Quantized Scalar Fields in a Closed Anisotropic Universe*

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We formulate the quantum theory of a neutral scalar field, either minimally or conformally coupled to gravity, in nonrotating Bianchi type IX (mixmaster) universes. Creation and annihilation operators in the Heisenberg picture develop in time under a general Bogolubov transformation, which we calculate for a particular definition of those operators. That transformation expresses mathematically the physical processes of particle creation and mode mixing, the latter being a new effect, absent in simpler models. Our results should be useful for investigating the possible damping of anisotropy in the expansion of closed, homogeneous universes as a result of particle creation and mode mixing.

INTRODUCTION

Classical waves propagating in a time-varying background geometry suffer backscattering and reflection. In the context of quantum field theory, the amplification of waves by nonadiabatic processes and parametric resonance corresponds to particle creation. In a slowly varying geometry the number of particles is an adiabatic invariant, but in strong or rapidly changing fields (near a singularity or under conditions of high curvature) particle number is no longer conserved.

Particle creation constitutes an important mechanism by which the anisotropy energy of geometry may be converted to matter energy. For isotropic Robertson-Walker (Friedmann) universes, there is no production of massless particles satisfying conformally invariant field equations, because of the conformal flatness of the metric.[1-3] Production of particles of small or zero mass is therefore expected to be enhanced in anisotropic metrics. According to the semiquantitative argument of Zel'dovich,[4,5] the production of elementary particles near the singularity in an anisotropic cosmological model can accumulate an energy density sufficient for isotropization of the expansion within the first 10^{-43} seconds of the history of the universe.

The present paper is the first step in a study of quantized fields in a closed, homogeneous, and anisotropic universe, Misner's "mixmaster universe"[6-8] (Bianchi type IX). Many of the results obtained for other cases remain valid here. But in the mixmaster universe another important feature is encountered, namely, the mixing of different modes. In universes of simpler types, such as Robertson-Walker, Kasner, or Taub, scalar fields decompose into independent modes. A change in the geometry mixes the positive- and negative-frequency solutions of each mode, bringing forth particle creation. In the mixmaster universe, on the other hand, scalar fields do not decompose into completely independent modes. Under the influence of a changing background, in addition to the mixing of positive- and negative-frequency parts of each mode, there is a mixing among the coupled modes themselves. Particles created in one mode in the mixmaster universe will appear in other coupled modes during the course of the evolution of the system. The resulting energy exchange among modes should help the particles to extract energy from the geometry. Mode mixing, therefore, ought to increase the effectiveness of the process of anisotropy damping in the early universe. It is toward an understanding of anisotropy damping resulting from particle creation and mode mixing that the present work is directed.

Quantum field theory in an external mixmaster gravitational field is of interest not only because of the application to the anisotropy problem but also because this is the first metric, beyond the relatively simple cases which can be solved by separation of variables, for which the canonical field theory has been studied in detail. New problems in defining particle observables and the energy-momentum tensor must therefore be dealt with.

We write down the canonical theory of a neutral scalar field in a mixmaster space-time, assuming "minimal coupling" at first, and discuss the solution of the operator field equations. Creation and annihilation operators are tentatively defined so that the states with a fixed number of quanta in each mode at a given time are the eigenstates of the Hamiltonian of the field theory at that time.

One can solve for the operators at one time in terms of those at another time, and the resulting transformation makes manifest the phenomena of particle creation and mode mixing. We calculate the coefficients of this transformation in terms of the quantities appearing in the c-number solutions of the field equation. Finally, we make the modifications necessary to treat the theory with "conformal coupling," and we describe the next steps in the program of investigating anisotropy damping.

