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Quantum Models for the Lowest-Order Velocity-Dominated Solutions of Irrotational Dust Cosmologies

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The lowest-order velocity-dominated solutions to the Einstein dust equations of Eardley, Liang, and Sachs are quantized using the canonical methods of DeWitt and of Arnowitt, Deser, and Misner. The quantum dynamics of these models is shown to be governed by the Einstein-Klein-Gordon (EKG) equation. Exact solutions of the decoupled EKG equations in the discrete limit are obtained, which have the striking feature that the state amplitude vanishes at the singularity for anisotropic models. The geometry of the manifold of the classical 3-metrics is studied and it turns out to be composed of conformally flat geodesic submanifolds. Other difficulties related to the quantum theory such as factor ordering, divergence, interpretation of the volume measure, etc. are also discussed.

I. INTRODUCTION

Recently, Eardley, Liang, and Sachs¹ introduced the concept of "velocity-dominated" singularities in irrotational dust cosmologies in general relativity and obtained the lowest-order solutions near these singularities by explicit integration. In this paper we are going to apply the methods of Dirac,² DeWitt,³ and Arnowitt, Deser, and Misner⁴ (ADM) to canonically quantize special models corresponding to these lowest-order velocity-dominated (LOVD) solutions. The purpose of this exercise is at least twofold: (a) to gain insight into the complicated formalism of canonical quantization in general relativity through the study of some simplified field models; (b) to obtain some meaningful physical results concerning the quantum structure of space-time singularities since the LOVD solutions may be a good approximation to the early universe. (It is at present still obscure whether or not the mixmaster⁵ or mixmaster-like models⁶ ultimately become velocity-dominated near the singularity.)

With irrotational dust as source, the dust flow lines provide a natural and unique 3+1 decomposition of space-time, which is necessary for the canonical approach. The "velocity-dominated" assumption then simply says that the spatial curvature (3R etc.) of the $t=\text{const}$ surfaces is small

compared to time-derivative terms in the Einstein equations, and can be dropped near the singularities (where the matter-energy density becomes infinite). This is true for a large class of exact solutions. The reduced equations can then be explicitly integrated to give the lowest-order approximations near the singularity. Some of the integration functions are restricted because of the constraint equations and self-consistency requirements.

These solutions may, of course, also be exact models whose spatial curvature is identically zero (i.e., exact models with flat 3-spaces). The crucial properties about these LOVD solutions are:

(a) They can be written in the form (8). (See Sec. III. This form is originally introduced by Lifshitz and Khalatnikov.⁷) In other words, they can be diagonalized by time-independent frame fields.

(b) They are spatially pointwise decoupled since all spatial derivatives are contained in the 3R terms. The situation is a little similar to that of ordinary quantum field theory when one ignores the coupling between particles at $t=\pm\infty$ and quantizes the free fields, except that here the individual "particles" are not particles but field variables evaluated at different dust world lines. The LOVD solutions obviously contain less degrees of freedom than a generic exact solution. For more details, the reader is referred to Ref. 1.

In Sec. III we develop the Hamiltonian formalism for the LOVD solutions, in terms of the now popular Misner⁸ coordinates. The momentum constraints (corresponding to $G_a^0=0$) are also reduced to the lowest-order canonical form. In Sec. IV we set up equal-time commutation relations for the conjugate pairs. Quantum dynamics is then formally described by the Einstein-Klein-Gordon⁹ (EKG) equation. Factor-ordering problems and divergence difficulties prevail. The role of the quantum momentum constraints is also discussed. In Sec. V we bypass the divergence difficulties by going to the discrete limit. The EKG equation is then reduced to an infinite decoupled system of "one-particle" Schrödinger-like equations. Exact solutions of these equations are obtained and their consequences discussed. In Sec. VI we follow the approach of DeWitt³ and Misner⁹ to recast the Hamiltonian equations in geometrical language. The LOVD dust solutions are shown to be the time-like or null geodesics in a pseudo-Riemannian manifold of LOVD 3-metrics with a metric structure induced by the form of the Hamiltonian. A covariant formulation of the quantum equation is presented after we make use of DeWitt's convention³ to avoid, temporarily, factor-ordering problems. Finally, we give some speculations concerning the relation between the structure of DeWitt's³ manifold of Riemannian 3-metrics and our manifold.

II. NOTATIONS AND CONVENTIONS

$\mu, \nu = 0, \dots, 3$; $a, b = 1, \dots, 3$; $A, B = 1, \dots, 3$.

Signature $g_{\mu\nu} = (-, +, +, +)$.

Units: $8\pi G = c = \hbar = 1$.

Riemann curvature tensor: $u_{\mu;[\nu\sigma]} \equiv \frac{1}{2}u_{\alpha}R_{\mu\nu\sigma}^{\alpha}$.

Ricci tensor: $R_{\mu\nu} \equiv R_{\mu\nu\alpha}^{\alpha}$.

Einstein tensor: $G_{\nu}^{\mu} \equiv R_{\nu}^{\mu} - \frac{1}{2}\delta_{\nu}^{\mu}R$; $R \equiv R_{\mu}^{\mu}$.

Four-dimensional co-derivative denoted by a semicolon (;).

III. HAMILTONIAN FORMULATION

Consider the Einstein dust equations

$$G_{\mu\nu} = -\rho u_{\mu} u_{\nu}, \quad (1)$$

where u_{μ} are the *irrotational* fluid 4-velocity ($\omega_{\mu\nu} \equiv u_{[\mu,\nu]} = 0$) and ρ is the proper matter-energy density. Using a method similar to that of Taub,¹⁰ one can show that (1) can be derived from the variational principle,

$$\frac{\delta I}{\delta g^{\mu\nu}} = 0, \quad I \equiv \int d^4x (-^4g)^{1/2} ({}^4R + 2\rho), \quad (2a)$$

where ρ is treated as a function of $g^{\mu\nu}$ through the subsidiary conservation equation

$$(\rho u^{\mu})_{;\mu} = 0. \quad (2b)$$

Here u^{μ} is in turn related to $g^{\mu\nu}$ via

$$u^{\mu} \equiv g^{\mu\nu} u_{\nu}, \quad u_{\mu} u_{\nu} g^{\mu\nu} = -1. \quad (2c)$$

