_b q_{ac})e^{ac}dS^b \equiv T\mid_S E^{\text{ADM}}(q)\ ,$$

and the positive-energy theorems ensure that E^{ADM} is non-negative on $\overline{\Gamma}$ and vanishes only at the points (q,p) corresponding to Minkowski space.[5] Using this result, we can now see how the peculiarity of general relativity, discussed in Sec. I, arises. Consider any three-metric q^0_{ab} in $\mathscr{C}$ for which the surface term in Eq. (2.7) is negative. (There exist a lot of such metrics. Example: Choose q^0_{ab} to be isometric to the negative-mass Schwarzschild three-metric outside, say, $r=17\mid m\mid$ and make any smooth extension inside.) Then, there cannot exist any tensor density p^{ab} such that the pair (q^0,p) satisfies the constraint equations (2.2) and (2.3): the existence of such a field will provide us with a point of $\overline{\Gamma}$ at which H_T is negative, thereby contradicting the positive-energy theorem. Thus, q^0_{ab} cannot belong to the image $\overline{\mathscr{C}}$ of $\overline{\Gamma}$ under the natural projection mapping from Γ to $\mathscr{C}$; $\overline{\mathscr{C}}\subset\mathscr{C}$. Note that the argument uses the fact that the surface term in Eq. (2.7), the ADM energy, is *independent* of the momentum variables, which is itself a peculiarity of general relativity.

To summarize, then, in the asymptotically flat contexts, there is a clear distinction between constraint functions C_{N^a} and C_N and the Hamiltonians H_{T^a} and H_T. In the Dirac[8] theory of constrained systems, constraints generate gauge and Hamiltonians generate dynamics. If one adopts this viewpoint, one is led to the conclusion that in the asymptotically flat contexts, there is a clear distinction also between gauge and dynamics. A detailed examination shows[12] that the group generated by the constraints—the gauge group *à la* Dirac— is a normal subgroup of the group generated by the constraints and Hamiltonians together, the quotient being the four-dimensional group of translations, representing "pure dynamics." (To simplify matters, we have left out rotations and boosts.) Although this viewpoint is simple and attractive, it is not necessary to adopt it for our main purpose in this paper. What we need is only the fact that the constraints are different from the Hamiltonians. The difference disappears in the spatially compact case. This situation is analogous to that in the Yang-Mills theory. On a compact spatial slice, just as the total charge of any source-free Yang-Mills field vanishes, so does the total four-momentum of any source-free graviational field.

We can now turn to the problem of quantization. Two lines of attack have been proposed in the literature. The first is the reduced phase-space approach. Here, one first constructs the space $\hat{\Gamma}$, each point of which represents an equivalence class of ("gauge-related") points of the constraint surface $\overline{\Gamma}$.[2] $\hat{\Gamma}$ inherits a natural symplectic structure from Γ and may be thought of as the phase space of true degrees of freedom of the gravitational field; constraints are eliminated. The price paid is that the reduced phase space $\hat{\Gamma}$ does not have a natural cotangent-bundle structure. Hence to obtain the quantum description, one has to find a new input, a polarization[13] on $\hat{\Gamma}$. Alternatively, one can try to take advantage of the existing cotangent-bundle structure of Γ. This leads to the second approach. Here, one considers wave functions $\Psi(q)$ on $\mathscr{C}$. However, one now has to incorporate the constraints explicitly. The prescription is to find quantum operators $\underset{\sim}{C}_{N^a}$ and $\underset{\sim}{C}_N$ corresponding to the classical constraint functions and permit as physical states only those wave functions $\Psi(q)$ which satisfy the quantum constraints[14]:

$$\underset{\sim}{C}_{N^a}\Psi(q)=0\ , \tag{2.8}$$

$$\underset{\sim}{C}_N\Psi(q)=0\ . \tag{2.9}$$

The significance of the first constraint is clear[15]: It requires that the wave functions $\Psi(q)$ should depend only on the equivalence classes of three-metrics, where q_{ab} and q'_{ab} are considered equivalent if they are related by a diffeomorphism on Σ *which is asymptotically identity.* The second constraint is not so easy to interpret. In fact, in this case, the formal expression of $\underset{\sim}{C}_N$ is divergent because it involves products of operator-valued-distributions and a canonical regularization is not yet available due to the difficult factor ordering problems. Thus, both approaches face difficulties. There are, nonetheless, indications that one may be able to use the presence of a nonvanishing Hamiltonian to resolve several of these problems. These indications, however, will be discussed elsewhere; the main purpose of this paper is to compare the two methods using a model system which mimics the appropriate features of general relativity. For now, we only note that for examples studied in this context so far, both methods are applicable and lead to equivalent quantum theories.

III. THE EXAMPLE

A. The system

Our aim is to construct a model which mimics certain features of general relativity and is yet sufficiently simple so that the two quantization methods referred to in Sec. II are applicable. The features of general relativity which we wish to mimic are the following. (i) There is a constraint, quadratic in momenta, such that the image $\overline{\mathscr{C}}$ of the constraint surface $\overline{\Gamma}$ under the natural projection is a proper subset of the configuration space $\mathscr{C}$; (ii) The constraint is preserved under time evolution, i.e., the Poisson bracket of the Hamiltonian and the constraint vanishes weakly; and, (iii) The Hamiltonian is non-negative on the constraint surface $\overline{\Gamma}$. Strictly speaking, the third property is not essential to compare the two quantization schemes. However, it will enable us to show explicitly that the differences between the resulting quantum theories are not just mathematical artifacts but can lead to distinct physical predictions.

