A Minisuperspace Example: The Gowdy T^3 Cosmology*

Charles W. Misner†
California Institute of Technology, Pasadena, California 91109
(Received 28 June 1973)

The Gowdy T^3 inhomogeneous cosmology is an exact vacuum solution of Einstein's equations representing gravitational waves propagating in an expanding closed universe. As shown by Berger, it provides an example showing graviton pair creation as a quantum effect near the initial singularity, together with the reaction this induces in the cosmological expansion. The truncated quantization given here by superspace methods develops the "single residual constraint" quantization method proposed by Moncrief. The quantum wave equation is soluble by separation of variables, and shows that graviton number is a concept unsuited to the description of the initial (velocity-dominated) singularity. Thus a good description of the pair creation occurring in even this soluble model has not yet been developed.

I. INTRODUCTION

The Gowdy T^3 cosmology[1] is the simplest inhomogeneous empty universe. It is studied here to illuminate superspace quantization methods, and questions of particle creation in the early universe. Near the singularity it is an example of a velocity-dominated cosmological singularity. Far from the singularity the solution can be described as an expanding universe with flat space sections filled with plane gravitational waves that move only in the z direction, but with arbitrary wave forms. The assumed symmetries in this model universe reduce the intrinsic nonlinearities of the Einstein equations to a minimum, and therefore allow a completely explicit treatment with a minimum of computational difficulties. In this paper a quantum treatment of the model is given in which the computations can be reduced to the solution of Schrödinger-type equations in finite-dimensional spaces.

The methods used here are extensions of those I have applied previously[2] to cosmological models with a finite number of degrees of freedom. The model here has an infinite number of degrees of freedom, but is somewhat simpler computationally than the Einstein-Rosen cylindrical waves which Kuchař[3] has treated so successfully using very similar techniques. One important aspect of the paper, however, is the difference between the "single residual constraint" approach to quantization taken here, and the more clear-cut limiting cases of the Arnowitt-Deser-Misner (ADM)[4] or Dirac[5] quantization methods illustrated in Kuchař's paper.[3] Because of these differences, the present example serves as a useful illustration of, and provides part of the motivation for, a method for deciding critical factor-ordering questions in the quantization of the gravitational field by superspace methods.[6]

Another important application of this quantum cosmology model is to the problem of particle creation in the early universe. The limited aspects of this problem that can be modeled within the universes treated here are formulated, but not solved, in Sec. VII of this paper. A semiclassical solution is given in Sec. IX. The class of cosmological models which are studied here were introduced by Gowdy[1] and have been further studied by Berger.[7] Her work included a quantization of the models by the ADM methods and an application to the questions of particle creation.

The creation of particle-antiparticle pairs as a consequence of a strong gravitational field existing near the cosmological singularity was studied by Parker[8] and subsequently by Zel'dovich and Starobinsky.[9,10] Current interest in this particle-creation process centers not so much on the particles themselves, as upon the reaction to the particle-creation process by the universe which induced it. Thus, one is not importantly concerned at present with whether there are particles in the universe that were not produced by such a pair-creation process. (This would be necessary if the total baryon number of the universe is to be nonzero.) Two quite different effects are the center of attention. One focuses upon the highly dissipative nature of the particle-creation process which, as pointed out by Zel'dovich,[9] could require that the universe achieve a highly isotropic expansion already as early as the Planck time. The second question is the puzzling relationship between the observed homogeneity of the early universe (as deduced from the isotropy of the microwave radiation) and the severe horizon limitations which exist within the homogeneous Friedmann cosmological models especially at early times. These limitations exclude a causal synchronization of the distinct regions emitting the microwave radiation within the model. Attempts to overcome horizon limitations by using the mixmaster cosmological model at early time[11] have not been successful.[12,13]

That the particle-creation process may bear on the horizon question may be proposed on the basis of Zel'dovich's[14] analysis of causality in the completely understood pair-creation process in quantum electrodynamics. Here, one sees that attempts to describe the particle-creation process in a purely classical language result in apparent causality violations. Consider a pair of particles that are spontaneously created by electric fields exceeding a critical strength. These particles already materialize with a spacelike separation so that the work done in separating them as virtual particles before they materialize supplies the energy to produce their rest mass. The classical-world lines upon which the pair of particles materialize are hyperbolas in an assumed uniform background electric field, but in the spacetime diagram they are hyperbolas that have a common focus but lie entirely outside each other's light cones. Thus, in this completely understandable case, a causal and relativistically invariant quantum theory of electrodynamics leads to a result which appears completely acausal if one attempts to describe it in a purely classical language. It is therefore a significant and urgent question to inquire concerning the apparent acausality of the Friedmann cosmological models (in which physical conditions are synchronized at distant points whose past light cones do not overlap) and to ask whether this apparent acausality is not merely the result of using a classical language to describe the results of a phenomena whose quantum origins were entirely causal.

There are three principal differences between the Berger treatment of this minisuperspace example in quantum cosmology and the present extension of her work. The first of these differences is in methodology. Berger used the ADM Hamiltonian as a principal tool, whereas I will use a vanishing super-Hamiltonian. The other differences reflect a reformulation of the physical problem which is being studied. One of these further differences is that one additional degree of freedom is treated as a dynamical variable subject to quantum fluctuations in the present paper, but treated as a fixed classical background parameter in Berger's work. (Both papers omit infinitely many modes of the gravitational field by treating them as fixed classical parameters and ignoring even their vacuum fluctuations in the quantization.) The other difference reflects the choice of initial states for the universe near the singularity upon which to concentrate attention. Berger defined a graviton number in each mode in the same way that I will, and studied the particle creation subsequent to some (nonsingular) initial time at which it was assumed that there were no gravitons in any mode. The major extension of Berger's work which this paper provides is a more extensive analysis of the state of the universe near the singularity within the quantum language. It will be argued here that the graviton numbers are an unnatural and singular language for describing the initial state of the early universe. An alternate language is presented which fits very well. The description of the corresponding classical singularity was given by Lifshitz and Khalatnikov[15] and subsequently rewritten from a more global viewpoint by Eardley, Liang, and Sachs.[16] The present treatment differs from the quantum theory of velocity-dominated singularities presented by Liang[17] in choosing a different metric for superspace. This results in a different factor ordering in the quantum problem and dramatically changes the behavior of the wave function near the singularity. The factor ordering chosen here preserves the singularity with essentially its classical significance and inevitablity, whereas Liang's choice allowed the wave function to vanish in those regions of superspace describing singular configurations of the universe. Some justification for the present choice of factor ordering will be given elsewhere.[8]

II. METRIC AND COORDINATE CONDITIONS

The superspace approach to relativity[18] views as the primary object a three-dimensional Riemannian metric geometry assigned to a three-dimensional manifold. The topology of the manifold is fixed once and for all, but its metric properties are variable. Each specification of a different set of metric properties constitutes a different point in superspace. A solution of Einstein's equations classically may be represented by a curve in superspace parametrized by time parameter t. Thus, the solution to Einstein's equations is seen as the time evolution of the three-dimensional Riemannian metric properties of a three-manifold. By auxilary constructions this sequence of three-manifolds can be sewn together into a four-dimensional manifold of Minkowski signature satisfying the Einstein equation. A different choice of time coordinate in this four-manifold would correspond to a different curve in superspace. The totality of such curves would form a submanifold of superspace which would represent in a coordinate-independent way the classical solution of the Einstein equations. In the quantum theory there would be defined a wave function Ψ on superspace satisfying a Klein-Gordon type equation there. At least in the case where a specific choice of time coordinate (slicing of the four-manifold) is agreed upon, there would be also defined a probability current vector constructed from Ψ and satisfying a conservation law. This probability current would then serve to describe the motion of a wave packet which, in appropriate limiting cases, would be centered upon and essentially define the classical curve giving an unquantized solution to the Einstein equation.

To define a minisuperspace, then, our first task is to specify the topology of that three-manifold to which points in the superspace will assign metric structure. The choice made in this paper is to always consider the underlying topological manifold for spacelike hypersurfaces to be the 3-torus T^3. This manifold can be described in terms of three coordinates which are treated as angles. We shall call the coordinates θ, σ, δ. Although our superspace will be infinite-dimensional, it is a minisuperspace simplified and limited by the restricted form admitted for the possible Riemannian metrics assigned to the 3-torus. These metrics are in the first instance those for which the spatial line element may be put in the form[1]

$$dl^2 = e^{-\tau-(\lambda/2)}\, d\theta^2 + e^{2\tau}(e^{\beta}d\sigma^2 + e^{-\beta}d\delta^2)\,. \tag{1}$$

Here the three functions τ, λ, β parametrize the three independent metric components. As a condition of symmetry we require that these functions τ, λ, β may depend only on the coordinate θ and upon the time t. After studying the ADM variational principal for metrics of this form, we will find it possible to impose as a coordinate condition the requirement that τ be independent of θ as well. The solution of the momentum constraints, which is described in Sec. III, will further reduce the configuration space of the problem to one in which λ has only one degree of freedom, although β will retain infinitely many degrees of freedom as an arbitrary function of θ. Thus the final configuration space is somewhat smaller than the minisuperspace which we have first defined here.