We now restrict ourselves to comoving Gaussian normal (CGN) coordinates in which

$$ds^2 = -dt^2 + g_{ab}(x^c, t) dx^a dx^b, \quad u^{\mu} = \delta_0^{\mu}. \quad (3)$$

Then variational principle (2a) is reduced to the following (3+1)-canonical (ADM)⁴ form:

$$I = \int d^3x dt (\pi^{ij} \partial_t g_{ij} - \mathcal{H}), \quad (4)$$

$$\mathcal{H} \equiv \frac{1}{\alpha} (\frac{1}{2} \pi^2 - \pi_j^i \pi_i^j) - \alpha^3 R - 2\alpha\rho,$$

where the "momenta" π^{ij} conjugate to g_{ij} are related to the second fundamental form $K_j^i \equiv \frac{1}{2} g^{ik} \partial_t g_{kj}$ of $t = \text{const}$ hypersurfaces by

$$\pi^{ij} = \alpha (K g^{ij} - K^{ij}), \quad K \equiv K_i^i, \quad \alpha \equiv ({}^3g)^{1/2}$$

and all indices are raised or lowered by the 3-metric g_{ij} . Equation (2b) can be explicitly integrated and substituted into the Hamiltonian density \mathcal{H} :

$$\rho = \frac{\mu(x^c)}{\alpha}, \quad \mu \text{ integration function}$$

$$\Rightarrow \mathcal{H} = \frac{1}{\alpha} (\frac{1}{2} \pi^2 - \pi_j^i \pi_i^j) - \alpha^3 R - 2\mu. \quad (5)$$

Equations (4) and (5), on independent variations with respect to g_{ij} and π^{ij} , will give the equivalents of the "evolution equations" $G_a^0=0$. The "constraint equations" $G_a^0=0$ and $G_0^0=\rho$, however, can no more be obtained from (4). Instead, they have to be considered as additional constraints supplementary to (4). In terms of g_{ij} and π^{ij} , they have the following forms:

$$(a) \text{ the "Hamiltonian constraint": } \mathcal{H} = 0 \quad (6)$$

and

$$(b) \text{ the "momentum constraints": } \mathcal{P}^i = -2\pi^{ij}{}_{|j} = 0, \quad (7)$$

where a stroke "|" denotes co-derivative with respect to g_{ij} .

We are interested in metrics with the following properties:

(a) They can be written in the form (no sum for capitals in general)

$$g_{ab}(x^c, t) = e^{2\Omega(x^c, t)} \sum_A e^{2\beta_A(x^c, t)} \omega_{Aa}(x^c) \omega_{Ab}(x^c), \quad A = 1, \dots, 3 \quad (8)$$

where $\sum_A \beta_A = 0$ and ω_A^a 's are a *given* set of 3-vectors orthonormal with respect to some prescribed "singularity metric"¹ ${}_0g_{ab}(x^c)$ (i.e., metrics with their singular time factors "stretched way"). (See Ref. 1 for details.)

$$\begin{aligned}
 {}_0g_{ab}(x^c)\omega_A^a\omega_B^b &= \delta_{AB}, \quad \omega_{Aa} = {}_0g_{ab}\omega_A^b, \\
 {}_0g_{ab}(x^c) &= \sum_A \omega_{Aa}(x^c)\omega_{Ab}(x^c), \quad \text{etc.}
 \end{aligned}
 \tag{9}$$

We then have $\alpha = e^{3\Omega}\omega$, where $\omega \equiv +\det|\omega_{Aa}| > 0$,
 $-\infty < \Omega < +\infty$, and $\Omega \rightarrow -\infty \leftrightarrow \alpha \rightarrow 0$ (10)

at the singularity.

(b) $g_{ab}(x^c, t)$ satisfies field equations generated by (4) and (5) with the 3R term dropped.

Property (a) is satisfied by the LOVD solutions of Ref. 1. What (a) says is essentially that the metric can be diagonalized by time-independent frame fields, which is in turn equivalent to the assumptions of Lifshitz and Khalatnikov.⁷ As is obvious from (8), the metric now has only three degrees of freedom contained in the diagonal components. Assumption (b) is equivalent to the "velocity-dominated" assumption of Ref. 1. Since all spatial derivatives are contained in 3R , solutions obtained by dropping it in the field equations are spatially pointwise decoupled. In all, the restricted models we are considering represent two possibilities:

- (i) They correspond to those exact solutions of Einstein equations which have flat 3-spaces (e.g., flat Friedmann,¹¹ Heckmann-Schucking,¹² etc.),
- (ii) They represent the *lowest-order* approximate solutions of the Einstein equations near a singularity which satisfy the "velocity-dominated" assumption. In this case there will in general be additional constraints on the initial data (e.g., ω_{Aa} 's) required by the self-consistency of the approximation. For convenience, we will always call our models the LOVD solutions.

Equation (8) now implies that we can put π_j^i in the form

$$\pi_j^i = \sum_A [\pi_A(x^c, t) + \frac{1}{3}\pi(x^c, t)] \omega_A^i(x^c) \omega_{Aj}(x^c), \tag{11}$$

where $\sum_A \pi_A = 0$ and $\pi \equiv \pi_i^i$. Note that Ω , β_A 's transform as scalars and π , π_A 's transform as scalar densities. Using assumptions (a) and (b) and Eq. (11), Eqs. (4) and (5) reduce to

$$I = \int dt d^3x (2\pi\partial_t\Omega + 2\sum_A \pi_A \partial_t \beta_A - \mathcal{H}) \tag{12a}$$

and

$$\mathcal{H} = -2\mu + \frac{e^{-3\Omega}}{\omega} \left(\frac{1}{6}\pi^2 - \sum_A \pi_A^2 \right). \tag{12b}$$

Following Misner,⁸ we now redefine

$$\begin{aligned}
 h &\equiv 2\pi, \\
 \beta_A &\equiv (\beta_+ + \sqrt{3}\beta_-, \beta_+ - \sqrt{3}\beta_-, -2\beta_+), \\
 12\pi_A &\equiv (\pi_+ + \sqrt{3}\pi_-, \pi_+ - \sqrt{3}\pi_-, -2\pi_+).
 \end{aligned}
 \tag{13}$$

Then Eqs. (12) become

$$I = \int d^3x dt (h\partial_t\Omega + \pi_+ \partial_t \beta_+ + \pi_- \partial_t \beta_- - \mathcal{H}) \tag{14}$$

and

$$\mathcal{H} = -2\mu + \frac{e^{-3\Omega}}{24\omega} (h^2 - \pi_+^2 - \pi_-^2). \tag{15}$$

The system is thus reduced to Hamiltonian form with $\{h, \Omega\}$, $\{\pi_\pm, \beta_\pm\}$ as conjugate pairs. They are, however, not completely independent, but are subject to the constraint equations (6) and (7). We now show that this system is completely equivalent to the LOVD equations of Ref. 1.