Let the configuration space $\mathscr{C}$ be R^3 and let Γ be the cotangent bundle over $\mathscr{C}$. Introduce spherical coordinates (r,θ,ϕ) on $\mathscr{C}$. Let the constraint be

$$C\equiv p_\theta{}^2-R(\phi)=0\ , \tag{3.1}$$

where $R(\phi)$ is a smooth function of ϕ which takes on both positive and negative values. The constraint is quadratic in momentum variables, and, since $p_\theta{}^2$ is non-negative, the image $\overline{\mathscr{C}}$ of the constraint surface $\overline{\Gamma}$ is not all of $\mathscr{C}$: $\overline{\mathscr{C}}$ contains only those points of $\mathscr{C}$ at which $R(\phi)\geq 0$. The regions of $\overline{\Gamma}$ with $P_\theta \gtrless 0$ will be referred to as $\overline{\Gamma}_\pm$, respectively; on $\overline{\Gamma}_\pm$, $p_\theta=\pm[R(\phi)]^{1/2}$.

Next, we have to introduce a Hamiltonian such that conditions (ii) and (iii) above are satisfied. Several choices are available. Perhaps the simplest of these is

$$H(\vec{q},\vec{p})\equiv C(\vec{q},\vec{p})+E(\phi) \tag{3.2}$$

with $E(\phi)$ satisfying the condition $E(\phi)\cdot R(\phi)\geq 0$. Thus, in particular, $E(\phi)\geq 0$, where $R(\phi)\geq 0$. This definition mimics the situation in relativity, $E(\phi)$ playing the role of the surface term $E^{\rm ADM}(q)$. The Poisson bracket of C and H clearly vanishes. Finally, since $H(\vec{q},\vec{p})=E(\vec{q},\vec{p})$ on $\overline{\Gamma}$, the energy is non-negative on $\overline{\Gamma}$; a positive-energy theorem is satisfied classically. Furthermore, just as $E^{\rm ADM}(q)$ fails to be positive outside the constraint surface in general relativity, so does $E(\phi)$ in our example. Another possible choice of the Hamiltonian is

$$H'(q,p)\equiv p_r{}^2/2+p_\theta{}^2/2r^2+V(r)R(\phi)\ , \tag{3.3}$$

where $V(r)$ is a smooth, non-negative function of r with $\int V(r)r^2dr<\infty$. Again, it is easy to check that conditions (ii) and (iii) are satisfied.

Both choices have the feature that p_ϕ does not appear in the Hamiltonian although ϕ does. Consequently, ϕ is a constant of motion although p_ϕ is not. This makes it awkward to interpret the model directly in terms of particles and potentials that one usually comes across. The feature could probably have been avoided at the cost of making the constraint and the Hamiltonian more complicated. However, the situation in general relativity is similar to that in the present model: the kinetic energy term

$$(\tfrac{1}{2}q_{ab}q_{cd}-q_{ac}q_{bd})p^{ab}p^{cd}$$

in the Hamiltonian (2.7) has a degenerate supermetric so that the momentum variables satisfying $p^a{}_a p^b{}_b = 2p_{ab}p^{ab}$ make no contribution to the Hamiltonian. We have therefore refrained from introducing more complicated models.

For simplicity, in what follows, we shall use H of Eq. (3.2) as our Hamiltonian. However, all the basic results would remain unaltered had H' of Eq. (3.3) been used instead. Furthermore, the proofs would have to be modified only in inessential ways.

B. Quantization with operator constraint

Let $\mathscr{H}$ denote the Hilbert space of square-integrable functions on $\mathscr{C}$; $\mathscr{H}=L^2(R^3)$. A physical state Ψ of the system is an element of $\mathscr{H}$ satisfying the quantum constraint equation

$$\underline{C}\Psi \equiv [\underline{p}_\theta{}^2-\underline{R}(\phi)]\Psi(r,\theta,\phi)=0 \,. \tag{3.4}$$

Fortunately, the system is simple enough so that no factor-ordering problems are encountered here. The operator $\underline{R}$ just multiplies Ψ by the function $R(\phi)$ and the operator $\underline{p}_\theta$ is given, as usual,[16] by

$$\underline{p}_\theta = (\hbar/i)(\partial_\theta+\tfrac{1}{2}\cot\theta) \,. \tag{3.5}$$

(Note that $\underline{p}_\theta$ is a symmetric operator on the dense subspace of $\mathscr{H}$ consisting of, say, C^∞ functions of compact support of R^3 and admits a self-adjoint extension.) It is straightforward to solve Eq. (3.4). The solutions are given by

$$\Psi_\pm(r,\theta,\phi)=K(r,\phi)(\sin^{-1/2}\theta)\times\exp\left[\pm\frac{i}{\hbar}\sqrt{R(\phi)}\theta\right] , \tag{3.6}$$

where $K(r,\phi)$, an arbitrary function of r and ϕ, is the "integration constant." It is important to note that the support of $K(r,\phi)$ is not necessarily contained in $\overline{\mathscr{C}}$, and, consequently, $R(\phi)$ is not necessarily real everywhere in the support of $\Psi_\pm$. The solutions $\Psi_\pm$ are nonetheless normalizable provided $K(r,\phi)$ falls off appropriately at infinity,

$$|\Psi(r,\theta,\phi)|^2=\int_{\overline{\mathscr{C}}}|K(r,\phi)|^2 r^2 dr\,d\theta\,d\phi+\int_{\mathscr{C}-\overline{\mathscr{C}}}|K(r,\phi)|^2\exp\left[\mp\frac{2}{\hbar}\theta\,|R(\phi)|^{1/2}\right]r^2 d\theta\,d\phi\,dr \,. \tag{3.7}$$

Denote by $\overline{\mathscr{H}}_\pm$ the space of normalizable solutions $\Psi_\pm$ to the constraint equation. Each $\overline{\mathscr{H}}_\pm$ is a complex subspace of the Hilbert space $\mathscr{H}$. Set $\overline{\mathscr{H}}=\overline{\mathscr{H}}_+\oplus\overline{\mathscr{H}}_-$. $\overline{\mathscr{H}}$ is the *physical subspace* of $\mathscr{H}$ (and is the quantum analog of $\overline{\Gamma}$). For simplicity, we shall restrict ourselves to $\overline{\mathscr{H}}_+$ in detailed calculations. The analysis and results for $\overline{\mathscr{H}}_-$ are identical.

