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Quantization of a Friedmann universe filled with a scalar field

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The problem of quantizing a Robertson-Walker metric with a scalar field as source is discussed within the framework of a true canonical theory. A discussion is given of the role played by different choices of time.

I. INTRODUCTION

A number of approaches to the problem of quantizing the gravitational field have appeared in the last 40 years.[1,2] That this should be so is hardly surprising, bearing in mind the great complexity of the subject—from both the technical and conceptual points of view—and the very different backgrounds of various workers in this field. One of the most interesting approaches is surely that of so-called quantum models or quantum cosmology. This approach was inaugurated by DeWitt[3] and then followed up by Misner[4] and his collaborators and by many other people in the last few years.[5] The basic idea is to freeze out all but a finite number of degrees of freedom of the system and then quantize the remaining ones. The significance of this approach lies in two different directions. On the one hand, by restricting the system to one of a finite number of degrees of freedom attention can be focused on the problems of quantum gravity which are peculiar to the gravitational field rather than on those which are common to any quantum field theory. In particular the phenomenon of gravitational collapse and the influence upon it of quantum effects can be sensibly discussed in this framework, as indeed can a whole range of conceptual and technical problems concerning the choice of time, the interpretation of state vectors and probability, the choice of canonical variables, etc. On the other hand, one can regard this approach as an actual perturbation scheme in which the perturbation is not in terms of any coupling constants (as it usually is in the Feynman-diagram-oriented "covariant" quantization schemes), but rather in terms of the number of modes quantized. From this point of view one would naturally ask if the models with finite numbers of degrees of freedom can ever realistically describe true physical systems (so that the answers can be believed as genuine approximations), and, more theoretically, if the limit as this number is taken to infinity actually exists. This latter question will inevitably reintroduce the usual problems of quantum field theories such as, for example, the existence of unitarily inequivalent representations of the canonical commutation relations and ultraviolet divergences.

Most of the work which has been done in the past has been concerned either with empty universes or with ones where matter is made up of the usual standby of general relativity—dust and perfect fluids. However, it seems to us that from a physical point of view this is unrealistic. Actual matter is itself quantized and the characteristic lengths of such matter, for example, 10^{-13} cm for hadrons, are many orders of magnitude higher than the characteristic Planck length (10^{-33} cm) of pure quantum gravity. In particular if one is interested in the problem of the gravitational collapse of matter then it seems very reasonable to attempt to describe the matter quantum mechanically, and the easiest way of doing this is to use a quantum field for it. Thus we discuss in this paper the problem of a scalar matter field coupled to a Robertson-Walker metric in which both are quantized in the quantum-model sense. Initially a massive scalar field was considered as we were partly motivated by the remarkable results of Parker and Fulling[6] who showed that if such a system was quantized in the semiclassical sense of choosing the expectation value of the energy-momentum tensor of the quantized matter as the source of the classical gravitational field, then the system did not collapse, but rather had a minimum radius of of the Compton wavelength of the particles described by the scalar fields. There are a number of problems which arise in their work, some of which are related to the use of an infinite number of degrees of freedom, and we hoped to circumscribe these by using the quantum-model approach. However, we found that a number of interesting problems arise even in the (technically) simpler massless case, and so most of the work reported in this paper is concerned with that situation. The massive case will be discussed elsewhere. In particular the difficulties which arise from the occurrence in these types of models of a square-root, time-dependent Hamiltonian are frequently treated in a way which seems to us a little dubious.

The usual resolution of the square-root problem is to use a Klein-Gordon equation instead of a Schrödinger equation. However, these are *not* equivalent at all in the case where the Hamiltonian is time-dependent, and we prefer to use the original Schrödinger equation and define the square root via the spectral theorem. This means of course that we must first show that the quantity H^2 really is a positive self-adjoint operator, but this is fairly easy in the present model. Our approach has the advantage that the state vectors belong to a genuine Hilbert space, whereas in the Klein-Gordon-oriented approach a nonpositive inner product tends to occur bringing with it a number of difficulties. The only previous work[7] (to our knowledge) on the combined Robertson-Walker scalar-field system uses the Klein-Gordon superspace approach, so our work can be regarded as complementary to that. Perhaps one should also observe that the present two-mode system can, by a series of canonical transformations, be made to look like almost any other two-mode system and in particular (in the massless case) to some purely gravitational ones.[8] However, quantum mechanics frequently does not respect canonical transformations and so the significance of such relations should not be overstated.

The model we discuss is clearly related to that in the original work by DeWitt on the Friedmann universe. In his case he was forced to introduce a cloud of "clocks" in order to support a Robertson-Walker metric. His discussion of the correlation between various choices of time is mirrored in our work by the possibility of choosing the matter field itself, or some function of it, as the time for the system.

II. THE CLASSICAL THEORY

The geometries of interest are those provided by the usual homogeneous and isotropic Robertson-Walker metrics

$$ds^2 = N(t)^2 dt^2 - R(t)^2 \mathcal{S}_{ij} dx^i dx^j, \tag{2.1}$$

where $\mathcal{S}_{ij}$ is the metric for a three-space of constant curvature K. The case $K=1$ is that of a three-sphere, while $K=0$ and $K=-1$ correspond to the flat and hyperbolic cases, respectively. Such a space-time leads to a nonvanishing Einstein tensor $G_{\mu\nu}$ and therefore requires a source of matter. In our case we use a massive scalar field described by the Lagrangian

$$\mathcal{L} = \tfrac{1}{2}(-\det g)^{1/2}(g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - m^2\phi^2), \tag{2.2}$$

in which ϕ is the scalar field and $g_{\mu\nu}$ is the metric in Eq. (2.1) and the corresponding energy-momentum tensor is