The Hamiltonian equations associated with (15) are

$$\partial_t \Omega = \frac{\delta H}{\delta h} = \frac{-h}{12\omega} e^{-3\Omega}, \tag{16a}$$

$$\partial_t h = -\frac{\delta H}{\delta \Omega} = -6\mu \quad (\text{after using } \mathcal{H} = 0), \tag{16b}$$

$$\partial_t \beta_\pm = \frac{\delta H}{\delta \pi_\pm} = \frac{\pi_\pm}{12\omega} e^{-3\Omega}, \tag{16c}$$

$$\partial_t \pi_\pm = -\frac{\delta H}{\delta \beta_\pm} = 0, \tag{16d}$$

where $H \equiv \int d^3x \mathcal{H}$. The "Heckmann-Schucking-like" (general) solutions of (16) are

$$\begin{aligned}
 h &= -6\mu \left(t - \frac{{}_0t + {}_0t'}{2} \right), \\
 e^{3\Omega} &= \frac{3\mu}{4\omega} (t - {}_0t)(t - {}_0t'), \\
 \pi_\pm &= {}_0\pi_\pm, \\
 \beta_\pm &= {}_0\gamma_\pm [\ln(t - {}_0t) - \ln(t - {}_0t')] + {}_0\beta_\pm, \\
 {}_0\gamma_\pm &\equiv \frac{{}_0\pi_\pm}{9\mu({}_0t - {}_0t')},
 \end{aligned}
 \tag{17}$$

where ${}_0t, {}_0t', {}_0\pi_\pm$, and ${}_0\beta_\pm$ are arbitrary functions of integration. Putting solution (17) back into metric (8) we see that in order that $\sum_A \omega_A \otimes \omega_A$ be the metric of the singularity we need $\mu = \frac{4}{3}\omega$ and ${}_0\beta_\pm = 0$. If we now put ${}_0\pi_\pm = ({}_0t - {}_0t')$ and take the limit ${}_0t \rightarrow {}_0t'$, we obtain the "Friedmann-like"¹ (isotropic) solutions

$$h = -8\omega(t - {}_0t), \quad e^{3\Omega} = (t - {}_0t)^2, \quad \pi_\pm = \beta_\pm = 0. \tag{18}$$

On the other hand, if we put $\mu = \frac{4}{3}\omega/{}_0t'$, rewrite ${}_0\gamma_\pm = {}_0\gamma'_\pm \ln(-{}_0t')$, and take the limit ${}_0t' \rightarrow -\infty$, we obtain the "Kasner-like"¹ (anisotropic) solutions

$$\begin{aligned}
h &= 4\omega, \quad e^{3\Omega} = (t - {}_0t), \\
\beta_{\pm} &= {}_0\gamma'_{\pm} \ln(t - {}_0t), \quad \pi_{\pm} = {}_0\pi_{\pm}.
\end{aligned} \tag{19}$$

This is equivalent to putting $\mu = 0$ in (15), so that "matter does not matter near an anisotropic singularity." One can easily check that the equivalents of ${}_0K_b^a {}_0K_a^b = {}_0K_a^a = 1^1$ are satisfied by the above solutions. In fact, the eigenvalues (p_1, p_2, p_3) of ${}_0K_b^a$ can be explicitly computed to be

$$\begin{aligned}
p_1 &= \frac{1}{12\omega} ({}_0\pi_+ + \sqrt{3} {}_0\pi_-) + \frac{1}{3}, \\
p_2 &= \frac{1}{12\omega} ({}_0\pi_+ - \sqrt{3} {}_0\pi_-) + \frac{1}{3}, \\
p_3 &= -\frac{1}{6\omega} ({}_0\pi_+) + \frac{1}{3}.
\end{aligned} \tag{20}$$

Let us now look at the constraint equations (7). Multiplying (7) by ξ_i and integrating over all 3-space, one obtains

$$\begin{aligned}
2 \int d^3x \xi_i \pi^{ij}{}_{|j} &= 0 \\
&= \int d^3x \pi^{ij} (\xi_{i|j} + \xi_{j|i}) \\
&= \int d^3x \pi^{ij} \mathcal{L}_{\xi} g_{ij},
\end{aligned} \tag{21}$$

where \mathcal{L}_{ξ} is the Lie derivative with respect to ξ^i , and we have assumed that 3-space is either closed or $\pi^{ij} \xi_j \rightarrow 0$ at spatial infinity so that the surface terms vanish. In terms of $\{\Omega, \beta_{\pm}, h, \pi_{\pm}\}$ and the ω_A^a 's (21) has the form

$$\int d^3x \left[\xi^a (h\Omega_{,a} + \pi_+ \beta_{+,a} + \pi_- \beta_{-,a}) + \frac{1}{3} h \xi^a_{|a} + 2 \sum_A \pi_A \omega_{Aa} \mathcal{L}_{\xi} \omega_A^a \right] = 0, \tag{22}$$

where " $|$ " denotes co-derivative with respect to ${}_0g_{ab}$. Equation (22) is an exact relation. However, using solutions (17), (18), or (19) one can check that the last two terms contain only higher-order terms in $(t - {}_0t)$. Thus to lowest order we need only keep the first three terms. We therefore take

$$\int d^3x \xi^a (h\Omega_{,a} + \pi_+ \beta_{+,a} + \pi_- \beta_{-,a}) = 0 \tag{23}$$

as the new "momentum constraints" for our models. Note that ξ^a is arbitrary up to the boundary condition $\xi_a \pi^{ab} \rightarrow 0$ at spatial infinity if we do not require closed 3-topologies.