Note that if the support of $K(r,\phi)$ is chosen to lie in $\mathscr{C}-\overline{\mathscr{C}}$—which can always be done since $K(r,\phi)$ is freely specifiable except for a normalization condition—we obtain physical states whose support lies *entirely* in the classical forbidden region. Let us consider the expectation value of the Hamiltonian operator $\underline{H}=\underline{p}_\theta{}^2-\underline{R}(\phi)+\underline{E}(\phi)$ in such a state Ψ_+. One obtains

$$\begin{aligned}\langle\Psi_+,\underline{H}\Psi_+\rangle&=\langle\Psi_+,\underline{E}(\phi)\Psi_+\rangle\\&=\frac{\hbar}{2}\int_{\mathscr{C}-\overline{\mathscr{C}}}E(\phi)|K(r,\phi)|^2|R(\phi)|^{-1/2}\left[1-\exp\left[-\frac{2\pi}{\hbar}|R|^{1/2}\right]\right]r^2dr\,d\phi \,.\end{aligned} \tag{3.8}$$

Since $E(\phi)$ is negative in $\mathscr{C}-\overline{\mathscr{C}}$, we have

$$\langle\Psi_+,\underline{H}\Psi_+\rangle<0 \,. \tag{3.9}$$

Thus, although the classical energy is positive on the surface of physically admissible states, the quantum Hamiltonian admits negative expectation values on certain states in the physical subspace $\overline{\mathscr{H}}$. As is clear from the above calculations, this comes about because the elements of $\overline{\mathscr{H}}$ *can* tunnel in to the classically forbidden region $\mathscr{C}-\overline{\mathscr{C}}$. Finally, since $\underline{H}\Psi=E(\phi)\Psi$ for all Ψ in the physical subspace $\overline{\mathscr{H}}$ of $\mathscr{H}$, and since $E(\phi)$ is a C^∞ (and hence bounded) function on R^3, it follows that the Hamiltonian $\underline{H}$ is a bounded self-adjoint operator on $\overline{\mathscr{H}}$. The spectrum of $\underline{H}$ is bounded below and, by Eq. (3.9), the lower bound is negative.[17]

The existence of quantum states with support entirely in the classical forbidden region is very surprising at first. For, since these states satisfy the quantum constraint $\underline{p}_\theta{}^2\Psi=\underline{R}(\phi)\Psi$, and since $R(\phi)$ is negative on $\mathscr{C}-\overline{\mathscr{C}}$, one obtains

$$\langle \Psi,\underline{p}_\theta{}^2\Psi\rangle = \langle \Psi,\underline{R}(\phi)\Psi\rangle < 0 \,, \tag{3.10}$$

contradicting one's intuition about the positivity of $\underline{p}_\theta{}^2$. How does this result come about? Let us reexamine the steps leading to Eq. (3.10) one by one. Consider, to begin with, solutions Ψ to the quantum constraint equation (3.4). Does Ψ define, unambiguously, an element of $\mathscr{H}$? Note, first, that although Ψ contains a factor of $\sin^{-1/2}\theta$, its singularities are confined to a set of measure zero, the z axis. Furthermore, since the volume element of R^3 contains a factor of $\sin\theta$, the L^2 norm of Ψ *is* finite. Thus, it does define a unique element of $\mathscr{H}$. Next, we ask: Is $\underline{p}_\theta\Psi_+$ again in $\mathscr{H}$ for all Ψ_+ in $\overline{\mathscr{H}}_+$? Since[18]

$$\underline{p}_\theta\Psi_+ = [R(\phi)]^{1/2}\Psi_+ \,,$$

we have

$$\langle \underline{p}_\theta\Psi_+,\underline{p}_\theta\Psi_+\rangle \le |R(\phi)|_{\sup}\langle \Psi_+,\Psi_+\rangle \,, \tag{3.11}$$

where $|R(\phi)|_{\sup}$ is the maximum value of $|R(\phi)|$ in R^3. [Recall $R(\phi)$ is a bounded function on R^3.] Therefore, if Ψ_+ belongs to $\overline{\mathscr{H}}_+$, $\underline{p}_\theta\ \Psi_+$ belongs to $\mathscr{H}$. Furthermore, since the quantum constraint operator $\underline{C}$ contains derivatives only with respect to θ, it follows that $\underline{p}_\theta\Psi_+ = R^{1/2}\Psi_+$ is again in $\overline{\mathscr{H}}_+$. Thus, $\underline{p}_\theta$ leaves $\overline{\mathscr{H}}_+$ invariant and consequently $\underline{p}_\theta{}^2$ is a well-defined operator on $\overline{\mathscr{H}}_+$. How then can $\underline{p}_\theta{}^2$ admit negative expectation values? The answer is simply that $\underline{p}_\theta$ (as well as $\underline{p}_\theta{}^2$) fails to be self-adjoint (in fact, even symmetric) on $\overline{\mathscr{H}}$, which is to be expected since $R^{1/2}$ is imaginary on $\mathscr{C}-\overline{\mathscr{C}}$. Thus, if $\tilde{\Psi}_+$ and Ψ_+ are any two elements of $\overline{\mathscr{H}}_+$ with support entirely in $\mathscr{C}-\overline{\mathscr{C}}$, we have