The form of the space metric in Eq. (1) is adopted, with minor changes in notation, from the work of Berger.[7] The ADM variational integral for this metric is also computed there. With the corresponding notational changes it reads

$$2\pi I = \int\!\!\int dt\, d\theta (p_\lambda \dot{\lambda} + p_\tau \dot{\tau} + p\dot{\beta} - N_\mu \mathfrak{C}^\mu)\,, \tag{2}$$

provided that units $G = 1 = c$ have been adopted, and the periods of the angles σ and δ are chosen so that

$$\int\!\!\int d\sigma\, d\delta = 8\,. \tag{3}$$

Dot and prime indicate differentiation with respect to t and θ, respectively, and θ is assigned a 2π period. The quantities $N_0 \equiv N$ and N_i here are the standard lapse and shift functions and the $\mathfrak{C}^\mu$ are the constraints. The appearance of the constraints is improved slightly by the definitions

$$\overline{N} \equiv \overline{N}_0 = Ng^{-1/2} = N\exp(-\tfrac{3}{2}\tau + \tfrac{1}{4}\lambda)\,, \tag{4a}$$

$$\overline{N}_\theta = N_\theta \exp(\tau + \tfrac{1}{2}\lambda)\,. \tag{4b}$$

With these redefinitions the variational integral can be rewritten as

$$2\pi I = \int\!\!\int dt\, d\theta (p_\lambda \dot{\lambda} + p_\tau \dot{\tau} + p\dot{\beta} - \overline{N}_\mu\, \overline{\mathfrak{C}}^\mu)\,, \tag{5}$$

where

$$\overline{\mathfrak{C}}^0 = \tfrac{1}{2}p^2 + p_\lambda p_\tau + \tfrac{1}{2}e^{4\tau}\beta'^2 + e^{4\tau}(4\tau'' + 8\tau'^2 + \tau'\lambda')\,, \tag{6}$$

and

$$\overline{\mathfrak{C}}^\theta = 4p_\lambda' + p_\tau \tau' + p\beta' + p_\lambda \lambda'\,. \tag{7}$$

The two other constraints vanish identically:

$$\overline{\mathfrak{C}}^\delta = 0 = \overline{\mathfrak{C}}^\sigma\,. \tag{8}$$

In this transformation, the variables N_μ were replaced by linear combinations of themselves ($\overline{N}_\mu$) in which the coefficients in the transformation were functions of the g_{ij}, p^{ij}, and their spatial derivatives. Such a transformation does not alter the resulting system of differential equations since the additional terms which are introduced are all linear combinations of the constraints or of their spatial derivatives. Of course, the variational principle itself requires that these constraints vanish as a result of varying $\overline{N}_\mu$ or the N_μ, as the case may be.

The variational principle (5) leads immediately to the following equations for $\dot{\tau}$ and $\dot{p}_\lambda$:

$$\begin{aligned}\dot{\tau} &= -\,\delta(\overline{N}_\mu \overline{\mathfrak{C}}^\mu)/\delta p_\tau \\ &= \overline{N}p_\lambda + \overline{N}_\theta \tau'\,, \\ \dot{p}_\lambda &= -\,\delta(\overline{N}_\mu \overline{\mathfrak{C}}^\mu)/\delta\lambda \\ &= (\overline{N}e^{4\tau}\tau')' + (\overline{N}_\theta p_\lambda)'\,.\end{aligned} \tag{9}$$

From these equations it is easy to see that a coordinate condition can be imposed which will considerably simplify the study of the remaining equations. Suppose that $\overline{N}$ and $\overline{N}_\theta$ are required to be constant for all time. Then Eqs. (9) show that the initial condition $p_\lambda' = 0 = \tau'$ would be preserved for all future time. We therefore restrict the time development of the coordinates off the initial surface by the coordinate condition

$$\overline{N} = 1, \quad \overline{N}_\theta = 0\,, \tag{10}$$

and further restrict the coordinates by imposing as initial conditions the coordinate requirements

$$\tau' = 0 = p_\lambda'\,. \tag{11}$$

Since we have just verified that these initial conditions (11) will be preserved throughout all times we will incorporate them in the variational principle and constraints immediately to achieve a further simplification. The procedure adopted by imposing Eq. (11) is of course equivalent to Fourier analyzing τ and p_λ in space (that is, as functions of θ) and setting all of the nonconstant modes in this expansion to zero. Since choosing a well-defined coordinate system prevents a single intrinsic geometry from being represented in more than one way, this procedure of imposing coordinate conditions is equivalent to passing from the space of Riemannian metrics on T^3 to the minisuperspace of T^3, i.e., the space in which each distinct point represents a distinct three-geometry. Another equivalent way of stating the significance of imposing completely well-defined coordinates on our manifold is to say that all remaining quantities in the problem now become observables.

III. REDUCTION TO A SINGLE HAMILTONIAN CONSTRAINT

When Eqs. (11) are imposed upon the system, the equations governing the time development of the conjugate variables can no longer be obtained from the variational principle. One could adjoin these equations to the variational principle to supply a complete statement of the problem. This is, of course, necessary for the constraint equations once conditions (10) have been imposed. However, the equations lost by imposing (11) will in fact not be needed, since we will find that the conjugate variables themselves can be eliminated from the problem. Let us then rewrite the variational integral (5), incorporating the simplifications which result from Eqs. (10) and (11). The result is

$$I=\int dt\,(p_\lambda\dot{\lambda}_0+p_*\dot{\tau})+(2\pi)^{-1}\iint dt\,d\theta(p\dot{\beta}-\mathcal{H})\,. \tag{12}$$

Here we have been able to carry out the θ integration in the first two terms as a consequence of the θ independence of τ and p_λ. The quantities canonically conjugate to these two variables are thus found to be

$$\lambda_0\equiv(2\pi)^{-1}\oint\lambda d\theta\,,$$

and (13)

$$p_*\equiv(2\pi)^{-1}\oint p_\tau d\theta\,.$$

The variational integral (12) is now in canonical form, and the Hamiltonian density $\mathcal{H}$ which appears in it is

$$\mathcal{H}=p_\lambda p_\tau+\tfrac{1}{2}p^2+\tfrac{1}{2}e^{4\tau}(\beta')^2\,. \tag{14}$$

The assertion that the variational integral is in canonical form can be made because the spatially variable parts of p_τ disappear from the total Hamiltonian just as they have done from the $p\mathring{q}$ terms in the integral. The total Hamiltonian is

$$\begin{aligned}\mathfrak{H}&\equiv p_\lambda p_*+(2\pi)^{-1}\oint(\tfrac{1}{2}p^2+\tfrac{1}{2}e^{4\tau}\beta'^2)d\theta\\&=(2\pi)^{-1}\oint\mathcal{H}d\theta\,.\end{aligned} \tag{15}$$

In addition to the dynamical equations which result from the statement $\delta I=0$ applied to Eq. (12), it is also necessary to impose the constraints

$$\mathcal{H}\equiv\overline{N}_\mu\overline{\mathfrak{C}}^\mu=0 \tag{16}$$

and

$$\overline{\mathfrak{C}}^\theta\equiv p\beta'+p_\lambda\lambda'=0\,. \tag{17}$$

All but one of this double infinity of constraints can be solved to provide the quantities which have disappeared from the variational principle. Thus we write

$$\begin{aligned}\lambda&=\lambda_0+\lambda_+\,,\\p_\tau&=p_*+p_+\end{aligned} \tag{18}$$

to separate out the spatially variable parts λ_+ and p_+ of λ and p_τ. Then from Eq. (14) the constraint $\mathcal{H}=0$ can be solved to give p_τ. One linear combination of these constraints, namely,

$$\mathfrak{H}=0\,, \tag{19}$$

could be solved to give p_*, while the remaining infinitely many constraints (one for each value of θ) can be solved to give p_+. However, p_+ appears nowhere else in the physical problem, neither in the variational principle nor in the formulas for reconstructing the metric from the solution of the differential equations. Therefore it is not necessary to actually inspect these equations, simple as they may be. An explicit solution of the single residual constraint (19) can be readily found from Eq. (15) and reads

$$\begin{aligned}H_{\text{ADM}}&=-p_*\\&=(2\pi p_\lambda)^{-1}\oint(\tfrac{1}{2}p^2+\tfrac{1}{2}e^{4\tau}\beta'^2)d\theta\,.\end{aligned}$$

Our decision not to adopt this equation, which would eliminate p_* from the discussion at this point, marks the turnoff at which we depart from the standard ADM approach. Thus we prefer not to regard the constraint (19) as solved, but as a remaining condition on the initial data for the dynamic equations. The momentum constraint (17), however, we do wish to regard as defining the function λ_+. [The spatially constant dynamical variable λ_0 clearly does not enter Eq. (17).] Thus, λ_+ is to be defined as follows:

$$\lambda_+ = -(p_\lambda)^{-1}\left[\int_0^\theta p\beta' d\theta - (2\pi)^{-1}\oint d\theta' \int_0^{\theta'} p d\beta\right], \tag{20}$$

where the constant second term is chosen so that $\langle\lambda_+\rangle = (2\pi)^{-1}\oint \lambda_+ d\theta = 0$. It is necessary to pay explicit attention to this equation for λ_+ because the function λ_+ occurs in the metric of Eq. (1). This equation also leads to an additional condition or constraint not from the local differential equations, but from the boundary conditions implicit in the assumed T^3 topology. Thus, since λ must be a periodic function of θ, $\lambda(\theta+2\pi)=\lambda(\theta)$, the same must hold true for λ_+ and consequently the condition

$$\mathfrak{P} \equiv -(2\pi)^{-1}\oint p\beta' d\theta = 0, \tag{21}$$

must be imposed upon the initial conditions for β and p. This condition, which can be interpreted as saying that the total momentum of the gravitational waves in this closed universe must add up to zero, can easily be seen to be preserved in time by the differential equations satisfied by p and β.