IV. CANONICAL QUANTIZATION

We now consider $\{\Omega, \beta_{\pm}\}$ etc. as q numbers and ω_{Aa} 's as c numbers and set up (equal-time) commutation relations for the conjugate pairs:

$$\begin{aligned}
[\Omega(\vec{x}, t), h(\vec{x}', t)] &= i \delta^3(\vec{x}, \vec{x}'), \\
[\beta_{\pm}(\vec{x}, t), \pi_{\pm}(\vec{x}', t)] &= i \delta^3(\vec{x}, \vec{x}')
\end{aligned} \tag{24}$$

(other commutators vanish). Here \vec{x} denotes a matter line with coordinates x^c and $\delta^3(\vec{x}, \vec{x}')$ is a distribution density (at each slot) with the usual δ -function properties. The unequal-time commutators $[\Omega(\vec{x}, t), \Omega(\vec{x}', t')]$ etc. are in general q numbers because of the nonlinearity of the field equations (16), and cannot be computed explicitly.

However, because the field equations are pointwise decoupled, it is clear that all commutators must be proportional to $\delta^3(\vec{x}, \vec{x}')$. So there is no "propagation" of quantum interference from one world line $x^c = \text{const}$ to another, as commutators with any time difference vanish if $\vec{x} \neq \vec{x}'$.

From now on we work in the Schrödinger picture and freeze out the variable t . Instead, one can, following Misner⁸ or DeWitt,³ consider the volume measure Ω as an "intrinsic" time variable. (Compare Kuchar.¹³) The dynamics of the system is then described in terms of Ω alone. Since Ω is in general a function of spatial variables, it corresponds in some sense to the "many-fingered" time of Schwinger¹⁴ and Tomonaga.¹⁵ However, in both the Misner and Schwinger and Tomonaga cases, Ω is treated as a c number, whereas in our case, Ω is a q number, coming closer to the ζ time of DeWitt.³

The Dirac quantization involves transforming the classical constraints (6) and (7) into quantum constraints on the state vector $|\Psi\rangle$ of the total system. \mathcal{K} and \mathcal{P}^i become operators in a Hilbert space (with yet undefined inner product):

$$\mathcal{K}|\Psi\rangle = 0, \tag{25a}$$

$$\mathcal{P}^i|\Psi\rangle = 0. \tag{25b}$$

We see immediately that there is ambiguity in factor ordering in \mathcal{K} . Different factor orderings lead to different quantum models and they are in general inequivalent. This is one of the basic difficulties in canonical quantization of gravity, or, nonlinear field theories in general. In fact, since all operators in \mathcal{K} are evaluated at the same space-time point, in general this will bring about divergences of the form $\delta^3(\vec{x}, \vec{x})$. DeWitt³ has argued (or suggested) that this should be set equal to zero. In our opinion, however, setting $\delta^3(\vec{x}, \vec{x}) = 0$ corresponds to throwing away some divergence and should be done only in cases when it is physically required or justified. For instance, in the functional formulation of the spin-zero boson field, say, setting $\delta^3(\vec{x}, \vec{x})$ equal to zero in the ground-state equation corresponds exactly to the removal of the infinite energy term $\sum_{\vec{k}} \frac{1}{2} \hbar \omega_{\vec{k}}$ in the particle representation, a practice well justified. How-

ever, in our case there is not yet any interpretable physical guideline, and the meaning of such practice is obscure.

In any case, one can formally write equations (25a) in the functional representation³ $h = (1/i) \times (\delta/\delta\Omega)$, $\pi_{\pm} = (1/i)(\delta/\delta\beta_{\pm})$ as

$$: \left[e^{-3\Omega} \left(-\frac{\delta^2}{\delta\Omega^2} + \frac{\delta^2}{\delta\beta_+^2} + \frac{\delta^2}{\delta\beta_-^2} \right) - 48\omega\mu \right] \Psi[\Omega, \beta_{\pm}] = 0 \quad (26)$$

modulo some factor ordering (represented by $::$) adjustments. Equation (25b), however, has no ordering problem because $[\Omega, \delta(\vec{x}), h(\vec{x})]$ etc. vanishes $[\delta_{,a}^3(\vec{x}, \vec{x}) = 0]$,

$$i \int d^3x \xi^a \left(\Omega, \delta_{,a} \frac{\delta}{\delta\Omega} + \beta_{+,a} \frac{\delta}{\delta\beta_+} + \beta_{-,a} \frac{\delta}{\delta\beta_-} \right) \Psi[\Omega, \beta_{\pm}] = 0. \quad (27)$$

Here $\Psi[\Omega, \beta_{\pm}] \equiv \langle \Omega, \beta_{\pm} | \Psi \rangle$, in general a functional of $\{\Omega(\vec{x}), \beta_{\pm}(\vec{x})\}$, is interpreted as the wave function of state $|\Psi\rangle$ having the geometric configuration $\{\Omega(\vec{x}), \beta_{\pm}(\vec{x})\}$. We call Eq. (26) the "Einstein-Klein-Gordon" (EKG) equation.⁹ It is the sole equation governing the quantum dynamics of our system. On the other hand, Eq. (27) says that the functional Ψ , considered as dependent on $\{\Omega, \beta_{\pm}\}$ alone, is invariant under the infinitesimal spatial coordinate transformations (gauge transformations) $x^a \rightarrow x^a + \xi^a$. Strictly speaking, Ψ depends on $\omega_{\lambda}^a(\vec{x})$ too. But since in the classical case terms involving ω_{λ}^a 's are of higher order, we assume that variations of Ψ due to ω_{λ}^a 's are also of higher order and ignore them in our models. How Eq. (27) actually affects the form of Ψ is not yet clear. In the following we will leave it aside and concentrate on (26) alone.