$$\begin{aligned}\langle \tilde{\Psi}_+,\underline{p}_\theta\Psi_+\rangle - \langle \underline{p}_\theta\tilde{\Psi}_+,\Psi_+\rangle &= \frac{\hbar}{i}\int \partial_\theta\left[\tilde{K}^*K\exp\left[-\frac{2}{\hbar}\theta\,|R(\phi)|^{1/2}\right]\right]r^2dr\,d\theta\,d\phi\\ &= \frac{h}{i}\int(\tilde{K}^*K)\left[\exp\left[-\frac{2\pi}{\hbar}|R(\phi)|^{1/2}\right]-1\right]r^2dr\,d\phi\\ &\neq 0\end{aligned}$$

in general. Consequently,

$$\begin{aligned}\langle \Psi_+,\underline{p}_\theta{}^2\Psi_+\rangle &= \langle \underline{p}_\theta^\dagger\Psi_+,\underline{p}_\theta\Psi_+\rangle\\ &\neq \langle \underline{p}_\theta\Psi_+,\underline{p}_\theta\Psi_+\rangle\end{aligned}$$

in general. Thus, the classical constraint is transcended at the quantum level by a subtle phenomenon. Although the physical subspace *is* in the domain of the differential operator $\underline{p}_\theta$,[18] it contains elements which fail to belong to that domain which makes $\underline{p}_\theta$ self-adjoint.[19] An intuitive "explanation" of this behavior lies in the fact that $\overline{\mathscr{H}}$ contains wave functions Ψ (namely with support outside $\overline{\mathscr{C}}$) for which $|\Psi(r,\theta,\phi)|^2r^2\sin\theta$ fails to vanish at the poles $\theta=0$ and $\theta=\pi$. Physically, of course, there is nothing abnormal with these wave functions; there is no physical reason as to why the quantity should vanish at the poles or why the operators which constitute the quantum constraint should be self-adjoint on the physical subspace.

To summarize, then, the physical subspace $\overline{\mathscr{H}}$ consisting of elements of $\mathscr{H}$ satisfying the operator constraint admits states with support entirely in the classically forbidden region $\mathscr{C}-\overline{\mathscr{C}}$. These states have an exponential—rather than oscillatory—behavior with respect to θ which is characteristic of quantum tunneling. Because of this tunneling, the classical positive-energy theorem is violated in quantum mechanics and the energy spectrum extends into the negative part of the real line. In spite of this extreme tunneling, the quantum Hamiltonian *is* self-adjoint on the physical subspace.

C. Quantization via reduced phase space

The reduced phase space $\hat{\Gamma}$ is the manifold of orbits, restricted to $\overline{\Gamma}$, of the Hamiltonian vector field generated by the constraint function. Let us for simplicity, restrict ourselves to $\overline{\Gamma}_+$ defined by $0<p_\theta(\equiv +R^{1/2})$. Analysis on $\overline{\Gamma}_-$ will be identical.[20] The Hamiltonian vector field $\vec{C}_+$ generated by the constraint function $C(q,p)$ on $\overline{\Gamma}_+$ is given by

$$\begin{aligned}\vec{C}_+ &= 2p_\theta\frac{\partial}{\partial\theta}+R'(\phi)\frac{\partial}{\partial p_\phi}\\ &\equiv 2R^{1/2}\frac{\partial}{\partial\theta}+R'(\phi)\frac{\partial}{\partial p_\phi} \,.\end{aligned} \tag{3.12}$$

Hence, to obtain a chart on the manifold $\hat{\Gamma}_+$ of orbits of $\vec{C}_+$, we need to find four independent functions f on Γ satisfying

$$\mathscr{L}_{\vec{C}_+} f \,|_{\bar{\Gamma}_+} = 0 \; . \tag{3.13}$$

By inspection, a set of solutions is given by

$$r, p_r, \phi \text{ and } \tilde{p}_\phi^+ = p_\phi - \frac{R'}{2}\theta R^{-1/2} \; . \tag{3.14}$$

Each integral curve of $\vec{C}_+$ on $\bar{\Gamma}_+$ can be specified by fixing the values of these four functions with $0<r<\infty$, ϕ such that $R(\phi)>0$, $-\infty<p_r<+\infty$, and $-\infty<\tilde{p}_\phi^+<+\infty$. Therefore, modulo the usual problems associated with the spherical coordinates r, p_r, ϕ, and $\tilde{p}_\phi^+$ provide us with a global chart on $\hat{\Gamma}_+$. It is straightforward to verify that the obvious symplectic structure induced on $\hat{\Gamma}_+$ by these coordinates,

$$\hat{\Omega} \equiv dr \wedge dp_r + d\phi \wedge d\tilde{p}_\phi^+ \; , \tag{3.15}$$

is in fact the natural symplectic structure induced on $\hat{\Gamma}_+$ by Ω on Γ. Hence, it is consistent[21] to interpret $\hat{\Gamma}_+$ as the cotangent bundle over a manifold $\hat{C}$ defined by

$$\hat{C} \equiv \{ r, \phi \,/\, 0<r<\infty \text{ and } R(\phi)>0 \} \; . \tag{3.16}$$

$\hat{C}$ is a two-manifold and may be regarded as the reduced configuration space obtained from $\hat{\Gamma}_+$. $\hat{\Gamma}_+$ is a four-manifold and may be regarded as the phase space of "true degrees of freedom" (obtained, according to the Dirac[8] theory, by factoring out gauge).