IV. CLASSICAL SOLUTIONS

All the degrees of freedom remaining in this problem can be treated as discrete variables by introducing the Fourier transforms of β and p. In order to make the transition to the Klein-Gordon-type wave equation more straightforward later, we use a real Fourier series

$$\begin{aligned}\beta &= q_0 + \sum_{n=1}^{\infty}(q_n\sqrt{2}\cos n\theta + q_{-n}\sqrt{2}\sin n\theta),\\ p &= k_0 + \sum_{n=1}^{\infty}(k_n\sqrt{2}\cos n\theta + k_{-n}\sqrt{2}\sin n\theta).\end{aligned} \tag{22}$$

With this choice of dynamical variables, the variational integral becomes

$$I = \int dt\,(p_\lambda\dot\lambda_0 + p_*\dot\tau + \sum_{n=-\infty}^{\infty} k_n\dot q_n - \mathfrak{H}), \tag{23}$$

where

$$\mathfrak{H} = p_\lambda p_* + \sum_{n=-\infty}^{\infty}\tfrac{1}{2}(k_n{}^2 + n^2 e^{4\tau} q_n{}^2). \tag{24}$$

The corresponding rewrite of the momentum constraint is

$$\mathfrak{P} = -\sum_{n=1}^{\infty} n(k_n q_{-n} - k_{-n} q_n) = 0. \tag{25}$$

As a consequence of the coordinate conditions we have imposed in Eq. (10), the metric form for the spacetime metric [which can be reconstructed as a solution of the Einstein equations from any solution of the variational principle and remaining constraints (24) and (25)] is as follows:

$$\begin{aligned}ds^2 &= \exp(-\tau - \tfrac{1}{2}\lambda_0 - \tfrac{1}{2}\lambda_+)(-e^{4\tau}dt^2 + d\theta^2)\\ &\quad + e^{2\tau}(e^{\beta}d\sigma^2 + e^{-\beta}d\delta^2).\end{aligned} \tag{26}$$

The Hamiltonian equations for this problem are, from Eq. (23), just

$$\dot\lambda_0 = p_*, \quad \dot p_\lambda = 0, \tag{27λ}$$

$$\dot\tau = p_\lambda, \quad \dot p_* = -2e^{4\tau}\sum_{n=-\infty}^{\infty} n^2 q_n{}^2, \tag{27τ}$$

$$\dot q_n = k_n, \quad \dot k_n = -n^2 e^{4\tau} q_n, \tag{27β}$$

$$\dot{\mathfrak{H}} = 0. \tag{27$\mathfrak{H}$}$$

From these equations one sees that p_λ is a constant in time as well as in space, and that τ is therefore proportional to the coordinate time t.

One difference between the present approach and that of Berger[7] is that we treat p_λ as a dynamical variable rather than as an arbitrary fixed constant. As a consequence of this, the residual constraint $\mathfrak{H}=0$ of Eq. (24) remains quadratic in the momenta and allows the interpretation given in Sec. V in terms of a metric geometry on superspace.

The value of the constant p_λ may have geometrical significance in that it controls the relationship between the horizon sizes in the θ direction and the transverse ($\sigma\delta$) cross-sectional areas of these model universes. It is evident from Eqs. (3) and (26) that the transverse cross-sectional area of this universe is $8e^{2\tau}$. On the other hand, we may compute the coordinate size of the horizon at any time from Eq. (26) as follows:

$$\begin{aligned}\theta_{\text{horizon}} &= \int_{\text{null}} d\theta\\ &= \int e^{2\tau}dt\\ &= \int_{-\infty}^{\tau} e^{2\tau}\frac{d\tau}{p_\lambda}\\ &= \frac{1}{2p_\lambda}e^{2\tau}.\end{aligned} \tag{28}$$

In this computation we have evaluated the change in θ following a null ray on which σ and δ were both constant, starting from the singularity at $\tau=-\infty$. The variable of integration was changed from t to τ by the use of Eq. (27τ). Since the coordinate circumference of this universe is $\theta_{\text{circumference}}=2\pi$, we find the following geometrical interpretation of p_λ:

$$p_\lambda = \frac{(\sigma\delta \text{ proper area})}{32\pi(\theta_{\rm hor}/\theta_{\rm circ})} \ . \tag{29}$$

Because the boundary condition of spatial closure is imposed rather artifically in this model, the interpretation (29) of p_λ may have limited significance.

Another interpretation can be obtained from the behavior of the gravitational waves in these model universes. In order to study these classically,[7] it is convenient to introduce the relation $dt = d\tau/p_\lambda$ into the wave Eq. (27β) in order to obtain

$$\frac{d^2 q_n}{d\tau^2} + \frac{n^2 e^{4\tau}}{p_\lambda{}^2} q_n = 0 \ . \tag{30}$$

The solutions of this equation are

$$q_n = Z_0\left(\tfrac{1}{2}e^{2\tau}\left|\frac{n}{p_\lambda}\right|\right), \tag{31}$$

where Z_0 is any real Bessel function of order zero. Near the singularity, $\tau \to -\infty$, the Bessel function will be dominated by the Neumann term and q_n will be a linear function of τ. For large values of τ the q_n will become an oscillatory function of τ in a regime which, we will later see, corresponds to a WKB or adiabatic approximation in the wave equation. In this region, therefore, one may properly speak of gravitational-waves modes. The critical epoch which separates the behavior dominated by the singularity from the behavior describable in terms of gravitational waves, is that where the argument of the Bessel function is of order unity. The critical epoch for the nth mode is therefore characterized by a value τ_n given by

$$\tfrac{1}{2} e^{2\tau_n}\left|\frac{n}{p_\lambda}\right| = 1 \ . \tag{32}$$

By comparison with Eq. (28) this may also be written[7]

$$n\theta_{\rm hor}(\tau_n) = 1 \ , \tag{32$'$}$$

which is a statement that at this epoch the reduced coordinate wavelength (θ wavelength divided by 2π) of the mode in question is just equal to the θ-circumference of the universe. Since one knows from the work of Berger[7] that particle creation ceases at this critical epoch in each mode, the parameter p_λ controls how long (in the sense of increasing τ or equivalently increasing transverse cross section of the universe) the particle-creation process will continue.

Of course the solution of Eq. (30) in the limit $\tau \to -\infty$ presents no problem; however, it is interesting also to study this limit in the form of the Hamiltonian given in Eq. (15). There one sees that as $\tau \to -\infty$, the β'^2 term, the only term involving spatial derivatives, drops out of the Hamiltonian. As a consequence, there is no coupling between adjacent points in space. The solution of Hamilton's equations in this case makes every momentum a constant of motion. Therefore, to specify solutions, one must specify a value for p_λ and, in addition, an arbitrary function $p(\theta)$. The residual constraint $\mathfrak{H} = 0$ will then determine p_*. This solution near the singularity in which adjacent points are decoupled from each other is an example of a situation described by Khalatnikov and Lifshitz[15] in early work that has been reformulated by Eardley, Liang, and Sachs[16] under the characterization "velocity-dominated singularities." In this case the local behavior of the singularity at each value of θ is precisely that of some Kasner homogeneous universe, but the Kasner parameter can be assigned independently at each different θ. The details of the correspondence between the metric form used here and the canonical forms for the Kasner metrics are given in Ref. 7. For the parameter u which Lifshitz and Khalatnikov[15] introduce to parametrize the Kasner exponents $(p_\theta, p_\sigma, p_\delta)$ one finds

$$2u(\theta) = -1 + (2p_\lambda)^{-1}p(\theta) \ ,$$

with

$$p_\theta = \frac{u(u+1)}{(u^2+u+1)} \ . \tag{33}$$

Thus $u = \infty$, the particular choice of the Kasner parameter that washes out horizons in the θ direction, corresponds to $p_\lambda = 0$. This choice is not available as a local condition, to be satisfied at some points θ but not at others, in the present metric, however. Because of the equation $\mathfrak{H} = 0$, the choice $p_\lambda = 0$ requires $p(\theta) = 0$ and consequently leads to this special horizon-breaking Kasner form simultaneously at all points of the manifold, and, indeed, can only be achieved in the case of a homogeneous cosmology within the class of solutions considered in the present paper.

V. SUPERSPACE FORMULATION: KLEIN-GORDON EQUATION AND PROBABILITY FLUX VECTOR

The Einstein equations for a particular class of metrics have now been reformulated so that they consist of the variational principle (23) which is in canonical form, the two constraints (24) and (25) which must be imposed on the initial condition, a definition (20) of the quantity λ_+ in which the primary remaining nonlinearity of the Einstein equations is concentrated, and a formula (26) for the spacetime metric which results. The momentum constraint (25) which arose from global considerations (boundary conditions) is not at all troublesome, and could be satisfied term by term if desired by restricting the class of solutions under consideration. The residual Hamiltonian constraint (24) is even simpler, as one could solve this equation and adopt the ADM approach where τ would be used as a time variable and $-p_*=H_{\rm ADM}$ would become the ADM Hamiltonian. We do not adopt that approach because the superspace viewpoint, and analogies to methods that can be employed in the general case, as discussed elsewhere,[6] are more evident if one retains this residual Hamiltonian constraint.