V. SPATIALLY POINTWISE-DECOUPLED EKG EQUATION

Because of its nonlinearity and divergences, the functional equation (26) is very difficult to analyze. On the other hand, to see the qualitative quantum behavior of the system, one can approximate the 3-space continuum by ∞^3 infinitesimal cubes, one at each \vec{x}_i . Then the field system can be decoupled into ∞^3 independent "one-particle" systems. Let $\Omega_i, \beta_{\pm i}, \omega_i$, etc. be appropriate averaged values of $\Omega, \beta_{\pm}, \omega$, etc. over the volume at \vec{x}_i . Equation (26) is reduced to an infinite system of partial differential equations:

$$: \left[e^{-3\Omega_i} \left(-\frac{\partial^2}{\partial\Omega_i^2} + \frac{\partial^2}{\partial\beta_{+i}^2} + \frac{\partial^2}{\partial\beta_{-i}^2} \right) - 48\omega_i \mu_i \right] \Psi(\Omega_1, \beta_{1\pm}, \dots, \Omega_{\infty^3}, \beta_{\pm\infty^3}) = 0, \quad i = 1 \dots \infty^3. \quad (28')$$

To decide upon the factor ordering, let us first try to endow the Hilbert space of $\{\Psi\}$ with an inner product. Although we have previously discussed the option of thinking of Ω as a time variable, there is no *a priori* reason that one cannot treat it on equal grounds with $\{\beta_{\pm}\}$ as configuration variables. In that case, however, (28') is no more a "dynamical equation" in the ordinary sense, but rather becomes a stationary Schrödinger equation. It is then natural to define the inner product as

$$\langle \chi, \Psi \rangle \equiv \int \prod_{i=1}^{\infty^3} d\Omega_i d\beta_{+i} d\beta_{-i} \chi^* \Psi \quad \text{for any } \chi, \Psi,$$

in which case Ψ can be correctly interpreted as a probability amplitude. Note that the measure is coordinate-invariant since $\{\Omega, \beta_{\pm}\}$ are scalars. If we now require the Hamiltonian operator to be Hermitian, then the simplest symmetric form is

$$\left(-\frac{\partial}{\partial\Omega_i} e^{-3\Omega_i} \frac{\partial}{\partial\Omega_i} + e^{-3\Omega_i} \frac{\partial^2}{\partial\beta_{+i}^2} + e^{-3\Omega_i} \frac{\partial^2}{\partial\beta_{-i}^2} - 48\omega_i \mu_i \right) \Psi(\Omega_1, \dots, \beta_{\pm\infty^3}) = 0. \quad (28)$$

In the following discussion of this section we will tentatively adopt this point of view and take (28) as our quantum equation. In Sec. VI, however, we will go back to the Ω -time concept, which follows more naturally from geometrical considerations. Since (28) are decoupled, we can write Ψ in the form

$$\Psi = \prod_{i=1}^{\infty^3} \psi(\Omega_i, \beta_{\pm i}). \quad (29)$$

Putting (29) back into (28) and dropping the i 's for simplicity, we get the spatially pointwise-decoupled EKG equation (compare Misner⁸),

$$\left(-\frac{\partial}{\partial\Omega} e^{-3\Omega} \frac{\partial}{\partial\Omega} + e^{-3\Omega} \frac{\partial^2}{\partial\beta_+^2} + e^{-3\Omega} \frac{\partial^2}{\partial\beta_-^2} - 48\omega\mu \right) \psi(\Omega, \beta_{\pm}) = 0. \quad (30)$$

Linearity in β_{\pm} suggests we Fourier analyze ψ :

$$\psi = \int dp_+ dp_- e^{i(p_+ \beta_+ + p_- \beta_-)} \psi(\vec{p}, \Omega), \quad \vec{p} \equiv (p_+, p_-) \quad (31)$$

$$\Rightarrow \left(\frac{d}{d\Omega} e^{-3\Omega} \frac{d}{d\Omega} + e^{-3\Omega} p^2 + 48\omega\mu \right) \psi(\vec{p}, \Omega) = 0, \quad (32)$$

$$p^2 \equiv p_+^2 + p_-^2.$$

In terms of the variable $\rho \equiv e^{3\Omega/2}$, (32) reads

$$\left(\frac{d^2}{d\rho^2} - \frac{1}{\rho} \frac{d}{d\rho} + \frac{\lambda^2}{\rho^2} + k^2 \right) \psi = 0, \quad (33)$$

where

$$\lambda^2 \equiv \frac{4}{3} p^2, \quad k^2 \equiv \frac{64}{3} \mu\omega.$$

Suppose we forget for a moment about the origins of λ and k . Then k^2 resembles the "energy" eigenvalue of a one-particle stationary state, and $-\lambda^2$ the "angular momentum" eigenvalue. Now a quantum Heckmann-Schucking-like model is a general solution ψ with arbitrary eigenvalues k and λ , whereas a quantum Friedmann-like model corresponds to $\lambda=0$ (zero anisotropy eigenvalue), and a quantum Kasner-like model corresponds to $k=0$ (zero "energy" eigenvalue).

Classically, $k^2 \geq 0$ because we assume $\mu \geq 0$. However, it is at least conceivable that in the quantum theory one may "analytic continue" k into the complex axis so that there may exist $k^2 < 0$ (negative energy) states. In that case (33) becomes

$$\left(\frac{d^2}{d\rho^2} - \frac{1}{\rho} \frac{d}{d\rho} + \frac{\lambda^2}{\rho^2} - \kappa^2 \right) \psi = 0, \quad \kappa \equiv ik. \quad (33')$$

The general solutions to both equations are just the generalized Bessel functions

$$\Psi_k(\Omega) \sim e^{3\Omega/2} Z_{\pm(1-\lambda^2)^{1/2}}(\pm k e^{3\Omega/2}), \quad (34a)$$

$$\Psi_\kappa(\Omega) \sim e^{3\Omega/2} Z_{\pm(1-\lambda^2)^{1/2}}(\pm i\kappa e^{3\Omega/2}),$$

whenever $k^2 \neq 0$, where Z is any cylindrical function. For the Kasner-like case ($k^2=0$) however, only special combinations of the Z 's are allowed, and the solutions are of rather simple form:

$$\psi_0(\Omega) \sim e^{3\Omega[1 \pm (1-\lambda^2)^{1/2}]/2}. \quad (34b)$$

We note the following features about the solutions.

(a) For $|\lambda| \leq 1$ (or $|p| \leq \frac{3}{2}$), everything is all right. $\{\psi_k, \psi_\kappa\}$ form a complete orthonormal set with continuous spectrum $-\infty < k^2 < \infty$. If we choose Z to be the Hankel functions, H , then we get asymptotic waves for $k^2 > 0$ and normalizable bound states (exponentially decaying) for $k^2 < 0$. The state with $k^2 = 0$ (Kasner-like model) is *not* normalizable, as usual.