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \tfrac{1}{2}g_{\mu\nu}(g^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi - m^2\phi^2). \tag{2.3}$$

As might be expected the homogeneous Friedmann models can only be filled by a homogeneous scalar field. That is, we must take $\phi = \phi(t)$ (with no dependence on the spatial coordinates) in order to maintain the Robertson-Walker form of the metric. Thus in effect all but one mode of the scalar field drop out leaving us with just the three coupled variables $N(t)$, $R(t)$, and $\phi(t)$. The resulting equations of motion (in units in which the velocity of light c and the Newtonian constant G are related by $8\pi G/c^4 = \frac{1}{2}$) are as follows: The "G_{00} equation" is

$$3\frac{\dot{R}^2}{R^2} + \frac{3KN^2}{R^2} = \tfrac{1}{4}(\dot{\phi}^2 + m^2N^2\phi^2), \tag{2.4}$$

and the "G_{ij} equation" is (after dropping an overall factor $\mathcal{S}_{ij}$)

$$\frac{2\ddot{R}}{R} + \frac{\dot{R}^2}{R^2} - 2\frac{\dot{R}}{R}\frac{\dot{N}}{N} + \frac{KN^2}{R^2} = \tfrac{1}{4}(-\dot{\phi}^2 + m^2N^2\phi^2), \tag{2.5}$$

in which $\dot{R} \equiv dR/dt$, $\dot{\phi} \equiv d\phi/dt$, and $\ddot{R} \equiv d^2R/dt^2$. The "Klein-Gordon" equation for the scalar field is

$$\frac{d}{dt}\frac{(R^3\dot{\phi})}{N} + m^2(NR^3\phi) = 0, \tag{2.6}$$

which can also, by virtue of the Bianchi identities, be derived from Eqs. (2.4) and (2.5) by differentiation.

The equations above are of course underdetermined, and before they can be solved classically a choice of time must be made. This can be done in any of the usual ways within the context of these second-order equations.

As an example consider the case when the time variable is provided implicitly by the choice $N=R$. In order to simplify the calculations we will also consider the case $m=0$. This has the big advantage that the Klein-Gordon equation immediately leads to $R^3\dot{\phi}/N$ as a constant of the motion. Then Eqs. (2.4) and (2.5) can be solved readily to give (in the case $K>0$)

$$R^2(t) = R_m^2 \sin(2\sqrt{K}\,t + \delta), \tag{2.7}$$

$$\phi(t) = \phi_0 + \sqrt{3}\ln[\tan(\sqrt{K}\,t + \tfrac{1}{2}\delta)], \tag{2.8}$$

where δ, R_m, and ϕ_0 are constants. This shows clearly that in the positive-curvature case ($K>0$) the system has a maximum radius of expansion R_m and also experiences gravitational collapse. The solution for $K \leqslant 0$ can similarly be obtained from Eqs. (2.4) and (2.5) and exhibits the same gravitational-collapse phenomenon, although of course there is no longer a maximum value for the radius parameter. The parameter δ is merely an additive constant in the definition of time and can for convenience be set equal to zero. The values of $\phi - \phi_0$ range from $-\infty$ to $+\infty$, for example,

$t=0$ corresponds to $\phi - \phi_0 = -\infty$,

$t=\frac{\pi}{4\sqrt{K}}$ corresponds to $\phi - \phi_0 = 0$,

$t=\frac{\pi}{2\sqrt{K}}$ corresponds to $\phi - \phi_0 = +\infty$,

and in particular one notices that $\phi - \phi_0$ changes sign at the point of maximum expansion.

The parameter t can be eliminated from these equations to give

$$\phi(R) - \phi_0 = \mp\sqrt{3}\,\ln\frac{R_m^2 + (R_m^4 - R^4)^{1/2}}{R_m^2 - (R_m^4 - R^4)^{1/2}}\,, \tag{2.9}$$

or equivalently

$$R(\phi) = \frac{R_m}{\{\cosh[(\phi-\phi_0)/2\sqrt{3}\,]\}^{1/2}}\,. \tag{2.10}$$

For future reference we note that the corresponding flat-space ($K=0$) equations are

$$R(\phi) = R_0 e^{\pm(\phi-\phi_0)/2\sqrt{3}}. \tag{2.11}$$

These equations [in which the expansion or contraction phases are described by the minus and plus signs respectively in Eq. (2.9)] describe the intrinsic dynamics of the system expressed as a correlation between ϕ and R and are of course independent of the choice of time.

As we are interested ultimately in canonical quantization, it is worthwhile pursuing any further discussion of the choice of time within the framework of a first-order canonical scheme. The aim is to construct a set of genuine canonical variables whose first-order equations of motion (derived from the appropriate Hamiltonian) are equivalent to Eqs. (2.4)–(2.6). However, the latter equations are not *all* genuine dynamical equations since they contain variables which will at some stage be eliminated by making a choice of time. One possible solution to this problem is, implicitly or explicitly to fix the parameter representing time, to eliminate the redundant variables from Eqs. (2.4)–(2.6) and then convert the remaining true dynamical equations to canonical form. Alternatively it is possible to write Eqs. (2.4)–(2.6) directly in first-order form by introducing "canonical" moments π_ϕ, π_R, and π_N which are conjugates to ϕ, R, and N. However, the covariance of the equations of motion manifests itself by the G_{00} equation (2.4) appearing purely as a constraint amongst these variables and by the necessity of imposing as an additional constraint $\pi_N=0$. It is the existence of these constraint equations which provides the main obstacle to quantization. Another approach is the one which was developed from the work of Dirac[9] by Arnowitt, Deser, and Misner.[10,11] In this scheme the G_{00} constraint is still present, but the $\pi_N=0$ constraint is, in effect, replaced by the statement that the N variable is simply a Lagrange multiplier. Their technique can readily be used here (adapted to include the matter field), and we simply state the result that the system of equations above can be derived from the first-order Lagrangian