Quantization procedure is now straightforward since constraints are eliminated classically. Let $\hat{\mathscr{H}}_+$ be the Hilbert space of square-integrable functions on $\hat{C}$ with the volume element $r\,dr\,d\phi$.[22] This is the Hilbert space of quantum states determined by C_+. Since the classical Hamiltonian induced on the reduced phase space is given by

$$\hat{H}(r,p_r,\phi,\tilde{p}_\phi^+) = E(\phi) \; , \tag{3.17}$$

the quantum Hamiltonian on $\hat{\mathscr{H}}_+$ is given by

$$\underline{\hat{H}}\hat{\Psi}(r,\phi) = E(\phi)\hat{\Psi}(r,\phi) \; . \tag{3.18}$$

Finally, since $E(\phi)$ is positive on the support of $\hat{\Psi}$ for all $\hat{\Psi}$ in $\hat{\mathscr{H}}_+$, it follows that the Hamiltonian $\underline{\hat{H}}$ is a positive, bounded, self-adjoint operator on $\hat{\mathscr{H}}_+$.

The situation on $\hat{\Gamma}_-$ is completely analogous. The only difference is that $\tilde{p}_\phi^+$ is now replaced by $\tilde{p}_\phi^- \equiv p_\phi + (R'/2)\theta R^{-1/2}$. $\hat{\Gamma}_-$ is again a cotangent bundle on $\hat{C}$ whence $\hat{\mathscr{H}}_-$ is just a copy of $\hat{\mathscr{H}}_+$. The quantum Hamiltonian operator is again given by (3.18). Thus, the complete Hilbert space of quantum states $\hat{\mathscr{H}}$ is the direct sum of $\hat{\mathscr{H}}_+$ and $\hat{\mathscr{H}}_-$. The positivity of the quantum Hamiltonian $\underline{\hat{H}}$ on $\hat{\mathscr{H}}$ is a direct consequence of the positivity of the classical Hamiltonian on the constraint surface $\bar{\Gamma}$ (and hence also on the reduced phase space $\hat{\Gamma}$).

We now have two quantum descriptions of the model system and can therefore ask for the relation between them. We claim that there is a well-defined sense in which the quantum theory obtained via the reduced phase-space method is "contained" in the theory obtained via the operator constraint approach. To see this, define mappings $I_\pm$ from $\hat{\mathscr{H}}_\pm$ into $\bar{\mathscr{H}}_\pm$ as follows:

$$I_\pm \circ \hat{\Psi}_\pm(r,\phi) \equiv (\pi r \sin\theta)^{-1/2} \hat{\Psi}_\pm(r,\phi) \times \exp\left[\frac{i}{\hbar}\theta R^{-1/2} \right] \tag{3.19}$$

for all $\hat{\Psi}_\pm$ in $\hat{\mathscr{H}}_\pm$. It is easy to verify that the mapping is norm preserving:

$$\begin{aligned} |\, I_\pm \circ \hat{\Psi}_\pm(r,\phi) \,|^2_{\bar{\mathscr{H}}_\pm} &= \frac{1}{\pi} \int_{\bar{\mathscr{C}}} |\, \hat{\Psi}_\pm(r,\phi) \,|^2 r\,dr\,d\phi\,d\theta \\ &= \int_{\hat{\mathscr{C}}} |\, \hat{\Psi}_\pm(r,\phi) \,|^2 r\,dr\,d\phi \\ &= |\, \hat{\Psi}_\pm \,|^2_{\hat{\mathscr{H}}_\pm} \; . \end{aligned} \tag{3.20}$$

Here we have used the fact that function $R(\phi)$ is non-negative on $\bar{\mathscr{C}}$ to get rid of the phase factors in the norm integral. Equation (3.20) implies that $I_\pm$ are (proper) imbeddings of $\hat{\mathscr{H}}_\pm$ into $\bar{\mathscr{H}}_\pm$ as Hilbert spaces. Finally, since

$$\begin{aligned} I_\pm \circ (\underline{\hat{H}}\hat{\Psi}_\pm) &= I_\pm \circ [E(\phi)\hat{\Psi}_\pm] \\ &= E(\phi) I_\pm \circ \hat{\Psi}_\pm \\ &= \underline{H}(I_\pm \circ \hat{\Psi}_\pm) \; , \end{aligned}$$

the imbeddings commute with the action of the Hamiltonians. Thus, the reduced phase-space method yields only a part of the description provided by the operator constraint method. One may summarize the situation as follows. The θ dependence of elements of $\bar{\mathscr{H}}$ is predetermined by the quantum constraint equation. Thus, as in $\hat{\mathscr{H}}$, the freedom in $\bar{\mathscr{H}}$ is to choose a function of r and ϕ only, namely the function $K(r,\phi)$. Indeed the mapping $I_\pm$ essentially sends $\bar{\Psi}_\pm(r,\phi)$ to $K(r,\phi)$. Thus, it is not the availability of θ variables that makes $\bar{\mathscr{H}}$ larger than $\hat{\mathscr{H}}$. Rather, the difference arises because, whereas $\hat{\Psi}_\pm(r,\phi)$ is allowed to have support only in the classically permissible region where $R(\phi)$ is non-negative, there is no such restriction on the support of $K(r,\phi)$. Consequently,

$\hat{\mathscr{H}}$ corresponds only to the subspace of $\overline{\mathscr{H}}$ in which the wave functions $\Psi_{\pm}$ have support only in $\overline{\mathscr{C}}$. It is precisely the orthogonal complement of this subspace in $\overline{\mathscr{H}}$ that contains the wave functions representing quantum tunneling, wave functions which are responsible for lowering the quantum energy below the classically permissible values.