(b) For $|\lambda| > 1$ (or $|p| > \frac{3}{2}$), the order of the Bessel functions becomes imaginary. According to Case,¹⁶ different $k^2 < 0$ eigenstates are in general not orthogonal to each other, unless the solutions are

constructed in a special way. Suppose we take the Z 's as the I 's:

$$\psi \sim e^{3\Omega/2} I_{\pm i(\lambda^2-1)^{1/2}}(\kappa e^{3\Omega/2}).$$

Take a linear combination of the form

$$\psi = e^{3\Omega/2} [e^{i\gamma} I_{i(\lambda^2-1)^{1/2}}(\kappa e^{3\Omega/2}) + e^{-i\gamma} I_{-i(\lambda^2-1)^{1/2}}(\kappa e^{3\Omega/2})].$$

To make ψ 's with different κ 's orthogonal to each other, we need

$$\gamma = B - (\lambda^2 - 1)^{1/2} \ln \kappa, \quad B \text{ some constant} \quad (35)$$

after some calculation, and asymptotically

$$\psi \sim \frac{1}{(2\pi\kappa)^{1/2}} [(e^{i\gamma} + e^{-i\gamma})e^{\kappa x} + (\text{const})e^{-\kappa x}], \quad x \equiv e^{3\Omega/2}$$

to be decaying. Then we need $\cos \gamma = 0 \Rightarrow \gamma = (n + \frac{1}{2})\pi$. Thus

$$B - (\lambda^2 - 1)^{1/2} \ln \kappa = (n + \frac{1}{2})\pi$$

$$\Rightarrow \kappa_n = \exp\{[B - (n + \frac{1}{2})\pi]/(\lambda^2 - 1)^{1/2}\}$$

$$\Rightarrow -\kappa_n^2 = -\exp\{2[B - (n + \frac{1}{2})\pi]/(\lambda^2 - 1)^{1/2}\}. \quad (36)$$

In ordinary quantum mechanics, B is determined by the cutoff of the potential term. (I.e., the attractive potential ceases to become effective within a radius of ${}_0x$, and gets replaced by, say, an infinite repulsive potential. Then B is determined by ${}_0x$ through boundary conditions.) However, in our case, we want to *assume no cutoff* (i.e., gravity predominates up to the singularity $x=0$). So B is arbitrary and can be put to zero without loss of generality. In any case, (36) predicts "energy-level quantizations" for bound states. Thus we conclude: *For quantum states of the lowest-order velocity-dominated universes with shear eigenvalues $|p| > 3/2$, and energy-density eigenvalues $k^2 < 0$, discrete energy levels appear.*

(c) Solutions (34) have the peculiar property that $\psi(\Omega) \rightarrow 0$ as $\Omega \rightarrow -\infty$ for any choice of Z as long as $\lambda^2 \neq 0$. For $\lambda=0$, one solution goes to a constant at $\Omega = -\infty$. Thus we conclude: *For quantum states of the lowest-order velocity-dominated universes with nonzero shear eigenvalues ($|p| \neq 0$), the amplitude of finding the universe at the singularity $\Omega = -\infty$ is zero.*

This is the strongest statement on how quantization may "remove" the classical singularity in general relativity so far obtained. This special property of our quantum solutions may be traced to the factor ordering we choose. Whether other factor ordering choices might give similar results is not known. (Compare Misner.⁸)

VI. GEOMETRY OF THE MANIFOLD OF LOVD METRICS

For a fixed-frame field $\{\omega_A(x^c)\}_{A=1,2,3}$ defined on a spacelike 3-manifold, consider the set of all Riemannian 3-metrics which are diagonal with respect to $\{\omega_A\}$ [i.e., the metric can be put into the form (8)]. Then each 3-metric is uniquely and invariantly characterized by the three scalar functions $\{\Omega, \beta_{\pm}\}$. Thus $\{\Omega, \beta_{\pm}\}$ enter as natural ‘‘coordinates’’ g^A on this manifold of 3-metrics, which we call \mathfrak{M} . \mathfrak{M} is both the configuration space in which our LOVD solution (for a fixed set of $\{\omega_A\}$) evolves as well as the domain space of our quantum state functional Ψ . \mathfrak{M} as a function space is very hard to handle. Naively, we can realize it by decomposing it into an ∞^3 -fold topological product of pointwise-decoupled subspaces $M(\vec{x})$, each consisting of all points $\{\Omega(\vec{x}), \beta_{\pm}(\vec{x})\}$ at a particular \vec{x} :

$$\mathfrak{M} = \prod_{\vec{x}}^{\infty^3} M(\vec{x}), \tag{37}$$

$$\dim M(\vec{x}) = 3 \Rightarrow \dim \mathfrak{M} = 3 \times \infty^3.$$

Now the form of the Hamiltonian (15) suggests that we introduce a Minkowski-type metric on $M(\vec{x})$: At each \vec{x}

$$ds^2(\vec{x}) = \omega(\vec{x})e^{3\Omega(\vec{x})}[-d\Omega^2(\vec{x}) + d\beta_+^2(\vec{x}) + d\beta_-^2(\vec{x})] \\ \equiv G_{AB}dg^A dg^B, \quad \text{sgn}G_{AB} = (-, +, +), \tag{38}$$

$$G_{AB} = \omega e^{3\Omega} \eta_{AB},$$

$$\eta_{AB} \equiv \text{diag}(-1, +1, +1) \text{ in } \{\Omega, \beta_{\pm}\} \text{ coordinates}$$

(sum over repeated capital indices here and in the following). This induces, at least formally, a metric on \mathfrak{M} ,

$$d\mathfrak{S}^2 = \int d^3x G_{AB}(\vec{x}) dg^A(\vec{x}) dg^B(\vec{x}), \tag{39}$$

which is invariant under spatial coordinate transformations. It is remarkable to see that metric (38) is *conformally flat*. (Compare Misner.⁹)

So far we have been working in the particular coordinates $\{\Omega, \beta_{\pm}\}$. In the geometrical language there should be nothing particular about these coordinates, and one should be allowed to use arbitrary coordinates. Thus, (15), (16), etc. should be brought into covariant form.