$$\mathcal{L}(t) = \pi_R\dot{R} + \pi_\phi\dot{\phi} + N\left(\frac{\pi_R^2}{24R} + 6KR - R^3\phi^2\frac{m^2}{2} - \frac{\pi_\phi^2}{2R^3}\right), \tag{2.12}$$

in which π_R, R, π_ϕ, ϕ, and N are all to be varied independently. This Lagrangian is in fact just the usual one for general relativity with the matter Lagrangian equation (2.2) added on and the form of the metric given by Eq. (2.1) substituted. We have checked explicitly that the resulting equations are indeed precisely Eqs. (2.4), (2.5), and (2.6)—a step that is necessary as one cannot always guarantee that a reduced action principle of this type will reproduce the original equations of motion. Note that we have removed an overall factor of the spatial integral of $(\det\mathcal{S})^{1/2}$ in Eq. (2.12).

This Lagrangian demonstrates clearly the role played by N as a Lagrange multiplier. Furthermore the constraint equation obtained by varying N is precisely the G_{00} equation (2.4). The main virtue of introducing this Lagrangian is that it enables us quickly to reduce the system to a true canonical form after any concrete choice of time has been made.

If we were interested in superspace quantization techniques then the expression in the large parentheses in Eq. (2.12) would be regarded as the super-Hamiltonian H, and we would probably quantize by making the substitution $\pi_R \to -i\hbar\partial/\partial R$, $\pi_\phi \to -i\hbar\partial/\partial\phi$ and then imposing the classical G_{00} equation $H=0$ (which follows from varying N) in the form $\hat{H}\psi=0$ of an operator constraint on the allowed state vectors.

However, in this paper we are concerned with genuine canonical quantization in which the system is reduced to true canonical form *before* quantizing. Thus we must solve the constraint equation $H=0$ classically, make a choice of time and substitute the results in $\mathcal{L}$. These two steps are not independent. In fact in order to guarantee that the final Lagrangian is in a canonical form the correct variable for which to solve the constraint equation is the momentum that is conjugate to the time chosen in the second step. For example, if we chose $t=R$ which is the simplest "intrinsic" time (i.e., time expressed in terms of the intrinsic geometry) we must solve the constraint equation

$$\frac{\pi_R^{\,2}}{24R}+6KR-R^3\phi^2\frac{m^2}{2}-\frac{\pi_\phi^{\,2}}{2R^3}=0 \tag{2.13}$$

for π_R to get for the final Lagrangian

$$\mathcal{L}=\pi_\phi\dot{\phi}\pm(24t)^{1/2}\left(-6Kt+t^3\phi^2\frac{m^2}{2}+\frac{\pi_\phi^{\,2}}{2t^3}\right)^{1/2}, \tag{2.14}$$

which shows that the (positive) Hamiltonian is

$$H=(24t)^{1/2}\left(-6Kt+t^3\phi^2\frac{m^2}{2}+\frac{\pi_\phi^{\,2}}{2t^3}\right)^{1/2}. \tag{2.15}$$

Clearly $t=R$ is only appropriate for an expanding (with respect to local proper time) system. The negative square root would correspond to the contracting phase. In practice one needs to redefine the time at the point of maximum R (if there is one) in order to keep a positive Hamiltonian. There are various other possible times of interest, but discussion of them will be deferred until the next section on quantization.

III. QUANTIZATION OF THE MODEL

As mentioned already we are concerned in this paper with the approach to quantization which is based on a reduction of the equations of motion to true canonical form. Thus our Hilbert space of states will be square-integrable functions defined on the classical configuration space with the usual L^2 inner product. Canonical commutation relations will be imposed on the canonical variables and an irreducible representation of these by self-adjoint operators defined on the L^2 space must be constructed. The quantum Hamiltonian operator is then to be built up from these canonical operators and the time-dependent Schrödinger equation solved for states of interest.

There are, however, a number of subtleties which may arise in the implementation of this program for a given choice of time (and hence Hamiltonian). A major problem is that the Hamiltonian which arises is typically of a square-root form and is in addition time-dependent. This is well illustrated by the example in Eq. (2.15). This problem is sometimes dubiously treated in the existing literature and so we wish to discuss it a little further here. The time-dependent Schrödinger equation, with configuration variable and conjugate momentum written as x and p, is

$$H(t,\hat{x},\hat{p})\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t}(x,t), \tag{3.1}$$

in which the time t is merely a label (*not* an operator) in both the Hamiltonian and the state function. Because of the square-root form of H, it is very tempting to use a Klein-Gordon equation instead, namely (dropping the x,p in H for convenience)

$$H^2(t)\psi(x,t)=-\hbar^2\frac{\partial^2\psi}{\partial t^2}. \tag{3.2}$$

This indeed is frequently done in work on quantum-cosmology models, but we wish to emphasize that, in the case when H depends explicitly on time, Eq. (3.2) does *not* follow from Eq. (3.1). In fact operating with H on both sides of Eq. (3.1) leads to

$$H^2(t)\psi(x,t)=-\hbar^2\frac{\partial^2\psi}{\partial t^2}-i\hbar\frac{\partial H}{\partial t}\psi(x,t), \tag{3.3}$$

which of course by virtue of the extra term on the right-hand side still contains the awkward square root. [Note that Eq. (3.1) does *not* say that H acting on *any* function of the two variables (x,t) is $i\hbar(\partial/\partial t)$. This would of course lead to Eq. (3.2) but in fact is incorrect. It is only really an operator on functions of the single variable x, and Eq. (3.1) just gives the time evolution of an actual allowed state vector.] To be fair, since the axioms of quantum mechanics applied to cosmological systems of this type may well be different from the conventional ones, one cannot really object if Eq. (3.2) is *postulated* from the outset. This equation is in fact the same as one would get from a superspace quantization approach, although whether this is to be regarded as a point for or against it is unclear. In any event we prefer in this paper to deal with the true time-dependent Schrödinger equation (3.1) complete with its square-root Hamiltonian. This has the big advantage that we are not plagued by the difficulties which arise from the nonpositive definiteness of the scalar product which is usually associated with a Klein-Gordon type of equation.