IV. DISCUSSION

In Sec. II, we saw that the scalar constraint of general relativity restricts the physically permissible classical configurations to a proper subset of the configuration space and, being quadratic in momenta, prevents the reduced phase space from admitting a natural cotangent-bundle structure. To gain insight into this feature, in Sec. III we introduced a model system which mimics this feature. We saw explicitly that the operator constraint method and the reduced phase-space approach yield inequivalent quantum theories and, in particular, whereas the first method yields quantum states with negative energies, the second does not. What implications does this analysis have for quantum gravity? In the model, the difference between the two quantum descriptions occurred due to a tunneling phenomenon which, in turn, was possible because the operator $\underline{p}_\theta$ which enters the constraint fails to be self-adjoint on the physical subspace. Since there are independent reasons[23] to believe that the constraints of general relativity cannot be promoted to self-adjoint operators in the quantum theory, we expect the situation in general relativity to resemble that in the model.

In the model, both theories do agree if one restricts oneself only to those states which are common to both, i.e., which arise in the reduced phase-space method. Thus, it is not that the two theories are inconsistent. Rather, the second description is contained within the first. Hence, even if one adopts the viewpoint that the operator constraint method is the "correct" one, the appropriate label for the reduced phase-space approach would be "incomplete" rather than "wrong." *A priori*, of course, it is not clear as to which of the two methods is the physically correct one. Both would yield the right classical limit (provided of course the limits are taken appropriately); they both incorporate the classical constraint. This is not surprising: distinct quantum theories *can* have the same classical limit. Indeed, the existence of an ambiguity in quantization of complicated classical systems is only to be expected. For, quantization is essentially guesswork; one tries to guess the more complete quantum theory given only its classical limit. Hence, strictly speaking, the question as to which of the two theories is the correct one can be settled only by experiments. That is, there is no theoretical principle which can, by itself, decide unambiguously whether or not the extra quantum states provided by the operator constraint method actually occur in Nature. Unfortunately, the model only mimics certain mathematical features of general relatively and does not describe a simple physically realizable mechanical system. Therefore, the experimental avenue is not available.

The question, nonethelesss, is not completely unanswerable. For, although quantization is guesswork, it is guesswork which follows hints. Hints come from experiments with simpler systems, from semiclassical features and from mathematical analogies. Among these, there are two which can shed some light on the question as to which of the two methods should be preferred in the quantization of gravity. The first comes from the barrier penetration phenomena which lie at the heart of nonrelativistic quantum mechanics. To be specific, let us consider a particle in three (spatial) dimensions subject to a spherical potential $V(r)=V_0>0$ if $r<r_0$ and $V(r)=0$ if $r>r_0$, where r as usual is given by $r^2=\vec{q}\cdot\vec{q}$. Let us impose a constraint:

$$C(\vec{q},\vec{p})\equiv\vec{p}^2/2m+V(r)-E_0=0\ ,$$

where E_0 is a constant $0<E_0<V_0$. Then, classically, the configuration variables are restricted by the constraint: the region $r<r_0$ is inaccessible to the particle. The situation thus resembles the one in general relativity. Furthermore, a quantum-mechanical treatment of the problem is readily available. One knows that a barrier penetration can occur and is described by the Schrödinger equation. This is precisely the prediction of the operator constraint method. The constraint equation $\underline{C}(\vec{q},\vec{p})\Psi=0$ is precisely the Schrödinger equation. The reduced phase-space method, on the other hand, will not allow for this tunneling since the reduced phase space $\hat{\Gamma}$ has no knowledge of the classically forbidden region $r<r_0$. Thus, in this case, experimental evidence does support the operator constraint method.[24] The second hint, although not connected with experiments, is more direct as far as quantum gravity is concerned. It comes from semiclassical considerations. There is now ample evidence that the existence of a suitably regular (c-number) Euclidean solution to the field equations of

a theory connecting two configurations of the field—the instantons—signal the existence of a quantum transition between the two configurations, even when such transitions are forbidden classically. Therefore, in general relativity, one may ask: Do there exist Euclidean solutions to Einstein's equation which join two three-geometries, one of which is classically permissible (i.e., lies in $\overline{\mathscr{C}}$) and the other of which is not? The existence of such solutions would indicate that, even if one began with a wave function $\Psi(q)$ whose support lies entirely in $\overline{\mathscr{C}}$, generically, quantum time evolution will force its support off $\overline{\mathscr{C}}$. This, in turn will mean that to obtain a coherent quantum theory, we must allow the Hilbert space of physical states to contain some wave functions whose support is *not* restricted to lie in $\overline{\mathscr{C}}$; the penetration into $\mathscr{C}-\overline{\mathscr{C}}$ (permitted by the operator constraint) is essential. It turns out that it is trivial to obtain Euclidean solutions of the desired type. Consider the four-dimensional flat Euclidean space and introduce in it polar coordinates τ, r, θ, and ϕ. Let q_{ab} be the flat three-metric intrinsic to the surface $\tau=0$ and let q'_{ab} be the intrinsic metric on the surface defined by $\tau=1+f(r)$, where f is a smooth non-negative C^∞ function of compact support. A desired instanton is the four-dimensional region bounded by the two surfaces (equipped with the flat four-metric). It is clear that the metric q_{ab} belongs to the classically permissible region $\overline{\mathscr{C}}$ of the configuration space. However, unless $f(r)$ vanishes identically, the metric q'_{ab} cannot. [Proof: Since q'_{ab} is flat outside a compact region, its ADM energy is zero. Hence, if q'_{ab} were to belong to $\overline{\mathscr{C}}$, by the positive-energy theorem[5] it must be isometric to the metric of a spherically symmetric, spacelike three-surface in Minkowski space. But this is impossible, e.g., because if r_0 is in the support of $f(r)$, the distance between the spheres of radii r_0 and $r_0+\epsilon$, as measured by q'_{ab}, is greater than ϵ, while on Minkowski space surfaces, the distance would be equal to or less than ϵ.] Thus, the semiclassical analysis based on instantons also lends support in favor of the operator constraint method. Although these arguments do not constitute a proof, taken together they suggest quite strongly that the reduced phase-space method is likely to provide only an incomplete description of quantum gravity.