Let us first consider the ‘‘parageodesic’’ equation associated with metric (38),

$$\frac{\partial^2 g^A(\vec{x})}{\partial \tau^2} + \Gamma_{BC}^A \frac{\partial g^B}{\partial \tau}(\vec{x}) \frac{\partial g^C}{\partial \tau}(\vec{x}) = 0, \tag{40}$$

where

$$\Gamma_{BC}^A \equiv \frac{1}{2} G^{AD} (G_{DB,C} + G_{DC,B} - G_{BC,D})$$

and τ is some invariant affine parameter. In the

$\{\Omega, \beta_{\pm}\}$ system, we have

$$\Gamma_{BC}^A = \frac{3}{2} (\delta_B^A \delta_C^{\Omega} + \delta_C^A \delta_B^{\Omega} - \eta_{BC} \eta^{A\Omega}). \tag{41}$$

One then checks that Eqs. (16) are completely equivalent to the geodesic equations (40) provided one makes the identification $\tau = t$, so that the co-moving cosmological time serves as an invariant parameter in \mathfrak{M} . The Hamiltonian constraint $\mathcal{H} = 0$ is nothing but the statement that the tangent vectors to the ‘‘trajectories’’ of the solutions satisfy

$$\mathcal{H} = G^{AB} p_A p_B + \frac{1}{3} \mu = 0, \\ p_A \equiv G_{AB} \frac{\partial g^B}{\partial \tau} \\ = \frac{1}{12} (h, \pi_+, \pi_-) \text{ in } \{\Omega, \beta_{\pm}\} \text{ coordinates,} \tag{42}$$

$$\Rightarrow \begin{cases} p_A p^A = -\frac{4}{9} \omega < 0 & \text{for Heckmann-Schucking-like or Friedmann-like cases} \\ p_A p^A = 0 & \text{for the Kasner-like case.} \end{cases}$$

In other words, the curves in \mathfrak{M} corresponding to the LOVD solutions are either null or timelike geodesics. In the latter case they correspond to ‘‘particles’’ with ‘‘mass’’ $\frac{2}{3} \sqrt{\omega}$.

Equation (42) also leads to the ‘‘covariant’’ EKG equation

$$(\square^2 - 48\mu)\Psi[g^A] \\ = \frac{1}{\sqrt{-G}} \frac{\delta}{\delta g^A} \left(\sqrt{-G} G^{AB} \frac{\delta}{\delta g^B} \Psi \right) - 48\mu \Psi \\ = 0, \tag{43}$$

$$G \equiv \det G_{AB},$$

which prescribes a definite factor ordering. The momentum constraints (7) now read

$$i \int d^3x \frac{\delta \Psi}{\delta g^A} \mathfrak{L}_i g^A = 0. \tag{44}$$

However, as indicated earlier, functional derivatives in (43) will in general result in divergence of the form $\delta^3(\vec{x}, \vec{x})$. For the present discussion, let us tentatively adopt DeWitt’s convention of setting $\delta^3(\vec{x}, \vec{x}) = 0$, keeping in mind that such practice merits further justification. The following results are purely formal.

The ‘‘charge-current density’’ associated with a solution Ψ of (43) is

$$\psi \rho_A(\vec{x}) \equiv \left(\Psi^* \frac{\delta \Psi}{i \delta g^A(\vec{x})} - \Psi \frac{\delta \Psi^*}{i \delta g^A(\vec{x})} \right) \\ \Rightarrow \begin{cases} \psi \rho_A = \psi \rho_A^*, \\ \psi \rho_A = -\psi^* \rho_A^*. \end{cases} \tag{45}$$

$\psi \rho_A$ satisfies the ‘‘conservation equation,’’

$$\psi \rho^A{}_{;A} \equiv \frac{1}{\sqrt{-G}} \frac{\delta}{\delta g^A} (\sqrt{-G} G^{AB} \rho_B) = 0. \tag{43'}$$

From ${}_{\psi}\rho_A$ we can define the "total charge" P contained in some spacelike parahypersurface Σ with normal n^A ,

$${}_{\psi}P \equiv \int_{\Sigma} D^2\sigma \otimes \prod_{\vec{x}} {}_{\psi}\rho_A(\vec{x}) \sqrt{-G} n^A(\vec{x}), \quad (44')$$

where \int denotes functional integration. If we chose Σ to be the surface $\Omega = \text{const}$, we obtain (in $\{\Omega, \beta_{\pm}\}$ coordinates)

$${}_{\psi}P = \int_{\Omega=\text{const}} D\beta_+ D\beta_- \prod_{\vec{x}} [(-i)(\Psi^* \bar{\delta}_{\Omega} \Psi)(\omega e^{3\Omega})^{3/2}], \quad (45')$$

where

$$\bar{\delta}_{\Omega} \equiv \frac{\delta}{\delta\Omega} - \frac{\bar{\delta}}{\delta\Omega}.$$

${}_{\psi}P$ satisfies the conservation law $\delta P / \delta\Omega = 0$ provided functional surface terms vanish. Just as in ordinary Klein-Gordon theory, P can be both positive and negative. However, in our case it has an interesting physical interpretation. Let us consider an eigenstate Φ_h of

$$\frac{\delta}{i\delta\Omega} : \square \frac{\delta}{i\delta\Omega} \Phi_h = h\Phi_h$$

such that $h = h^*$. Classically we know that $h = -12e^{3\Omega}\omega\partial_t\Omega$ from (16a), so that

$$\begin{aligned} {}_{\Phi_h}P &= -24 \prod_{\vec{x}} \omega^{3/2} e^{9\Omega/2} \partial_t \Omega \left(\int D\beta_+ D\beta_- |\Phi_h|^2 \right) \\ &\propto - \prod_{\vec{x}} \partial_t \Omega \Rightarrow {}_{\Phi_h}P \geq 0 \iff \partial_t \Omega \leq 0 \text{ for all } \vec{x}. \end{aligned} \quad (46)$$

Thus ${}_{\Phi_h}P$ is proportional to the negative product of the "expansion rates" at all observers of the universe whose quantum state is Φ_h .