The square root itself can be correctly defined using the spectral theorem, provided that the operator whose square root is being constructed is a genuine positive, self-adjoint operator on the Hilbert space.

However, the integration of Eq. (3.1) needs to be discussed properly. The equation

$$\psi(x,t)=\left[\exp\left(-\frac{i}{\hbar}H(t-t_0)\right)\right]\psi(x,t_0)$$

is not correct for a time-dependent Hamiltonian. The correct form is

$$\psi(x,t)=T\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}H(s)\,ds\right)\right]\psi(x,t_0), \tag{3.4}$$

where T is the Dyson time-ordering symbol.

If the Hamiltonians at different times commute so that

$$[H(s),H(s')]=0 \tag{3.5}$$

then the time-ordering operation can be dropped and we have simply

$$\psi(x,t)=\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}H(s)\,ds\right)\right]\psi(x,t_0). \tag{3.6}$$

There is another important consequence of Eq. (3.5), namely that it is possible to find a complete set of basis states which are simultaneous eigenstates of the energy at all times. Thus if, say, $\psi_E(x)$ is such an eigenstate of $H(t_0)$ at some reference time t_0 so that

$$H(t_0)\psi_E(x)=E\psi_E(x), \tag{3.7}$$

there will exist numbers $E(t)$ [with $E(t_0)=E$] such that

$$H(t)\psi_E(x)=E(t)\psi_E(x). \tag{3.8}$$

Thus the time evolution of such a state is given simply via Eq. (3.6) as

$$\psi_E(x,t)=\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}E(s)\,ds\right)\right]\psi_E(x,t_0), \tag{3.9}$$

which, combined with the expansion of any state vector in terms of such eigenstates at $t=t_0$, gives a complete solution of the time-evolution problem.

On the other hand, if the Hamiltonians do *not* commute at different times then in general there will be no $E(t)$ such that Eq. (3.8) holds and the problem becomes much more complicated.

Let us now see how all this works for various choices of time. Let us take first the example considered in Sec. II with $t=R$. Then classically

$$H=\sqrt{24}\left(-6Kt^2+t^4\phi^2\frac{m^2}{2}+\frac{\pi_\phi^2}{2t^2}\right)^{1/2}. \tag{3.10}$$

The obvious Hilbert space for quantization is $L^2(-\infty,\infty)$ with the assignments

$$(\hat{\phi}\psi)(\phi)=\phi\psi(\phi), \tag{3.11}$$

$$(\hat{\pi}_\phi\psi)(\phi)=-i\hbar\frac{d\psi}{d\phi}(\phi), \tag{3.12}$$

which of course lead to genuine self-adjoint operators.

It is clear from the form of Eq. (3.10) that the quantity in the parentheses will only be a positive operator for all t if $K\leq 0$. Thus only in the hyperbolic or flat Friedmann cases is this choice of time immediately appropriate, although for nonzero mass and suitable ranges of t it can also be used with $K>0$. However, it is also clear from (3.10) that for nonzero mass $[H(s),H(s')]\neq 0$ and so this leads to the complicated time-evolution problem outlined above. For this reason we will set $m=0$ at this stage and will only return briefly to the massive case at the end of the paper. Since classically the system with $K\leq 0$ does not experience a turn-around there is no real problem with the two choices of sign in front of the square root.

Since Eq. (3.5) now holds we can use the time-evolution technique given by Eqs. (3.6) and (3.9) (for $K\leq 0$), provided that we can solve the energy eigenvalue equation (3.7):

$$\hat{H}(t_0)\psi_E(\phi)=E\psi_E(\phi).$$

We *can* eliminate the square root in this equation by using the form

$$H^2(t_0)\psi_E(\phi)=E^2\psi_E(\phi) \tag{3.13}$$

or

$$\frac{d^2\psi_E}{d\phi^2}+\frac{t_0^2}{12\hbar^2}(E^2+144t_0^2K)\psi_E(\phi)=0, \tag{3.14}$$

which can be readily solved.

In fact it is easy to see that $H^2(t)$ is a self-adjoint operator on $L^2(-\infty,\infty)$ with a purely continuous spectrum (when $m=0$) of $(-144t^2K,\infty)$, which for $K\leq 0$ is positive-definite as required. Clearly the generalized eigenfunctions $\psi_E(\phi)$ are

$$\psi_E(\phi)=ae^{i\lambda\phi}+be^{-i\lambda\phi}, \tag{3.15}$$

with

$$\lambda^2=\frac{t_0^2}{12\hbar^2}(E^2+144t_0^2K)\geq 0. \tag{3.16}$$

These eigenfunctions are also eigenfunctions of $H(t)$ with eigenvalue $E(t)$ given by

$$t^2E^2(t)=t_0^2E^2-144K(t^4-t_0^4), \tag{3.17}$$

and according to Eq. (3.9) have the time evolution

$$\begin{aligned}\psi_E(\phi,t)&=\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}E(s)\,ds\right)\right]\psi_E(\phi,t_0)\\&=\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\frac{1}{s}\left[t_0^2(E^2+144Kt_0^2)-144Ks^4\right]^{1/2}ds\right)\right]\psi_E(\phi,t_0)\\&=\left\{\exp\left[-\frac{i}{\hbar}\left(\tfrac{1}{2}[tE(t)-t_0E]\right.\right.\right.\\&\qquad\left.\left.\left.+\tfrac{1}{4}t_0(E^2+144Kt_0^2)^{1/2}\ln\frac{[tE(t)-t_0(E^2+144Kt_0^2)^{1/2}][E+(E^2+144Kt_0^2)^{1/2}]}{[tE(t)+t_0(E^2+144Kt_0^2)^{1/2}][E-(E^2+144Kt_0^2)^{1/2}]}\right)\right]\right\}\psi_E(\phi,t_0).\end{aligned} \tag{3.18}$$