The question of negative energies in quantum gravity is a more delicate one due to two factors. The first is that, due to the arbitrariness in the choice of lapse and shift fields [T and T^a in Eqs. (2.6) and (2.7)], the Hamiltonian in classical general relativity acquires ambiguities. On the constraint surface $\overline{\Gamma}$ these ambiguities essentially disappear: since the volume integrals in (2.6) and (2.7) vanish on $\overline{\Gamma}$, one can specify the Hamiltonian uniquely there just by picking a time translation at infinity. That is, on $\overline{\Gamma}$, the four-momentum is defined unambiguously. Off $\overline{\Gamma}$, however, the volume integrals also contribute and one has therefore to specify the lapse and the shift *everywhere* on the three-manifold Σ and not just at infinity; the freedom in the choice of the Hamiltonian is now "infinite dimensional, rather than just four." This ambiguity must be faced if we wish to permit tunneling off the classical constraint surface. What choice of lapse and shift is one to make to compute the quantum Hamiltonian? Although the ADM energy does become negative off $\overline{\Gamma}$, it is quite possible[25] that for specific choices of T and T^a, the Hamiltonian $H_T+H_{T^a}$ would be a non-negative function on *all of* Γ, although for a generic choice, of course, it would become negative off $\overline{\Gamma}$. Therefore whether quantum gravity admits states with negative energies appears to depend on the choice of the Hamiltonian to which energy refers. The model, however, suggests that this may not be so. For, in the model, the ground-state energy in quantum theory is dictated by $E(\phi)$ and not by $H={p_\theta}^2-R(\phi)+E(\phi)$. In particular, if $E(\phi)$ admits negative values, the quantum ground-state energy would be negative even when H is everywhere positive [i.e., $E(\phi)-R(\phi)$ is positive] on Γ.[26] This surprising situation can occur because the expectation value of $\underline{p_\theta}^2$ can become negative on physical states in quantum theory even though ${p_\theta}^2$ is everywhere non-negative classically. Hence, by analogy, one can conclude that, since $E^{\mathrm{ADM}}(q)$ does become negative off $\overline{\Gamma}$, the ground-state energy of quantum gravity would be negative irrespective of the choice of lapse and shift. The key question is: Is the analogy good enough? This brings us to the second reason which makes the issue of ground-state energy more subtle than that of the existence of tunneling. For, even if an operator constraint allows tunneling, in general, it will not permit wave functions whose support lies entirely in the classically forbidden region. Thus, *a priori*, it is quite possible that the wave functions $\Psi(q)$ in quantum gravity will be forced to have part of their support in the classically permissible region $\overline{\mathscr{C}}$. Because of this, the expectation value of $E^{\mathrm{ADM}}(q)$ on any physical state may still be non-negative; the contribution from $\overline{\mathscr{C}}$ may outweigh the contribution from $\mathscr{C}-\overline{\mathscr{C}}$. If this occurs, the quantum Hamiltonian may still be non-negative in spite of tunneling.

To summarize, tunneling into the classically forbidden region is likely to occur in quantum gravity since its existence depends only on the gross features of the constraint which are shared by the model system.[27] The occurrence of the negative energy states, on the other hand, depends on the detailed form of the constraint which decides whether or not the physical states of the quantum theory can have most of their support in the classically forbidden region. Therefore, on this issue, the situation is less clear; further information is needed on the properties of wave functions satisfying the quantum scalar constraint of general relativity. The model can nonetheless serve as a useful guide in the investigation of this issue since it presents an explicit mechanism for transcending the classical positive-energy theorems.

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[1]For recent reviews, see K. Kuchař, in *Quantum Gravity 2,* edited by C. J. Isham, R. Penrose, and D. W. Sciama (Oxford University Press, Oxford, 1981), and articles by J. Isenberg and J. Nester, C. Teitelboim, Y. Choquet-Bruhat and J. W. York; P. G. Bergmann and A. Komar, in *General Relativity and Gravitation 1,* edited by A. Held (Plenum, New York, 1980).

[2]The reduced phase space $\hat{\Gamma}$ is the manifold of orbits, restricted to the constraint surface $\bar{\Gamma}$, of the Hamiltonian vector field generated by the constraint function. Thus, each point of $\hat{\Gamma}$ is an equivalence class of (gauge related in the manner of Dirac) points of $\bar{\Gamma}$.

[3]See, e.g., A. Ashtekar and R. Geroch, Rep. Prog. Phys. 37, 1211 (1974), Appendix 3.

[4]See, e.g., articles by Kuchař and by Bergmann and Komar cited in Ref. 1.

[5]R. Schoen and S. T. Yau, Commun. Math. Phys. 65, 45 (1979); 79, 231 (1981); E. Witten, *ibid.* 80, 381 (1981).