The coordinates we are using in the present minisuperspace are λ_0, τ, and the q_n ($n=\ldots,-2,-1,0,1,\ldots$). They are analogs of the parameters one might specify to determine a unique 3-geometry in a genuine superspace problem. For this reason, we will denote them generically by g^A. Then the residual constraint (24) can be put in the form

$$\mathfrak{H}=\tfrac{1}{2}[G^{AB}(g)p_Ap_B-\mathcal{R}(g)], \tag{34}$$

which I have used previously in finite-dimensional examples.[2] From Eq. (24) one sees that the G^{AB} are all constants in the present examples whose values are given by

$$\begin{aligned}&G^{\lambda\tau}=G^{\tau\lambda}=1, \quad G^{\lambda\lambda}=0=G^{\tau\tau};\\&G^{mn}=\delta^{mn}, \quad m,n\neq\lambda,\ \tau.\end{aligned} \tag{35}$$

One interprets G^{AB} as contravariant components of a metric tensor (supermetric) which assigns a Riemannian structure to superspace. The line element corresponding to this supermetric is

$$d\mathfrak{s}^2=G_{AB}dg^Adg^B. \tag{36}$$

From the form given for G^{AB} in Eq. (35), one sees that λ and τ are null coordinates in this minisuperspace, and that the supermetric has a normal hyperbolic signature with one minus sign and all the remaining signs positive. A diagonal form for the supermetric is of course easily introduced by using sums and differences of λ and τ as new coordinates in the minisuperspace [Eq. (65)].

In order to better see the analogy between this example and a general superspace, it is useful to rewrite the residual constraints as follows:

$$\mathfrak{H}=(16\pi)^{-1}\int[\pi^{ij}\pi_{ij}-\tfrac{1}{2}(\pi^k{}_k)^2]\,d^3x-\tfrac{1}{2}\mathcal{R}, \tag{37}$$

where

$$\mathcal{R}=(8\pi)^{-1}\int(\sqrt{g}\,{}^3R)\sqrt{g}\,d^3x. \tag{38}$$

The transition from this form to that of Eq. (15) can be checked in detail using some computation from Berger's thesis[19]:

$$\pi^{ij}\pi_{ij}-\tfrac{1}{2}(\pi^k{}_k)^2=\tfrac{1}{2}p^2+p_\lambda p_\tau, \tag{39}$$

$${}^3R=-e^{\tau+\lambda/2}(\tfrac{1}{2}\beta'^2). \tag{40}$$

The correspondence can be drawn somewhat tighter if we interpret the operation $(16\pi)^{-1}\int\cdots d^3x$ to be the summation over discrete degrees of freedom such as occur, for example, in Eq. (23). Then Eq. (37) becomes the precise analog of Eq. (34) when we write it in the form

$$\mathfrak{H}=\tfrac{1}{2}\left[(16\pi)^{-1}\int G^{ijkl}\pi_{ij}\pi_{kl}d^3x-\mathcal{R}\right], \tag{41}$$

where

$$G^{ijkl}=g^{ik}g^{jl}+g^{il}g^{jk}-g^{ij}g^{kl}. \tag{42}$$

In this case the analog of Eq. (36) is

$$\begin{aligned}d\mathfrak{s}^2&=(16\pi)^{-1}\int G_{ijkl}\delta g^{ij}\delta g^{kl}\,d^3x\\&=(16\pi)^{-1}\int[-\tfrac{1}{2}\delta g_{ij}\,\delta g^{ij}-\tfrac{1}{2}(\delta\ln g)^2]\,d^3x.\end{aligned} \tag{43}$$

In this equation we have written δg^{ij} to take the place of dg^A in Eq. (36), and the covariant components of the superspace metric are then given by

$$G_{ijkl}=\tfrac{1}{4}(g_{ik}g_{jl}+g_{il}g_{jk}-2g_{ij}g_{kl}). \tag{44}$$

When Eq. (43) is evaluated for a metric of the form adopted in this paper and given in Eq. (1), the result is

$$d\mathfrak{s}^2=(2\pi)^{-1}\oint d\theta(2\delta\tau\delta\lambda+\delta\beta^2). \tag{45}$$

Under the further coordinate condition that τ should be independent of θ, this reduces further to

$$\begin{aligned}d\mathfrak{s}^2&=2\delta\tau\delta\lambda_0+(2\pi)^{-1}\oint d\theta(\delta\beta)^2\\&=2\delta\tau\delta\lambda_0+\sum_{n=-\infty}^{\infty}(\delta q_n)^2.\end{aligned} \tag{46}$$

This metric then assigns a metric geometry or a Riemann structure to the configuration space of the present example, a configuration space which we will refer to as minisuperspace. Actually, this configuration space is not simply superspace with a limited number of degrees of freedom. The reason for this is that a single point in our configuration space does not contain enough information to completely specify a 3-geometry by the use of Eq. (1). The missing information is that required to compute the function λ_+ from Eq. (20). Nevertheless, the analogy is close enough to justify our use of the word minisuperspace in this example. For instance, all of the preceding equations in this paragraph can be specialized directly from their general form by inserting the metric values implied by Eqs. (1) and result in equations that are meaningful and correct in our models.

The principal step taken in constructing this model for which analogs are not known in the general case is Eq. (20), which explicitly solves the momentum constraints and uses that solution to eliminate some variables from the dynamical equations. This step can, however, be circumvented by other means in the general case which will be more fully discussed elsewhere.[6] In particular, if one sets the problem in the framework of the classical Hamilton-Jacobi equation, or of the quantum wave functions subject to the Dirac constraint equations $\mathcal{C}^{\mu}(x)\Psi(^3G)=0$, then a procedure developed by Moncrief[20] allows one to avoid direct consideration of all but one of these infinitely many constraints, and this one residual constrant can be taken as $\mathfrak{H}=0$, with $\mathfrak{H}$ in the form given by Eq. (41). Thus, most aspects of the present example will provide valuable insight and hints for developing the general quantum theory of gravity, but contain enough simplifications that the formalism is not overwhelming and almost of the computations of interest can be carried out in complete detail.

A quantum theory is achieved by writing

$$p_A = \frac{1}{i}\frac{\partial}{\partial g^A} \tag{47}$$

in $\hbar = 1$ units so that the canonical commutation relations

$$[g^A, p_B] = i\,\delta^A_B \tag{48}$$

are satisfied. Then the residual constraint is imposed as a "subsidiary condition" on the state functional $\Psi(g)$, which in effect requires Ψ to satisfy a single Klein-Gordon type equation

$$\mathfrak{H}\Psi = 0\,. \tag{49}$$

In the general case for Eq. (34) where the metric components are functions of the supercoordinates g^A, there arise factor-ordering problems. These problems are the central issue treated in another paper.[6] For the present example, however, where the residual constraint is given by Eq. (24), no factor-ordering problems present themselves in an obvious way, and it requires considerable work and a broader viewpoint (all of which we omit here) to find them in this example. We can therefore immediately write the appropriate Klein-Gordon equation quite explicitly as follows:

$$\left[\frac{\partial^2}{\partial\lambda_0\partial\tau} + \sum_{-\infty}^{\infty}\frac{1}{2}\frac{\partial^2}{\partial {q_n}^2} - \tfrac{1}{2}e^{4\tau}\sum_{-\infty}^{\infty} n^2 {q_n}^2\right]\Psi = 0\,. \tag{50}$$

If all but a finite number of modes, say, $|n| < \mathfrak{N}$, are omitted from the expansion in Eq. (22), then one may even avoid problems associated with the infinite degrees of freedom in the problem and still retain a minisuperspace example with excellent analogies to important aspects of the general case.

The interpretation of this wave function describing the quantum evolution of the universe is based on a conserved probability current associated with Eq. (50). This is most simply illustrated in the minisuperspace based on the Kantowski-Sachs metric which has been worked out by Fishbone and myself,[21] but it can also be seen in the present example. For the purpose of defining this probability current it is convenient to rewrite Eq. (50) in the form

$$-2\mathfrak{H}\,\Psi \equiv G^{AB}\frac{\partial^2\Psi}{\partial g^A\partial g^B} + \mathfrak{R}\Psi = 0\,, \tag{51}$$

where the G^{AB} are the constants specified in Eqs. (35). In connection with this equation one defines probability current as

$$j^A = \frac{1}{2i}\left(\Psi^* G^{AB}\frac{\partial\Psi}{\partial g^B} - \frac{\partial\Psi^*}{\partial g^B}G^{AB}\Psi\right). \tag{52}$$

It is then quite easy to see that this current is conserved as a consequence of Eq. (51), that is

$$j^A{}_{;A} \equiv \frac{\partial j^A}{\partial g^A} = 0\,. \tag{53}$$

Let Σ be a hypersurface of limited extent in minisuperspace. For example, Σ could be that part of a τ = const hypersurface in which finitely many variables λ_0 and q_n were restricted to lie within finite intervals, while the remaining variables had their full range. Then the probability that the universe described by Ψ evolved across Σ is given by

$$P(\Sigma) = \int_\Sigma j^A |G|^{1/2} d\Sigma_A\,, \tag{54}$$

where

$$d\Sigma_A = \prod_{B\neq A} dg^B\,. \tag{55}$$

The hypersurface Σ is assumed to carry an orientation, and the products in Eq. (55) must also be properly oriented. If we describe this orientation by saying that Σ has a past and a future, then if P is positive, the probability is asserted for the universe having evolved from the past to the future side of Σ, while if P is negative, then the reverse is true.