I. QUANTIZED FIELD IN MIXMASTER SPACE-TIME

The covariant Klein-Gordon equation[9]

$$(g^{\mu\nu}\nabla_\mu\nabla_\nu - \mu^2)\Phi = 0\,, \tag{1}$$

which describes a spin-zero field "minimally coupled" to the geometry of a curved space-time, is derived from the scalar Lagrangian density

$$\mathcal{L} = -\tfrac{1}{2}(-g)^{1/2}(g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi + \mu^2\Phi^2)\,, \tag{2}$$

where ∇_μ and ∂_μ denote the covariant and ordinary derivatives, respectively. Equation (1) is not conformally invariant when the mass μ equals 0, unlike the simplest field equations for massless particles with spin. Zel'dovich and co-workers (Refs. 4 and 5) study the modified field equation containing an additional term $-\frac{1}{6}R\Phi$, where R is the scalar curvature of the space-time. That theory involves what may be called "conformal coupling" of the scalar field, since the field equation is conformally invariant when $\mu = 0$. Here we shall first study Eq. (1) because it is simpler, but the changes necessary to handle the conformally coupled field will be fully discussed in Sec. IV.

The mixmaster metric under study has the form (see Ref. 7)

$$ds^2 = -dt^2 + \sum_{a=1}^{3} l_a{}^2(\sigma^a)^2\,, \tag{3}$$

where the l_a (functions of the time t) are the three principal curvatures, and the σ^a are the invariant forms on a Bianchi type IX space, which obey the exterior differential relations $d\sigma^a = \frac{1}{2}\epsilon_{abc}\sigma^b\wedge\sigma^c$ (ϵ_{abc} being the completely antisymmetric tensor). By a "mixmaster universe" we mean any manifold with a metric of the form (3). The terms "Kasner" and "Taub" are to be understood in the analogous generalized sense, in which they only characterize the type of three-space geometry.

A convenient coordinate system in the space with metric (3) is provided by the Euler angles[10] (θ, ϕ, ψ), with the ranges

$$0 \le \theta \le \pi, \quad 0 \le \phi \le 2\pi, \quad 0 \le \psi \le 4\pi\,, \tag{4}$$

in terms of which the invariant forms are

$$\begin{aligned}
\sigma^1 &= -\sin\psi\, d\theta + \cos\psi \sin\theta\, d\phi,\\
\sigma^2 &= \cos\psi\, d\theta + \sin\psi \sin\theta\, d\phi,\\
\sigma^3 &= d\psi + \cos\theta\, d\phi\,.
\end{aligned} \tag{5}$$

The covariant metric tensor is then $[(x^1, x^2, x^3) \equiv (\theta, \phi, \psi)]$

$$\begin{aligned}
&g_{00} = -1, \quad g_{0a} = g_{a0} = 0, \quad \text{for } a = 1, 2, 3\\
&g_{11} = l_1{}^2\sin^2\psi + l_2{}^2\cos^2\psi,\\
&g_{22} = \sin^2\theta(l_1{}^2\cos^2\psi + l_2{}^2\sin^2\psi) + l_3{}^2\cos^2\theta,\\
&g_{12} = g_{21} = (l_2{}^2 - l_1{}^2)\sin\psi\cos\psi\sin\theta,\\
&g_{33} = l_3{}^2, \quad g_{13} = g_{31} = 0,\\
&g_{23} = g_{32} = l_3{}^2\cos\theta.
\end{aligned} \tag{6}$$

The square root of the negative of the determinant of $g_{\mu\nu}$ is

$$(-g)^{1/2} = l_1 l_2 l_3 \sin\theta \equiv V(t)\sin\theta\,. \tag{7}$$

When all the l's are equal, the metric reduces to that of a closed Robertson-Walker universe of radius $a(t) = 2l$ (where l is the common value). When two of the l's are equal, the space is a Taub universe.[11]

The field equation (1) takes the form

$$\ddot{\Phi} + 2\Gamma\dot{\Phi} - {}^{(3)}\Delta\Phi + \mu^2\Phi = 0, \tag{8}$$

where a dot denotes differentiation with respect to t.