Note that we could easily use Misner's exponential time $\Omega \equiv -\ln R$ which ranges between $(-\infty, \infty)$ rather than the $(0, \infty)$ range of R. This is advantageous in superspace-oriented approaches in which Ω is an actual self-adjoint operator, but in our case, when it is merely a parameter, there is no great virtue in this.

Another definition of time which is conjugate to the one above is $t = \pi_R$. This is the simplest example of an extrinsic time (i.e., one which is *not* expressed in terms of the intrinsic geometry). This time variable has the advantage of covering smoothly the point of maximum expansion (when $K>0$). Indeed $\pi_R \in (-\infty, 0)$ is the expansion phase and $\pi_R \in (0, \infty)$ is the contraction phase. The sign of the Hamiltonian (which is now simply R) is always positive. The constraint equation (2.13) must now be solved (as a quartic equation) for R leading to

$$H^2 = \frac{-\frac{1}{12}t^2 \pm (\frac{1}{144}t^4 + 48K\pi_\phi^2)^{1/2}}{24K}. \tag{3.19}$$

This is evidently most appropriate for the positive-curvature ($K>0$) case, and on choosing the plus sign leads to a positive self-adjoint operator with the same assignments for $\hat{\phi}$ and $\hat{\pi}_\phi$ as in Eqs. (3.11) and (3.12). Once again the Hamiltonians commute at different times and we can proceed essentially as before.

Thus we consider

$$H^2(t_0)\psi_E(\phi) = E^2\psi_E(\phi), \tag{3.20}$$

which gives

$$\left(H^2(t_0) + \frac{t_0^2}{288K}\right)^2 \psi_E = \left(E^2 + \frac{t_0^2}{288K}\right)^2 \psi_E = \frac{1}{576K^2}\left(\tfrac{1}{144}t_0^4 + 48K\pi_\phi^2\right)\psi_E \tag{3.21}$$

or

$$\frac{d^2\psi_E}{d\phi^2} + \frac{E^2}{12\hbar^2}(t_0^2 + 144E^2K)\psi_E = 0. \tag{3.22}$$

The spectrum of H^2 is purely continuous in $(0, \infty)$, and the eigenfunctions ψ_E are of the form

$$\psi_E(\phi) = ae^{i\lambda\phi} + be^{-i\lambda\phi}, \tag{3.23}$$

with

$$\lambda^2 = \frac{E^2}{12\hbar^2}(t_0^2 + 144E^2K) \geq 0. \tag{3.24}$$

As might be expected from the "conjugate" nature of the two choices of time, Eqs. (3.22), (3.24) and (3.14), (3.16) can be obtained from each other by interchanging E and t_0. In particular Eqs. (3.17) and (3.18) extend to the present case with these substitutions.

The two types of time discussed so far (intrinsic and extrinsic) have been used in the past by various authors studying the quantization of matter free cosmologies. A third type of time which has been discussed in other models is the "York" time, which is a very natural choice if the structure of the initial value equations is considered. The resulting Hamiltonian is rather complicated, and we prefer to defer discussion of this choice of time until a later date.[12] However, there is another type of time which naturally arises in the present model and that is one which is expressed in terms of the matter field itself. The obvious choice is $t = \phi$ which leads to the Hamiltonian

$$H^2 = (\tfrac{1}{12}R^2\pi_R^2 + 12KR^4 - R^6t^2m^2), \tag{3.25}$$

which has the virtue in the massless case of being time-independent. In general this time has the advantage (like π_R) of covering both the expansion and collapse phases. The classical range of R is $(0, \infty)$ and so we would use $L^2(0, \infty)$ as the Hilbert space in the quantum theory. However, care is required at this point as the usual assignments

$$R \to R, \quad \pi_R \to -i\hbar\frac{d}{dR} \tag{3.26}$$

will not work since the second one leads to a non-self-adjoint operator. More precisely the symmetric operator $-id/dR$ when defined on an appropriate domain (such as C^∞ functions vanishing at the end points) has no self-adjoint extensions.

One way out would be to use an $L^2(-\infty, \infty)$ space and interpret the negative values of R in an appropriate fashion. This would be related to the notion of extended superspace as advocated, for example, by DeWitt.[13]

However, the problem (which can arise even in ordinary quantum mechanics in a semi-infinite potential well) can be solved in a more direct way without changing the Hilbert space. The crucial observation is that the substitutions in Eq. (3.26) may lead to a self-adjoint form for the differential operator H^2 even if they are not in themselves self-adjoint. The momentum observable π_R can then be *defined* as a true self-adjoint operator *in terms* of H^2. To be more precise one can prove that $\hat{O} \equiv -(d/dR)R^2 d/dR$ is a positive self-adjoint operator (on an appropriate domain) in $L^2(0, \infty)$ and then define $\hat{\pi}_R$ as

$$\hat{\pi}_R \equiv \frac{1}{R}\sqrt{\hat{O}}. \tag{3.27}$$

For $K>0$, H^2 defined in this way is a positive self-adjoint operator whose positive square-root H therefore exists. In writing

$$H^2=-\frac{\hbar^2}{12}\frac{d}{dR}R^2\frac{d}{dR}+12KR^4 \tag{3.28}$$

a definite choice of factor ordering has been made. Other choices are of course possible, but the obvious ones, apart from shifting the spectrum of H around a little [for example, the choice $R^\nu(d/dR)R^{2-2\nu}(d/dR)R^\nu$ adds $\hbar^2\nu(\nu-1)$ to H^2], do not seem to affect anything very much so we will not consider that particular problem further.