The interpretation just given is tenable only if the surface element Σ is sufficiently small that the vector j^A points to the same side of Σ everywhere. It is quite possible even in elementary classical minisuperspace models[21] to find classical trajectories of the universe through superspace which cross a given hypersurface in superspace at different points at different directions. For instance, if the hypersurface were one of constant volume for the universe, a universe could first evolve across this hypersurface while expanding and then later on have its trajectory recross in the opposite direction while contracting. A description of this highly classical behavior in terms of a wave packet Ψ would of course show the probability-flux vector vanishing nearly everywhere except in the immediate neighborhood of the classical trajectory. Thus, the probability-flux vector would point towards one side of the constant-volume surface at one crossing and towards the other side on the other. The probability computed from Eq. (54) for evolution across the entire hypersurface of constant volume would integrate to zero. However, smaller sections of this hypersurface including a region around just one of the crossings of the classical trajectory would show probabilities +1 in the one region, and -1 in the other.

Because j^A is divergenceless, like a magnetic-field vector, the field lines of j^A may be pictured as defining tubes of flux. In this case it is a probability flux, not a magnetic flux. Such a tube could be defined by taking a limited hypersurface element Σ and moving it along the field lines of j^A which encounter it. Every cross section of this tube of flux would have the same total probability P as that for Σ given in Eq. (54). Thus if the universe evolves through Σ with 90% probability, its evolution would, with the same 90% probability, carry it across every cross section of the tube. Thus, these tube-of-probability-flux concepts in superspace serve as the quantum-mechanical description of the quantum uncertainties smearing out the single classical trajectory through superspace which describes a classical solution of the Einstein equations. These ideas will need further development in the case (which does not concern us at present) in which no preferred slicing or time-coordinate condition has been imposed upon the 4-geometry in the process of defining the superspace or configuration space for the problem.

VI. SEPARATED SCHRÖDINGER EQUATIONS

Solutions of Eq. (50) can be obtained in the form

$$\Psi = (2\pi)^{-1/2}\int \frac{dp_\lambda}{p_\lambda} f(p_\lambda)\exp(ip_\lambda\lambda_0) \times \prod_{n=0}^{\infty}\psi_n(q_n, q_{-n}, \tau; p_\lambda). \qquad (56)$$

(Here, and in what follows, we ignore the minor and the elementary modifications it would be necessary to take into account precisely the fact that q_n and q_{-n} are distinct only for the modes with n different from 0.) In order to assure that the wave functional Ψ given by Eq. (56) is a solution of the Hamilton-Jacobi Eq. (50), we require each of the factors ψ_n to satisfy a Schrödinger-type equation

$$ip_\lambda \frac{\partial \psi_n}{\partial \tau} = \mathfrak{H}_n \psi_n\,, \qquad (57)$$

where

$$\mathfrak{H}_n = -\frac{1}{2}\left(\frac{\partial^2}{\partial q_n{}^2} + \frac{\partial^2}{\partial q_{-n}{}^2}\right) + \tfrac{1}{2}n^2 e^{4\tau}(q_n{}^2 + q_{-n}{}^2)$$
$$= \tfrac{1}{2}(k_n{}^2 + k_{-n}{}^2) + \tfrac{1}{2}\omega_n{}^2(q_n{}^2 + q_{-n}{}^2) \qquad (58)$$

and

$$\omega_n = |n| e^{2\tau}. \qquad (59)$$

Let us now turn to questions of the normalization and the interpretations of Ψ. First notice that since the sub-Hamiltonians $\mathfrak{H}_n$ in Eq. (58) are clearly Hermitian, the norm

$$\int \psi_n^* \psi_n \, dq_n \, dq_{-n} = N_n(p_\lambda) \qquad (60)$$

is independent of τ and depends only on p_λ as indicated. All these normalization factors may therefore be absorbed in $f(p_\lambda)$ without changing Ψ, so that we may and do subsequently assume unit norms on each factor ψ_n:

$$\int |\psi_n|^2 dq_n \, dq_{-n} = 1\,. \qquad (61)$$

We will next see that the factor $f(p_\lambda)$ controls whether the transverse cross sections of the universe are expanding or contracting. As noted prior to Eq. (28), the transverse proper area in these model universes is given by $8e^{2\tau}$. Therefore the question of whether the transverse cross sections are expanding or contracting is determined by whether the evolution of the universe is proceeding towards increasing or decreasing τ. To determine this from the wave functional Ψ of Eq. (56), we must compute the probability flux of Eq. (52) and determine whether it flows across surfaces of constant τ. For simplicity we pose this question, not separately at limited regions of this hypersurface, but globally for the entire hypersurface τ = constant. We therefore wish to evaluate the (conserved) total weighted probability that the universe is expanding its cross section rather than decreasing it. This probability P_τ is defined by

$$P_\tau = \int_{\tau = \mathrm{const}} j^\tau d\Sigma_\tau$$
$$= \int j^\tau d\lambda_0 \prod_{n=-\infty}^{\infty} dq_n\,, \qquad (62)$$

corresponding to Eq. (54) since the supermetric G_{AB} has determinant $G = -1$. From Eq. (52) one immediately computes that

$$j^{\tau}=\frac{1}{2i}\left(\Psi^{*}\frac{\partial\Psi}{\partial\lambda_0}-\frac{\partial\Psi^{*}}{\partial\lambda_0}\Psi\right), \tag{63}$$

from which P_τ is readily evaluated as

$$P_\tau=\int\frac{dp_\lambda}{p_\lambda}|f(p_\lambda)|^2. \tag{64}$$

It is convenient to think in terms of a normalization $P_\tau=+1$, suggesting a universe which has evolved from the singularity at $\tau=-\infty$. This interpretation is only unambiguous, however, if one imposes the stronger conditions $j^\tau\geq 0$ in the neighborhood of a singularity $\tau\to-\infty$. These conditions, which are similar to positive frequency conditions in the normal Klein-Gordon equations, clearly have consequences (as a result of the uncertainty relationship) for the localizability of the values of λ_0, which controls the circumference of the universe in the θ direction. A careful analysis of these equations would be more appropriately carried out in coordinates which diagonalized the supermetric such as

$$\begin{aligned}\alpha&=2^{-1/2}(\tau-\lambda),\\ \zeta&=2^{-1/2}(\tau+\lambda).\end{aligned} \tag{65}$$

In the neighborhood of the singularity where $\mathcal{R}\to 0$, Eqs. (50) and (51), of course, simply represent a Klein-Gordon equation for a free particle, and not only p_λ but also all other momenta are constant in the neighborhood of $\tau\to-\infty$. A more complete analysis of the asymptotic states near the singularity, and their interpretation in terms of uncertainty relations and classical analogs, is one of several questions which arise within this model which we must leave for future analysis.

VII. MECHANICAL ANALOG FOR PARTICLE CREATION AT THE INITIAL SINGULARITY

As a prototype of Eq. (57), let us consider the equation

$$i\frac{\partial\psi}{\partial t}=H\psi, \tag{66}$$

with

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\tfrac{1}{2}e^{4t}x^2. \tag{67}$$

In order to understand the solutions of this differential equation in physical terms, it is useful to think of it as describing a ping-pong ball or some other unit mass attached to an origin in a one-dimensional space by a massless spring whose spring constant increases exponentially with time. In the distant past, $t\to-\infty$, this ball moves freely with no force acting. It is therefore natural to think of an initial state which is a wave packet of rather well-defined momentum, the major component of which is a plane wave $\psi\propto e^{-iEt+ikx}$, with $E=\frac{1}{2}k^2$. At later times the spring becomes more important and its influence will dominate the state of the system. The strength of the spring may be characterized by a natural frequency $\omega=e^{2t}$. When this frequency changes slowly over a period, the description of the system is again simple as the ball must then find itself in a simple harmonic-oscillator eigenstate of fixed quantum number, or a time-independent linear combination of such simple quantum states. The condition for this adiabatic approximation to be valid is

$$d\ln\omega/\omega dt=2e^{-2t}\ll 1. \tag{68}$$

Evidently, this condition is always satisfied for sufficiently large t. This can be easily understood since the natural period of oscillation becomes arbitrarily small for large t while the time interval in which the period changes significantly is always constant and order of magnitude unity. In this adiabatic limit the wave function can be expressed in terms of eigenfunctions of the operator H which are defined by the equation

$$H\varphi_n=(N+\tfrac{1}{2})e^{2t}\varphi_N. \tag{69}$$

In terms of these excitation-level eigenfunctions, the asymptotic solution of Eq. (66) may be rewritten as

$$\begin{aligned}\psi_N&=\exp\left[-i(N+\tfrac{1}{2})\int_{-\infty}^{t}\omega dt\right]\varphi_N(x,t)\\ &=\exp[-\tfrac{1}{2}i(N+\tfrac{1}{2})e^{2t}]\,\varphi_N(x,t),\end{aligned} \tag{70}$$

where φ_N may be assumed normalized:

$$\int|\varphi_N(x,t)|^2dx=1. \tag{71}$$

For negative values of t, Eq. (70) does not provide an approximate solution of Eq. (66). If the system is prepared so as to have a configuration ϕ_N at some given early time $t\ll-1$, then the time development according to Eq. (66) immediately will generate large numbers of other states corresponding to different numbers N. In particular, if the initial state were $N=0$, larger values of N would rapidly be generated in a process which could be referred to as the creation of oscillator excitations. The analogous phenomena in Eq. (57) would be called graviton creation. Calculations showing the details of this process have been given by Berger[7] and in somewhat related models by Parker,[8] Zel'dovich,[9] and Zel'dovich and Starobinsky.[10] In the context of Eq. (67), it is clear that this sort of initial condition is an unnatural one. One would prefer to think of a simple free-particle state for the ball moving in the absence of forces before the spring tension builds up. Let us try to see how such a simple free-particle motion appears if it is described in the language of excitation quantum numbers N. Thus we imagine a state of fixed momentum k and energy E at early times $t \ll -1$. This state provides a solution of the wave equation (66) and it evidently must continue to be a good solution until such a time as the rising potential walls (due to the increasing strength of the harmonic-oscillator force) become high enough that the wave packet representing the position of the ball bounces against them. Prior to this point, the motion of the ball is essentially uninfluenced by the harmonic-oscillator potential, but it is easy to see that the description of the motion in terms of harmonic-oscillator excitation numbers N is nevertheless changing very rapidly. One has only to write

$$E = (N + \tfrac{1}{2})e^{2t}, \tag{72}$$

which must relate the energy of the ball and the dominant excitation mode N in its wave packet, to see that at early times where E is constant the excitation level N is dropping extremely rapidly:

$$N(t) + \tfrac{1}{2} \propto e^{-2t}. \tag{73}$$

The reason for this, of course, is that the spacing in energy between the adjacent excitation levels of the harmonic oscillator is just $\omega = e^{2t}$, which is negligibly small at early times. Therefore, every state of finite momentum has arbitrarily large excitation number N at early times. This is quite without physical significance, however, since the harmonic-oscillator force is negligibly weak and without effect, and a description of the simple free particle motion in terms of these eigenstates of a singularly weak harmonic oscillator becomes asymptotically irrelevant.

VIII. IN AND OUT STATES: QUANTUM SINGULARITY AND GRAVITON-FILLED UNIVERSE

Cosmology is a scattering problem in superspace. This lesson has been pointed out previously,[2,21] and the present model provides another example of it. The quantum singularity is described by the "in" states which are solutions of a Klein-Gordon equation analogous to Eq. (49) but involving the asymptotic super-Hamiltonian

$$\begin{aligned}\mathfrak{H}_{-\infty} &= -\frac{\partial^2}{\partial\lambda_0\partial\tau} - \sum_{-\infty}^{\infty}\frac{1}{2}\frac{\partial^2}{\partial q_n{}^2}\\ &= -\frac{1}{2}\left[-\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial\zeta^2} + \sum_{-\infty}^{\infty}\frac{\partial^2}{\partial q_n{}^2}\right].\end{aligned} \tag{74}$$

The factorization of Eq. (56) can of course be used and leads to asymptotic forms for the sub-Hamiltonians in which each reduces to just its kinetic-energy term. Note that for (unnormalized) plane-wave solutions of $\mathfrak{H}_{-\infty}$, $\Psi = 0$, of the form

$$\begin{aligned}\Psi &= \exp\left(i p_\lambda \lambda_0 + i p_* \tau + i\sum k_n q_n\right)\\ &= \exp\left(-i\Omega\alpha + i k_\zeta \zeta + i\sum k_n q_n\right),\end{aligned} \tag{75}$$

the probability flux from Eq. (63) is positive everywhere, provided that p_λ, or equivalently Ω, is positive. Therefore, for plane wave states of this sort, or for wave packets which closely resemble such a plane wave over large regions, this information shows that not only can the wave function not vanish asymptotically near the singularity, which is already guaranteed in the general case by the conserved normalization condition

$$\int j^\tau d\lambda \prod dq_n = 1,$$

but the probability density j^τ is itself positive, so that the evolution is taking place exclusively away from the singularity and every tube of flux containing nonzero probability, if traced toward the past, will lead inevitably to the singularity.

The description of the singularity in this model is based upon a split of the super-Hamiltonian into two parts:

$$\mathfrak{H} = \mathfrak{H}_{-\infty} - \tfrac{1}{2}\mathfrak{R}, \tag{76}$$

in which the asymptotic part $\mathfrak{H}_{-\infty}$ governs the singularity behavior and describes a quantization of the the velocity-dominated singularity in these models in a way which differs from the work of Liang[17] in the choice of factor ordering. This factor ordering choice, which will be discussed separately,[6] is crucial to the difference between our conclusions and those of Liang concerning the inevitability of the singularity in these model quantum theories.

The "in" states of our scattering problem are characterized by the Hamiltonian $\mathfrak{H}_{-\infty}$, which is just the free particle or kinetic energy term in $\mathfrak{H}$. For the characterization of the "out" states, which will describe the universe in its evolved form representing an expanding universe containing a population of gravitons, a quite different split is necessary so that another asymptotic part $\mathfrak{H}_{+\infty}$ can be separated out from $\mathfrak{H}$ to represent the exactly soluble problem characteristic of late times in this model. In order to define this asymptotic operator, it will be necessary to first define graviton annihilation and creation operators, and the corresponding operators for characterizing the number of gravitons in each mode. One arrives at these operators by considering a Fourier series expansion for the basic field variables β and p

which is somewhat different from Eq. (22); it reads

$$\beta=\sum_{n=-\infty}^{\infty}\frac{1}{(2\omega_n)^{1/2}}(a_n e^{in\theta}+a_n^\dagger e^{-in\theta}),$$
$$p=\sum_{n=-\infty}^{\infty}(\tfrac{1}{2}\omega_n)^{1/2}(-ia_n e^{in\theta}+ia_n^\dagger e^{-in\theta}). \tag{77}$$

In order to relate the operators a_n introduced here to the operators q_n and k_n used previously, it is convenient, as an intermediate step, to consider also the very standard Fourier expansions

$$\beta=\sum_{-\infty}^{\infty}\beta_n e^{in\theta},\quad p=\sum_{-\infty}^{\infty}p_n e^{in\theta}. \tag{78}$$

Although β and p, and also the q_n and k_n, are Hermitian operators, the operators β_n, p_n, and a_n are not. The Hermitian property of β and p imposes, however, the following conditions:

$$\beta_n=\beta_{-n}^\dagger,\quad p_n=p_{-n}^\dagger. \tag{79}$$

The equations relating these operators can then be written down. For positive n, they read

$$2^{-1/2}(q_n-iq_{-n})=(2\omega_n)^{-1/2}(a_n+a_{-n}^\dagger)$$
$$=\beta_n,$$
$$2^{-1/2}(k_n-ik_{-n})=(\tfrac{1}{2}\omega_n)^{1/2}(-ia_n+ia_{-n}^\dagger)$$
$$=p_n, \tag{80}$$

while the Hermitian conjugates of these equations serve to define β_{-n} and p_{-n}. As a consequence of the the commutation relations $[q_n,k_n]=i$, etc., introduced in Eq. (47) and (48), one finds the following commutation relations among β_n and p_n:

$$[\beta_n,p_n]=0,\quad[\beta_n,p_n^\dagger]=i,$$
$$[\beta_n,\beta_n^\dagger]=0=[p_n,p_n^\dagger]. \tag{81}$$

Of course, all operators referring to distinct values of $|n|$ commute with each other. Using these commutation relations, and the formula

$$a_n=(\tfrac{1}{2}\omega_n)^{1/2}\beta_n+i(2\omega_n)^{-1/2}p_n, \tag{82}$$

one easily computes the standard creation- and annihilation-operator commutation relations which hold for the a_n:

$$[a_n,a_n^\dagger]=1,$$
$$[a_n,a_{-n}]=0=[a_n,a_{-n}^\dagger]. \tag{83}$$

In terms of these operators, the super-Hamiltonian and sub-Hamiltonians can be rewritten as follows:

$$\mathfrak{H}=-\frac{\partial^2}{\partial\tau\partial\lambda_0}-\frac{1}{2}\frac{\partial^2}{\partial q_0{}^2}+\sum_{n=1}^{\infty}\omega_n(a_n^\dagger a_n+a_{-n}a_{-n}^\dagger), \tag{84}$$

$$\mathfrak{H}_n=p_n^\dagger p_n+\omega_n{}^2\beta_n^\dagger\beta_n$$
$$=\omega_n(a_n^\dagger a_n+a_{-n}a_{-n}^\dagger). \tag{85}$$