The above experience suggests that we define an indefinite metric \langle, \rangle in the Hilbert space of states $\{\Psi\}$ such that ${}_{\Phi}P = \langle \Phi, \Phi \rangle$ in the preferential Ω -time coordinates. Then we need

$$\begin{aligned} \langle \chi, \Psi \rangle &= \int D\beta_+ D\beta_- \prod_{\vec{x}} [-i(\omega e^{3\Omega})^{3/2} (\chi^* \bar{\delta}_{\Omega} \Psi)] \\ &\text{for any } \chi, \Psi. \end{aligned} \quad (47)$$

One can check that this inner product satisfies the following properties:

- (a) Hermiticity: $\langle \chi, \Psi \rangle = \langle \Psi, \chi \rangle$,
- (b) bilinearity: $\langle \alpha\chi_1 + \beta\chi_2, \Psi \rangle = \alpha\langle \chi_1, \Psi \rangle + \beta\langle \chi_2, \Psi \rangle$,
 $\langle \chi, \alpha\Psi_1 + \beta\Psi_2 \rangle = \alpha\langle \chi, \Psi_1 \rangle + \beta\langle \chi, \Psi_2 \rangle$,
- (c) $\frac{\delta\langle \chi, \Psi \rangle}{\delta\Omega} = 0$, provided surface terms vanish.

The following discussions concerning the relation of our manifold \mathfrak{M} to DeWitt's manifold of

Riemannian 3-metrics (M_D^3) [also called Riem(M) by Fischer¹⁷; here M stands for space-time] are purely qualitative and speculative. We will not go into the mathematical details because many aspects of the problem are not yet well understood.

According to DeWitt,³ solutions of the Einstein equations without the 3R terms can be considered as geodesics in the manifold of all spacelike Riemannian 3-metrics (M_D^3) with a metric structure prescribed by the Hamiltonian. The pointwise-decoupled subspace $M_D(\vec{x})$ at each \vec{x} is 6-dimensional, since it is just the space of all 3×3 symmetric matrices. But the solutions of the Einstein equations without the 3R terms are precisely the LOVD solutions, which also live in our 3-dimensional $\{\Omega, \beta_{\pm}\}$ spaces $M(\vec{x})$ for fixed ω_{Aa} 's. In fact, one checks explicitly that DeWitt's geodesic solutions³ can actually be put in the form (8). Now at first glance the relation between our $M(\vec{x})$ and DeWitt's $M_D(\vec{x})$ is obscure because given an arbitrary tensor g_{ab} , there is no unique invariant way of separating it into diagonal components and frame components with respect to which it is diagonal. However, if one is given another "reference" metric ${}_0g_{ab}$ (in our case this is just the "singularity" metric), then one can uniquely diagonalize g_{ab} by requiring that the eigenvectors ω_{Aa} be *orthonormal with respect to* ${}_0g_{ab}$ (i.e., ${}_0g^{ab}\omega_{Aa}\omega_{Bb} = \delta_{AB}$). Then the six degrees of freedom of g_{ab} is translated into the three eigenvalues (corresponding to $\{\Omega, \beta_{\pm}\}$), plus the remaining three degrees of freedom in the ω_{Aa} 's ($\omega_{\Sigma=1,2,3}$, say) (nine ω_{Aa} 's modulo six orthonormality relations). Thus given a ${}_0g_{ab}$, there will be a corresponding 3-parameter family of $\{\Omega, \beta_{\pm}\}$ hypersurfaces in which geodesics lie. A different ${}_0g_{ab}$ will induce another 3-parameter family. Thus the $\{\Omega, \beta_{\pm}, \omega_{\Sigma}\}$ coordinates are uniquely related to the $\{g_{11}g_{12} \cdots g_{33}\}$ coordinates through ${}_0g_{ab}$. Another way to interpret this is to say that giving ${}_0g_{ab}$ prescribes in which family of 3-dimensional submanifolds the geodesics must lie. In any case, one result is definite: The geodesic submanifolds in M_D defined by $\{\Omega, \beta_{\pm}\}$ coordinates are conformally flat.

At this point we would like to stop conjecturing any further except to point out the following features:

(A) The special form (8) of the geodesics of $M_D(\vec{x})$ is definitely highly restrictive. How much does this restriction tell us about the structure of the manifold itself is not clear.

(B) The fact that $\{\Omega, \beta_{\pm}\}$ are scalars makes one inclined to believe that they may play a special role in superspace ($\equiv M_D^3$ /group of diffeomorphisms).

(C) The lowest-order mixmasterlike solutions of Belinski and Khalatnikov,⁶ if they really exist,

are also constrained to $\{\Omega, \beta_{\pm}\}$ submanifolds, although they are not geodesics. Thus it seems that a large class, if not all, of exact solutions of the Einstein equations becomes asymptotically "trapped" in conformally flat $\{\Omega, \beta_{\pm}\}$ submanifolds near the singularity.

VII. CONCLUSION

In this paper we have used canonical methods to quantize some restricted models of general relativity, corresponding classically to the lowest-order velocity-dominated solutions of the Einstein equations with irrotational dust source. Some partial success is obtained, but basic difficulties related to factor ordering and nonlinearity, divergence, inner products, and interpretation problems remain. The most striking result, however, is the prediction of the vanishing of the state amplitude at the singularity for anisotropic universes, at least for our choice of factor ordering. Although the interpretation may not be unique, this is evidently in contradistinction to Misner's previous result⁸ that quantization does not affect the structure of the classical singularity, which used a different factor ordering. Thus the ordering problem seems to be crucial in quantum gravity and more

detailed investigation in this direction is imperative.

DeWitt's manifold $M_D^{\infty 3}$ (superspace before diffeomorphism identifications) turns out to be beautifully decomposed into families of conformally flat geodesic submanifolds, according to our analysis. The structure of the 6-dimensional manifolds $M_D(\vec{x})$, however, is not completely understood in our terms because of the complicated relations between the g_{ab} coordinates and our $\{\Omega, \beta_{\pm}\}$ coordinates. Further studies of this problem are underway.

Two different attitudes toward the interpretation of the volume measure Ω are adopted. In the discrete case, we let Ω be on the same footing as β_{\pm} , and the quantum system is a stationary one. In the continuum case, however, we follow the more popular practice of treating Ω as an internal time coordinate, and we have a dynamical system. Naturally, they lead to different inner products and inequivalent quantum models.

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