The energy eigenfunction equation

$$H^2\psi_E(R)=E^2\psi_E(R) \tag{3.29}$$

becomes

$$\frac{d^2\psi_E}{dR^2}+\frac{2}{R}\frac{d\psi_E}{dR}+\frac{12}{\hbar^2}\left(\frac{E^2}{R^2}-12KR^2\right)\psi_E=0, \tag{3.30}$$

which has the general solution ($K>0$)

$$\psi_E(R)=\left[\exp\left(-\frac{6(KR^2)^{1/2}}{\hbar}\right)\right]R^{-1/2}\left[AR^{-(1-48E^2/\hbar^2)^{1/2}/2}F\left(\frac{1}{2}-\frac{1}{2}\left(1-\frac{48E^2}{\hbar^2}\right)^{1/2}\middle|1-\left(1-\frac{48E^2}{\hbar^2}\right)^{1/2}\middle|\frac{12\sqrt{K}}{\hbar}R^2\right)\right.$$
$$\left.+BR^{(1-48E^2/\hbar^2)^{1/2}/2}F\left(\frac{1}{2}+\frac{1}{2}\left(1-\frac{48E^2}{\hbar^2}\right)^{1/2}\middle|1+\left(1-\frac{48E^2}{\hbar^2}\right)^{1/2}\middle|\frac{12\sqrt{K}}{\hbar}R^2\right)\right], \tag{3.31}$$

where A and B are arbitrary constants and $F(\ |\ |\ )$ is the confluent hypergeometric function. A careful examination of the spectral properties of H^2 shows that the spectrum is purely continuous and occupies the interval $(\frac{1}{48}\hbar^2,\infty)$. This enables one to rewrite Eq. (3.31) in terms of Bessel functions of purely imaginary order by using the relation

$$I_\nu(x)=\frac{1}{\Gamma(\nu+1)}(\tfrac{1}{2}x)^\nu e^{-x}F(\tfrac{1}{2}+\nu|1+2\nu|2x). \tag{3.32}$$

Note that for small R (that is, near the point $R=0$ which classically corresponds to the singularity) the eigenfunctions behave as

$$\psi_E(R)\sim R^{-1/2}(AR^{-i\mu}+BR^{i\mu}), \tag{3.33}$$

where

$$\mu=\frac{1}{2}\left(\frac{48E^2}{\hbar^2}-1\right)^{1/2}\geqslant 0. \tag{3.34}$$

This shows that it is impossible to impose boundary conditions of the form $\psi_E(0)=0$ as suggested by DeWitt in his model, at least on these eigenstates.

This is a good stage at which to discuss the investigation of the effect of quantization on the gravitational collapse exhibited classically by the present model. The first question is: Given that the system is in some state $\psi(R)$, what do we mean by saying that a measurement leads to the singular (collapsed) geometry? In the present case since we have a genuine Hilbert space, $|\psi(R)|^2$ can certainly be interpreted as a probability density, so that

$$P_\epsilon\equiv\int_0^\epsilon|\psi(R)|^2dR \tag{3.35}$$

is the probability that if a measurement of R is made it will lie in the interval $[0,\epsilon]$. It is frequently asserted that the condition $\psi(0)=0$ leads to the absence of a singularity, but this clearly is an incorrect interpretation in the case when R has a purely continuous spectrum as it does in the model above and indeed in most of the models which other authors have considered. What is important presumably is rather the manner in which $P_\epsilon\to 0$ as $\epsilon\to 0$. Evidently the vanishing of ψ at $R=0$ will tend to increase the "rate" at which P_ϵ tends to zero, but it is completely unclear as to what sort of behavior (ϵ, $\epsilon^{1/3}$, $e^{-1/\epsilon}$, etc.) would be regarded as the border line between a collapse and noncollapse situation. This behavior can be investigated for any self-adjoint operator which corresponds to an observable which classically has a well-defined value (albeit ∞) at the singularity by using the spectral theorem and writing the state vector as a function on the spectrum. If the spectrum happened to contain an *isolated* point which corresponded to the singular value then the vanishing of the wave function at that point could reasonably be taken as an indication of the absence of collapse in that state.

Also one should augment the above discussion with some statement to the effect that presumably it is the transition rate (i.e., the transition probability per unit time) from the initial state into the various "singular" states which is relevant rather than just the long term behavior of the state function.

Because of this uncertainty in what is actually meant in the quantum case by an evolution into a singularity, it is difficult for us to say much concerning the implication of the present model for gravitational collapse. If one could find a wave packet which in its time evolution always avoided some neighborhood of $R=0$ so that $P_\epsilon=0$ for ϵ less than some finite value, then we could reasonably claim to have a noncollapse situation. However, the various wave packets that we have managed to construct all tail down in time to $R=0$. An illustration of this effect will be given within the context of the simplifications introduced in the next section, but clearly a proper discussion of this point must await an elucidation of the significance of the behavior of P_ϵ near $\epsilon=0$.