If we now turn to the solution of the separated Schrödinger-like Eqs. (57), the problem one faces in using Eq. (85) is the fact that the operators a_n do not commute with $\partial/\partial\tau$ because of the τ dependence of the frequency $\omega_n=|n|e^{2\tau}$ in Eq. (82). The commutator is easily evaluated from Eq. (82) and is

$$\left[i\frac{\partial}{\partial\tau},a_n\right]=ia_{-n}^\dagger. \tag{86}$$

As a consequence of these computation relations, it is convenient to introduce the operator

$$i\frac{D}{D\tau}=i\frac{\partial}{\partial\tau}+\sum_{n>0}i(a_n^\dagger a_{-n}^\dagger-a_{-n}a_n), \tag{87}$$

which, as can easily be seen, commutes with all the a_n and $a_n^\dagger$, and is therefore more convenient to use than $\partial/\partial\tau$. The operators as defined in Eq. (87) would be introduced into the super-Hamiltonian (84) and the corresponding full Klein-Gordon equation. A reduced form of the operator, which we will not distinguish notationally, containing only a single pair of terms corresponding to the appropriate value of $|n|$ would appear in the rewrite of the separated Eqs. (57) which follows:

$$i\frac{D\psi_n}{D\tau}=\tilde{\mathfrak{H}}_n\psi_n, \tag{88}$$

$$\tilde{\mathfrak{H}}_n\equiv p_\lambda{}^{-1}\omega_n(\tau)(a_n^\dagger a_n+a_{-n}a_{-n}^\dagger)+i(a_n^\dagger a_{-n}-a_{-n}a_n). \tag{89}$$

In terms of the annihilation and creation operators just introduced, it is easy to recognize the dominant terms in the residual constraint equation in the limit $\tau\to+\infty$. One evidently defines

$$\mathfrak{H}_{+\infty}=-\frac{D}{D\tau}\frac{\partial}{\partial\lambda_0}-\frac{1}{2}\frac{\partial^2}{\partial q_0{}^2}+\sum_1^\infty\omega_n(a_n^\dagger a_n+a_{-n}a_{-n}^\dagger) \tag{90}$$

by neglecting in Eq. (89) the second pair of terms which do not have the exponential increase with τ of the first pair, which is retained.

To solve the separated equation

$$i\frac{D\psi_n}{D\tau}=\mathfrak{H}_{n,+\infty}\psi_n, \tag{91}$$

where

$$\tilde{\mathfrak{H}}_{n,+\infty}=p_\lambda{}^{-1}\omega_n(a_n^\dagger a_n+a_{-n}a_{-n}^\dagger), \tag{92}$$

one introduces the eigenstates of fixed graviton number $\varphi(N_+,N_-)\equiv\varphi(N_{+n};q_{+n},q_{-n},\tau)$ which satisfy the eigenvalue equations

$$a_n^\dagger a_n \varphi = N_+\varphi, \quad a_{-n}^\dagger a_{-n}\varphi = N_-\varphi . \tag{93}$$

Since the number operators in these eigenvalue equations commute with $iD/D\tau$, these graviton-number eigenstates can also be assumed to be eigenstates of this operator $iD/D\tau$. Since in addition, the annihilation and creation operators which also commute with $iD/D\tau$ connect these various eigenstates, they must all belong to a single eigenvalue of $iD/D\tau$,

$$i\frac{D}{D\tau}\varphi(N_+, N_-) = f(\tau)\varphi(N_+, N_-) . \tag{94}$$

To verify this in detail, evaluate matrix elements of the commutator

$$\left[i\frac{D}{D\tau}, a_n\right] = 0$$

and assume the usual normalization s for the $\varphi(N_+, N_-)$ so that, for example,

$$a_n \varphi(N_+, N_-) = (N_+)^{1/2}\varphi(N_+ - 1, N_-) .$$

In order to evaluate $f(\tau)$ it is sufficient to consider only the ground state. We assume that all the number eigenstates φ are normalized to unity, and then one consequence of Eq. (94) is

$$\begin{aligned} f(\tau) &= \int dq_{+n}\, dq_{-n}\, \varphi^*(0,0) i\frac{D}{D\tau}\varphi(0,0) \\ &= \int dq_{+n}\, dq_{-n}\, \varphi(0,0) i\frac{\partial}{\partial\tau}\varphi(0,0) \\ &= 0 . \end{aligned} \tag{95}$$

The first equality in this formula is an immediate consequence of Eq. (94). To obtain the next line one notes that the additional term in Eq. (87) has no diagonal matrix element in this occupation-number representation. We have, in addition, used the fact that the ground states can be taken as real:

$$\varphi(0,0) = \left[\frac{\omega_n(\tau)}{\pi}\right]^{1/2} \exp[-\tfrac{1}{2}\omega_n(\tau)(q_n{}^2 + q_{-n}{}^2)] , \tag{96}$$

and then the final step appears as immediate consequence of the normalization condition

$$\int dq_{+n}\, dq_{-n}\, \varphi^2(0,0) = 1 .$$

We have therefore succeeded in constructing a set of basis vectors $\varphi(N_+, N_-)$ which are "covariantly constant" with respect to the operator $iD/D\tau$. Using this set of basis vectors, one then immediately obtains solutions of the asymptotic Eq. (91) in the form

$$\begin{aligned} \psi_n^{\text{out}}(N_+, N_-) &= \exp\left[-ip_\lambda{}^{-1}(N_+ + N_- + 1) \times \int_{-\infty}^{\tau} \omega_n\, d\tau\right]\varphi(N_+, N_-) \\ &= \exp\left[-i(N_+ + N_- + 1)|n|\frac{e^{2\tau}}{2p_\lambda}\right] \\ &\quad \times \varphi(N_+, N_-) . \end{aligned} \tag{97}$$

The global momentum constraint $\mathfrak{P} = 0$ can be represented in terms of the annihilation and creation operators. It reads

$$\mathfrak{P} = \sum_1^\infty n(a_n^\dagger a_n - a_{-n}^\dagger a_{-n}) . \tag{98}$$

Since the perturbation term

$$\tilde{\mathfrak{V}}_n = i(a_n^\dagger a_{-n}^\dagger - a_{-n} a_n), \tag{99}$$

only creates or annihilates graviton pairs with equal and opposite values of n, it is clear that this constraint is conserved under the perturbation as a consequence of the conservation of $N_+ - N_-$.

In order to reconstruct the metric from these asymptotic solutions of the residual constraint equations, it is necessary to also construct the metric component λ_+. By inserting the expansions (78) into formula (20) one finds readily that

$$\lambda_+ = \frac{-1}{p_\lambda}\sum_{m=-\infty}^{\infty}\sum_{n>m}\frac{np_m^\dagger\beta_n}{n-m}e^{i(n-m)\theta} + \text{H.c.}, \tag{100}$$

where H.c. means Hermitian conjugate. Then Eq. (80) can be used to write

$$p_m^\dagger \beta_n = \frac{1}{2}i\left|\frac{m}{n}\right|^{1/2}(a_m^\dagger a_{-n}^\dagger - a_{-m}a_n + a_m^\dagger a_n - a_{-m}a_{-n}^\dagger) . \tag{101}$$

The most important thing to note about this expression is that it contains no explicit τ dependence. It is thus of the same order of magnitude as $\tilde{\mathfrak{V}}_n$ in Eq. (99) which has been neglected in Eq. (88) in obtaining the asymptotic wave functions (97). Notice that β is even smaller asymptotically:

$$\beta = e^{-\tau}\sum_{-\infty}^{\infty}|2n|^{-1/2}a_n e^{in\theta} + \text{H.c.} \tag{102}$$

As a consequence, the metric (26) becomes asymptotically homogeneous (independent of θ) as τ approaches infinity. This is a result of the gravitational waves being red shifted to negligible amplitude, and does not imply that the distribution of the gravitational waves becomes homogeneous.

IX. SEMICLASSICAL SOLUTION OF THE SCATTERING PROBLEM

It should be possible to give quite complete quantum-mechanical solutions of the scattering problem we have posed—namely, to compute and discuss the S matrix defined by Eq. (50) relating incoming states of the form (75) to outgoing states of the form (97). We will here, however, only attempt a preliminary semiclassical analysis based on the exact classical solution (31). Since the residual constraint Eq. (50) separates, we can restrict our attention to a single mode. In doing this we shall omit all subscripts n whenever possible. Thus, the differential equation we study governs one of the two modes described in Eq. (57) and reads

$$ip_\lambda \frac{\partial\psi}{\partial\tau} = \mathfrak{H}_s\psi\,, \qquad (103)$$

where

$$\mathfrak{H}_s = -\frac{1}{2}\left(\frac{\partial}{\partial q}\right)^2 + \tfrac{1}{2}n^2 e^{4\tau}q^2$$
$$= |n|e^{2\tau}(b^\dagger b + \tfrac{1}{2})\,. \qquad (104)$$

The standing-wave annihilation and creation operators used here are defined by

$$b_n = e^\tau |\tfrac{1}{2}n|^{1/2} q_n + i\,e^{-\tau}|2n|^{-1/2}p_n\,, \qquad (105)$$

and also commute with the operator $D/D\tau$ [Eq. (87)], which can be rewritten as

$$i\frac{D}{D\tau} = i\frac{\partial}{\partial\tau} + \sum_{\substack{n=-\infty \\ n\neq\infty}}^{\infty} \tfrac{1}{2}i\,(b_n^\dagger b_n^\dagger - b_n b_n)\,. \qquad (106)$$

In the limit $\tau\to-\infty$, one finds conventional free-particle wave-packet solutions of Eq. (103). Let k^{in} be the central momentum in this wave packet, and let the (classical) motion of the center of the wave packet be written as

$$q = \frac{k^{\text{in}}}{p_\lambda}(\tau - \tau_c) + q_c\,; \qquad (107)$$

here q_c is a constant and τ_c is the critical τ value at which an adiabatic approximation begins to be valid:

$$\frac{1}{2}\left|\frac{n}{p_\lambda}\right| e^{2\tau_c} = 2e^{-\gamma}$$
$$= 1.12292\ldots\,. \qquad (108)$$