[6]G. T. Horowitz, Phys. Rev. D 21, 1445 (1980); in *Quantum Gravity 2,* Ref. 1; J. B. Hartle and G. T. Horowitz, Phys. Rev. D 24, 257 (1981).

[7]This has a curious history. DeWitt pointed out as early as 1967 that there is a significant difference between the spatially compact and asymptotically flat cases. However, he confined his investigations within the canonical approach to the first case because he felt that the so-called covariant method was better suited to handle the second. After that, most work on canonical quantization became focused on the spatially compact case and the question of boundary conditions was not discussed. [See, however, Choquet-Bruhat and York, Ref. 1, and T. Regge and C. Teitelboim, Ann. Phys. (N.Y.) 88, 286 (1974).] Indeed, some recent papers do not even mention that a restriction is involved; vanishing of Hamiltonians is presented as an intrinsic feature of general relativity without any reference to boundary conditions.

[8]P. A. M. Dirac, Can. J. Math. 2, 129 (1950); *Lectures in Quantum Mechanics* (Academic, New York, 1965).

[9]Actually, one could have considered a more general situation and required only that the complement of a compact subset of Σ be diffeomorphic to the complement of a ball $r \leq r_0$ of R^3, with r_0 a fixed constant. We have made the restriction for simplicity only; issues of interest to this paper are insensitive to topology.

[10]D. Christodoulou and N. Ō'Murchadha, Commun. Math. Phys. 80, 271 (1981).

[11]A. Ashtekar, in *General Relativity and Gravitation 2,* edited by A. Held (Plenum, New York, 1980).

[12]T. Regge and C. Teitelboim, cited in Ref. 7; A. Ashtekar, D. C. Christodoulou, and A. Magnon-Ashtekar, in preparation.

[13]See, e.g., N. M. J. Woodhouse, *Geometric Quantization* (Clarendon, Oxford, 1980).

[14]It has also been argued that a weaker form of Eqs. (1.8) and (2.9) should be imposed; to obtain the correct classical limit, for example, it suffices that the expectation values of C_{N^a} and C_N vanish on physical states. In this paper we shall show that, *even with the stronger condition,* wave functions can tunnel into the classically forbidden region.

[15]P. W. Higgs, Phys. Rev. Lett. 1, 373 (1958); 3, 66 (1959).

[16]Let V^a be any vector field on the configuration space. The quantum operator corresponding to the classical observable $p_a V^a$ is $(\hbar/i)V^a\nabla_a + (\hbar/2i)\nabla_a V^a$. Setting $V^a = \partial/\partial\theta$, one obtains Eq. (3.5).

[17]The lower bound, however, belongs to the continuous spectrum of H. Thus, strictly speaking, there is no ground state.

[18]The wave functions $\Psi_\pm$ are defined everywhere on R^3 except for the z axis. *On this domain,* $\underline{p}_\theta \Psi_\pm = \pm R^{1/2}\Psi_\pm$ whence $\Psi_\pm$ satisfies Eq. (3.4). Note, however, $\Psi_\pm$ is not a solution to (3.4) in the distributional sense. This is why it does not belong to the domain which makes $\underline{p}_\theta$ self-adjoint.

[19]In fact, the situation is rather curious: p_θ is an unbounded self-adjoint operator with a dense domain in $\mathscr{H}$ and a bounded linear but non-self-adjoint operator on an infinite-dimensional subspace $\overline{\mathscr{H}}$ of $\mathscr{H}$.

[21]This is but one way to endow a cotangent-bundle structure on $\hat{\Gamma}$. $\hat{\Gamma}$ does not admit a natural cotangent-bundle structure in the sense that one must introduce on $\hat{\Gamma}$ additional structure, not inherited from Γ and $\overline{\Gamma}$, to make it a cotangent bundle.

[20]For simplicity, we are ignoring the set of measure zero at which p_θ vanishes on $\overline{\Gamma}$. The set would be incorporated in the quantum description in the process of Cauchy completion of the space of wave functions.

[22]It is more natural to regard quantum states as densities of weight $\frac{1}{2}$ than as functions. When this is done, a specific choice of volume element is not needed on the configuration space. For details, see, e.g., Ref. 13.

[23]See, e.g., the review by Bergmann and Komar cited in Ref. 1 and the references therein.

[24]In this case, the constraint is easy to realize experimentally. One only needs to prepare an incident beam of specific energy and find a repulsive central potential.

[25]In fact, there is a strong indication that the lapse and the shift fields obtained by solving the Witten equation (see Ref. 5) have this property.

[26]Note also that, although one can add to H any smooth function of the type $f(q,p)\cdot C(q,p)$ without changing the classical dynamics, this ambiguity does not affect the quantum ground-state energy since the expectation value $\langle \Psi_{\pm}, \underline{f}(q,p)\underline{C}(q,p)\Psi_{\pm} \rangle$ of the extra term vanishes in all physical states. The situation would be the same in quantum gravity.

[27]Linearization of the classical scalar constraint (off the datum $q_{ab} \equiv$ flat, $p_{ab}=0$) yields $R'=0$, a constraint independent of momenta. Hence, the operator constraint $R'\Psi=0$ implies that, in the weak-field limit, there is no tunneling; support of Ψ is restricted precisely to the classically permissible linearized metrics. A simple-minded expansion of the constraint equation (2.9) in powers of the coupling constant suggests that the situation would be analogous to higher orders in the perturbation expansion since the "kinetic energy term" in (2.9) is always one order higher than the "potential energy" term. Thus, the tunneling appears to be genuinely nonperturbative phenomenon.