IV. THE SIMPLIFIED MODEL

It is clear from the complicated form of the eigenfunctions in the case $t=\phi$ (or the complicated time dependence when $t=\pi_R$) that the investigation of the behavior in time of a typical wave packet in a curved $K>0$ space will be very complicated. It is useful and interesting to simplify and alter the model slightly by considering the flat-space case $K=0$. This simplifies the calculations since the energy eigenfunctions (for $t=\phi$) become

$$\psi_E(R)=R^{-1/2}(AR^{-i\mu}+BR^{i\mu})\ , \tag{4.1}$$

where

$$\mu=\tfrac{1}{2}\left(\frac{48E^2}{\hbar^2}-1\right)^{1/2}\geqslant 0$$

and the actual spectrum of H^2 is as before. Note that this is exactly the same as the small-R behavior, Eq. (3.32), of the wave functions in the general case, thus confirming the general impression gained in other models (see, for example, Liang in Ref. 14) that the curvature term affects the large R behavior, but does not play much role in the behavior of the system near the singularity.

To investigate this case further it is useful to map the $L^2(0,\infty)$ space onto a $L^2(-\infty,\infty)$ space by the unitary map U, defined by $(U\psi)(y)=e^{-y/2}\times\psi(e^{-y})$. This map (which is the analog in our case of Misner's choice of an exponential time) has the big advantage that the transformed operator is simply

$$\tilde{H}^2\equiv UH^2U^{-1}=\frac{\hbar^2}{12}\left(-\frac{d^2}{dy^2}+\frac{1}{4}\right)\ , \tag{4.2}$$

which is easy to handle. Indeed in the case when $K>0$ we get

$$UH^2U^{-1}=\frac{\hbar^2}{12}\left(-\frac{d^2}{dy^2}+\frac{1}{4}\right)+12Ke^{-4y}\ , \tag{4.3}$$

and this is the easiest form in which to discuss self-adjointness and the general spectral properties of H^2.

Returning to Eq. (4.2) we see at once that $\tilde{H}^2$ is essentially self-adjoint on the domain of all infinitely differentiable functions of compact support and has a purely continuous spectrum of $(\frac{1}{48}\hbar^2,\infty)$ with corresponding generalized eigenvectors:

$$\psi_E(y)=Ae^{i\mu y}+Be^{-i\mu y}\ , \tag{4.4}$$

where

$$\mu=\frac{1}{2}\left(\frac{48E^2}{\hbar^2}-1\right)^{1/2}\geqslant 0\ .$$

[These functions of course are just the images of those in Eq. (4.1) under the map U.] Thus the complete set of generalized (δ-function normalized) eigenvectors is $\{\chi_\lambda(y)=(1/\sqrt{2\pi})e^{i\lambda y}|\lambda\in\mathbb{R}\}$ which can now be used via the spectral theorem (in the guise of Fourier-transform theory) to discuss the time evolution of any state. As an extreme example consider a δ-function idealized state localized at some point y_0 at a time t_0, so that

$$\delta(y-y_0,t_0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\lambda\, e^{i\lambda(y-y_0)}\ . \tag{4.5}$$

Then

$$\delta(y-y_0,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[-\frac{i}{\hbar}E(t-t_0)\right]\times e^{i\lambda(y-y_0)}\,d\lambda\ ,$$

and so

$$\begin{aligned}\delta(y-y_0,t)&=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\lambda\,e^{i\lambda(y-y_0)}\exp\left[-\frac{i}{\hbar}(\lambda^2+\tfrac{1}{4})^{1/2}\frac{\hbar}{\sqrt{12}}(t-t_0)\right]\\&=\frac{1}{2\pi}\lim_{\epsilon\to 0+}\frac{\epsilon-i(t-t_0)}{\{12(y-y_0)^2+[\epsilon-i(t-t_0)]^2\}^{1/2}}K_1\left(\frac{1}{\sqrt{48}}\{12(y-y_0)^2+[\epsilon-i(t-t_0)]^2\}^{1/2}\right)\ ,\end{aligned} \tag{4.6}$$

where $\epsilon\to 0_+$ is in the sense of distributions. The distribution at the right is peaked around

$$12(y-y_0)^2-(t-t_0)^2=0\ , \tag{4.7}$$

which is

$$y-y_0=\pm\frac{1}{2\sqrt{3}}(t-t_0)$$

or

$$\ln\frac{R}{R_0}=\pm\frac{1}{2\sqrt{3}}(t-t_0)\ , \tag{4.8}$$

but tails down to $R=0$ whenever $t \neq t_0$. Equation (4.8) is precisely the classical motion of the flat $K=0$ system as given in Eq. (2.11). Thus a state which is localized at some initial time splits up into two wave packets whose peaks move classically. The appearance of two such packets is to be expected for the time evolution of an eigenstate of position by virtue of the uncertainty principle which in particular makes the sign of the conjugate momentum equally likely to take either value. The "contracting" packet eventually hits the $R=0$ singularity although, as discussed above, the significance of this is not clear.

We would like to complete this section by remarking that a possible way (albeit *not* within the framework of conventional quantization) of imitating the maximum expansion of the $K>0$ model in the context of the present $K=0$ case is to limit artificially the Hilbert space of functions of R to be $L^2(0, R_m)$ (with $R_m = 1$ for convenience, say) rather than $L^2(0, \infty)$, and to impose some boundary conditions on the wave function at $R=1$ such as $\psi(1)=0$ or $\psi'(1)=0$ which mimic the classical "turn around" behavior by forcing the system to reflect off the fixed point $R=1$. The unitary map U now maps $L^2(0,1)$ onto $L^2(0,\infty)$ and the boundary conditions are to be imposed at $y=0$. The choice of such conditions is related to the different possible self-adjoint extensions of the formal differential operator, each one of which can potentially lead to a different model.[15] For example, the choice $\psi(1)=0$ translates in $L^2(0,\infty)$ to $\psi(0)=0$ and the resulting operator $\tilde{H}^2$ has a purely continuous spectrum $(\frac{1}{48}\hbar^2, \infty)$. However, the choice $\psi'(1)=0$ translates into $2\psi'(0)+\psi(0)=0$, and the resulting operator now has the remarkable feature of possessing a single *discrete* eigenvalue $E^2=0$ as well as the continuous part $(\frac{1}{48}\hbar^2, \infty)$.