With these initial conditions the exact classical solution (31) is

$$q = q_c J_0\!\left(\frac{1}{2}\left|\frac{n}{p_\lambda}\right|e^{2\tau}\right) + \left(\frac{\pi}{4p_\lambda}\right)k^{\text{in}}\,Y_0\!\left(\frac{1}{2}\left|\frac{n}{p_\lambda}\right|e^{2\tau}\right)\,. \qquad (109)$$

One may then pass to the opposite asymptotic limit, $\tau\to+\infty$ and evaluate for this same classical solution the single-mode Hamiltonian as follows:

$$\mathfrak{H}_s = \tfrac{1}{2}(k^2 + \omega_n{}^2 q^2)$$
$$= \frac{2}{\pi}|p_\lambda|\,\omega_n\left[q_c{}^2 + \left(\frac{\pi}{4p_\lambda}\right)(k^{\text{in}})^2\right]. \qquad (110)$$

However, from the second form of Eq. (104), this may be interpreted in terms of the number of gravitons in this mode, $\mathfrak{H}_s = \omega_n(N+\tfrac{1}{2})$. In this way one arrives at a formula for the total number of gravitons in this mode in the asymptotic outgoing state:

$$N+\tfrac{1}{2} = \frac{1}{2}\left[\left|\frac{4p_\lambda}{\pi}\right| q_c{}^2 + \left|\frac{\pi}{4p_\lambda}\right|(k^{\text{in}})^2\right]. \qquad (111)$$

This relationship is consistent with quantum uncertainty relationships. Thus q and k are canonically conjugate variables restricted by uncertainty relationships which result from $k=-i\partial/\partial q$. The classical initial conditions k^{in} and q_c in Eq. (107) must be regarded as uncertain by amounts restricted by the conditions

$$\Delta q_c\,\Delta k^{\text{in}} \gtrsim \tfrac{1}{2}\,. \qquad (112)$$

If in Eq. (111) one sets $q_c = \Delta q_c$ and $k^{\text{in}} = \Delta k^{\text{in}}$ and minimizes subject to the condition (112), one finds the results $(N+\tfrac{1}{2})_{\min} = \tfrac{1}{2}$. The choices which achieve this minimum result are $2^{1/2}\Delta q_c = |\pi/4p_\lambda|^{1/2} = (2^{1/2}\Delta k^{\text{in}})^{-1}$.

Because spreading of the wave packet is inevitable as a consequence of Eq. (103), a final state with $N=0$ can only be achieved by a very carefully formed initial packet. Not only must the optimal spread in initial momentum k_n be used, but also the packet must be focused so as to achieve its minimum uncertainty in q precisely at the critical time appropriate to the mode in question:

$$\tau_c = -\tfrac{1}{2}(\gamma + \ln|n| - \ln|4p_\lambda|)\,. \qquad (113)$$

In order to display more clearly the dependence of the final state N upon this feature of the initial packet, it would be more appropriate to restate the initial conditions in the form

$$q = \frac{k^{\text{in}}}{p_\lambda}(\tau - \tau_0) + q^{\text{in}}\,,$$

where

$$\tau_0 = \tfrac{1}{2}\gamma - \ln 2 = -0.40454\ldots \qquad (114)$$

is a fiducial time chosen independently of n and p_λ. Then Eq. (111) could be rewritten, eliminating q_c as follows:

$$q_c = q^{\text{in}} - \frac{k^{\text{in}}}{2p_\lambda}\ln\left|\frac{n}{p_\lambda}\right|\,. \qquad (115)$$

There appear to be no particularly natural choices for the initial conditions q^{in} and k^{in}, or even for statistical ensembles of them. However, the present model may be too oversimplified, even in its most qualitative features, to be useful for the problem for characterizing quantum initial conditions. Thus the work of Belinski, Khalatnikov, and Lifshitz[22] shows that it is more reasonable to expect a mixmasterlike singularity behavior independently at each point on the initial surface, rather than the Kasner-like behavior displayed in this model. But the initial conditions for a mixmaster universe are rather simpler to control than those for a Kasner universe. The basis for this statement is the fact, established by Jacobs, Misner, and Zapolsky,[23] that the initial states are defined by an asymptotic Hamiltonian with discrete eigenvalues so that the S matrix is more an association of the form $N^{\text{in}} \rightarrow N_{\text{out}}$, rather than the more complicated form of Eq. (111) $(q^{\text{in}}, k^{\text{in}}) \rightarrow N^{\text{out}}$ in which there is no basis for restricting the values of q^{in}, even if one were willing to adopt an asymptotically stationary statistical distribution with $\rho_s \propto \exp(-c\mathfrak{H}_{s,-\infty})$ to define the initial states. The laws determining the initial conditions of the universe are obviously not understood, and current studies of quantum cosmology merely represent the beginnings of an attempt to recast the question in a new way in the hope that this might reveal new approaches to the formulation and resolution of the question.

---

*Supported in part by the National Science Foundation Grant No. GP-17673 at the University of Maryland, and Grant Nos. GP-36687X and GP-28027 at the California Institute of Technology.

†Guggenheim Fellow 1972–73 on sabbatical leave from the University of Maryland, College Park.

[1]R. H. Gowdy, Ann. Phys. (N.Y.) (to be published); Phys. Rev. Lett. 27, 826 (1971); 27, 1102 (1971).

[2]C. W. Misner, in *Magic Without Magic: John Archibald Wheeler*, edited by J. Klauder (Freeman, San Francisco, 1972), pp. 441–473.

[3]K. Kuchař, Phys. Rev. D 4, 955 (1971); see also K. Kuchař, in *Relativity, Astrophysics and Cosmology*, edited by W. Israel (Reidel, Dordrecht, 1973).

[4]R. Arnowitt, S. Deser, and C. W. Misner, in *Gravitation: An Introduction to Current Research*, edited by L. Witten (Wiley, New York, 1962), pp. 227–265.

[5]P. A. M. Dirac, Phys. Rev. 114, 924 (1959); see also B. S. DeWitt and C. J. Isham as cited in Ref. 18.

[6]C. W. Misner, lecture given at the Conference on Gravitation and Quantum Mechanics, Osgood Hill, Boston University, North Andover, Mass., November 1972 (unpublished).

[7]B. K. Berger, Ph.D. thesis, Center for Theoretical Physics, University of Maryland, College Park, 1972 (unpublished), see Diss. Abstr. 33, 5114-B (1973); B. K. Berger, Ann. Phys. (N. Y.) (to be published).

[8]L. Parker, Phys. Rev. 183, 1057 (1969); Phys. Rev. Lett. 28, 705 (1972); an early treatment is given by B. S. DeWitt, Phys. Rev. 90, 357 (1953).

[9]Ya. B. Zel'dovich, Comments Astrophys. Space Phys. 3, 179 (1971).

[10]Ya. B. Zel'dovich and A. A. Starobinsky, Zh. Eksp. Teor. Fiz. 61, 2161 (1971) [Sov. Phys.–JETP 34, 1159 (1972)].

[11]C. W. Misner, Phys. Rev. Lett. 22, 1071 (1969).

[12]A. G. Doroshkevich, V. N. Lukash, and I. D. Novikov, Zh. Eksp. Teor. Fiz. 60, 1201 (1971) [Sov. Phys.–JETP 33, 649 (1971)].

[13]D. Chitre, Phys. Rev. D 6, 3390 (1972).

[14]Ya. B. Zel'dovich, in *Magic Without Magic: John Archibald Wheeler*, edited by J. Klauder (Freeman, San Francisco, 1972), pp. 277–288.

[15]E. M. Lifshitz and I. M. Khalatnikov, Adv. Phys. 12, 185 (1963); more general (mixmaster type) singularities are described in Ref. 22.

[16]E. Eardley, E. Liang, and R. Sachs, J. Math. Phys. 13, 99 (1972).

[17]E. P. T. Liang, Phys. Rev. D 5, 2458 (1972).

[18]J. A. Wheeler, *Battelle Rencontres 1967: Lectures in Mathematics and Physics*, edited by C. DeWitt and J. A. Wheeler (Benjamin, New York, 1968), pp. 242–307; B. S. DeWitt, Phys. Rev. 160, 1113 (1967); U. Gerlach, *ibid.* 177, 1929 (1969); also see Ref. 2 and the review by C. J. Isham, Imperial College, London Report No. ICTP-72-8, 1972 (unpublished).

[19]B. K. Berger, Appendix C of thesis cited in Ref. 7.

[20]V. Moncrief, Phys. Rev. D 5, 277 (1972); for further aspects, see also V. Moncrief and C. Teitelboim, *ibid.* D 6, 966 (1972).

[21]L. Fishbone and C. W. Misner (unpublished), reported in M. P. Ryan, Jr., *Hamiltonian Cosmology* (Springer, Berlin, 1972), and in Ref. 2.

[22]V. A. Belinski, I. M. Khalatnikov, and E. M. Lifshitz, Usp. Fiz. Nauk. 102, 463 (1970) [Adv. Phys. 19, 525 (1970)].

[23]K. Jacobs, C. W. Misner, and H. S. Zapolsky (unpublished), reported in part by C. W. Misner, in *Relativity*, edited by M. Carmeli, S. K. Fickler, and L. Witten (Plenum, New York, 1970), pp. 55–79. and in Ref. 2.