The fact that the (isolated) discrete point is at vanishing energy means that it corresponds to a state in which the matter in some sense does not contribute so that the space is empty, a situation which of course cannot occur classically. This evidently corresponds to Misner's Robertson-Walker "quantum puff" universe,[16] but with the advantage that in the present formalism it appears as an eigenvalue as part of the spectrum of a genuine self-adjoint operator. However, this discrete part disappears in the full theory (that is $K>0$ without the arbitrary imposition of a boundary condition at $R=R_m$), and so the status of Misner's idea is still not entirely clear.

V. CONCLUSIONS

We have discussed the canonical decomposition of the coupled scalar-field–Robertson-Walker metric system and have shown that a canonical quantization based on a normal Hilbert space (rather than a space equipped with the indefinite inner product associated with the Klein-Gordon equation) is possible. In this approach a reasonably careful discussion of the self-adjointness and positivity of various operators is necessary in order to ensure the actual existence of the square-root Hamiltonian. In particular these technical requirements lead to a choice of time which is to some extent dictated by the sign of the curvature constant K. A particularly suitable time for $K>0$ is the choice $t=\phi$, which leads in the massless case to a time-independent Hamiltonian. An illustration of the motion of a wave packet was given for the flat $K=0$ case, but we have not exhibited any more complicated examples because as emphasized in the text the criteria which would enable one to judge whether a given time-evolving state leads in some sense to a collapse situation have not yet been properly formulated. Finally by imposing an artificial boundary condition in the $K=0$ case (and by changing the Hilbert space) we showed that Misner's Robertson-Walker "quantum puff" universe arises as the single discrete, isolated point of the spectrum of the Hamiltonian.

There are obviously a number of points which need further discussion. The most pressing one is an investigation of the case in which the mass m of the scalar fields is nonzero since one of the original motivations of the work was to look at the Parker-Fulling results from a different point of view. It is clear that this case will be qualitatively very different from the massless one in many respects. An inspection of the Hamiltonian in Eq. (3.10) (choosing $t=R$, for example) reveals two points immediately. On the one hand, the noncommutativity of $H(t)$ at different times leads to a complicated time evolution of an initial eigenstate. On the other hand, it is clear that at any given time the Hamiltonian is effectively that of a simple harmonic oscillator and as such will have a *discrete* spectrum only, rather than the purely continuous spectrum of the mass-zero case. Thus one might reasonably hope to be able to make a better discussion of the gravitational collapse problem. It is also possible that the Misner "quantum puff" will finally reemerge in a genuine way as the lowest energy eigenstate of the system. A thorough investigation of this case is now under way and the results will form the contents of a separate publication.

It would also be useful to investigate the effect of adding a cosmological term and perhaps of greater interest to see what happens when the theory is rendered conformally invariant by the addition of the appropriate coupling of the scalar field to the contracted curvature scalar. Similarly it would be worthwhile to replace the Robertson-Walker metric by one of the other more complicated Bianchi-type universes so as to introduce some anisotropic degrees of freedom into the metric and hence into the scalar field.

At a somewhat deeper conceptual level a question must be asked concerning the significance of the possibility of quantizing these types of models using different choices of time. The role played in the classical theory of general relativity by different sets of space-time coordinates and reference frames is well understood. However, in the quantized theory the situation is very different, and it is not always clear in what sense one would expect such a theory to be invariant under the general coordinate group. If a genuine canonical scheme, such as the one in this paper, is adopted then it is perfectly possible that the canonical variables corresponding, for example, to two different choices of time could be related classically by a canonical transformation which is not unitarily implementable in the Hilbert spaces of either of the two quantum theories. On the other hand, in a superspace-based approach the problem is rather to choose an operator ordering which makes the Lie algebra generated by the quantized constraint equations consistent with the classical Poisson-bracket equivalent (which is a reflection of the general coordinate invariance), and then to discuss the role played by the different possible choices of time in the interpretation of the Wheeler-DeWitt Hamiltonian constraint equation. Insofar as the different choices of time in the genuine canonical scheme may be related by *q numbers* it is likely that the problems in these two different schemes are closely connected.

This feature of q-number related times can easily be seen in the cases considered in the present paper. We have tended to choose these times for their different technical qualities, such as, for example, leading to a time-independent Hamiltonian, or covering both an expansion and a collapse phase (with respect to proper time) or, for us rather importantly, leading to a form for $\hat{H}^2$ which is self-adjoint and positive and hence enabling the spectral theorem to be used in defining $+\sqrt{\hat{H}^2}$. The physical significance of our specific choices or indeed even the more general technical significance could only be discussed within the framework of an investigation into the general problems mentioned above.

Finally it is of great interest both technically and conceptually to investigate the system in which fermions rather than bosons form the matter source for the geometry. Preliminary results in this direction indicate that the anticommutation relations and first-order differential equations obeyed by a massive Fermi field significantly alter the point of view which one takes to quantization. In particular the role played by the canonical decomposition and the Schrödinger equation is diminished at the expense of the increase in significance of the Heisenberg equations of motion for the spinor fields. A full account of this topic has appeared elsewhere.[17]

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