$$\Gamma \equiv \tfrac{1}{2}\sum_{a=1}^{3} \dot{l}_a/l_a\,, \tag{9}$$

and

$${}^{(3)}\Delta \equiv (-g)^{-1/2}\partial_a[(-g)^{1/2}g^{ab}\partial_b] \tag{10}$$

is the Laplace-Beltrami operator on the three-dimensional mixmaster space. The negative of this covariant Laplacian (which depends on t) is the Hamiltonian, expressed in Euler angle variables, of an asymmetric top[12] with principal moments of inertia $I_a = \frac{1}{2}l_a{}^2$ $(a = 1, 2, 3)$.

The metric is treated in the present work as an unquantized external field. The scalar field is quantized canonically by imposing the equal-time commutation relations

$$\begin{aligned}
&[\Phi(x, t), \Phi(x', t)] = 0,\\
&[\pi(x, t), \pi(x', t)] = 0,\\
&[\Phi(x, t), \pi(x', t)] = i\delta^{(3)}(x - x'),
\end{aligned} \tag{11}$$

where $\pi = \partial\mathcal{L}/\partial\dot{\Phi} = (-g)^{1/2}\dot{\Phi}$ is the conjugate momentum to Φ.

The solutions of the wave equation (8) in a mixmaster universe have been studied previously by one of the authors.[13,14] We shall treat the purely mathematical problem of the time development separately from the question of defining annihilation and creation operators.

On the one hand, the general Hermitian solution of Eq. (8) is conveniently written as

$$\Phi(x,t)=2^{-1/2}\sum_k [C_k(t)w_k(x)+C_k^\dagger(t)w_k(x)], \tag{12}$$

where the C_k are operators satisfying Eq. (14) below and the $w_k(x)$ form a complete set of *time-independent* functions. (The symbol k stands for a multiple index to be specified below.) We choose the normalization [cf. Eq. (7)]

$$\int dx \sin\theta\, w_k^*(x) w_{k'}(x)=\delta_{kk'}$$
$$[x=(\theta,\phi,\psi),\quad dx=d\theta\, d\phi\, d\psi]. \tag{13}$$

In particular, the w_k are chosen to be linear combinations of the familiar hyperspherical harmonics,[15] eigenfunctions of the Laplacian on the metric three-sphere [not of the actual mixmaster Laplacian ${}^{(3)}\Delta$ of Eq. (10)]. When two of the quantities l_a are equal at all times (the case of a Taub universe or a symmetrical top), the w_k are eigenfunctions of ${}^{(3)}\Delta$ if the polar axis of the harmonics is chosen to be the axis of symmetry. (The metric three-sphere is, of course, the special case of all three l's being equal.) The existence of time-independent eigenfunctions in the symmetrical situation is responsible for the breaking of the field into uncoupled modes (i.e., solvability by separation of variables). We are interested in the case that the symmetry is absent, when the eigenfunctions are different at each time and solving the equation directly in terms of them becomes inconvenient.

The functions $w_k(\theta,\phi,\psi)$ are linear combinations of the representation functions[16] $e^{iM\phi}d^J_{KM}(\theta)\, e^{iK\psi}$ of the three-dimensional rotation group. (Here both M and K range from $-J$ to J in integral steps.) The basis w_k includes the eigenfunctions of the quantum-mechanical Hamiltonian for a symmetric top. In such a case the index k stands for (J,M,γ,K), where (1) J is an integer, (2) $M=-J, J+1,\ldots,J$, (3) $\gamma=0$ or 1, (4) $K=0,1,\ldots,J$ for $\gamma=0$; $K=1,\ldots,J$ for $\gamma=1$. The J multiplet is thereby split into four submultiplets, labeled by γ and the parity of K, of different behavior under certain discrete symmetries (see Refs. 12–14). However, half-integral J's appear in the mixmaster problem and not for the top because the three-sphere is in two-to-one correspondence with the configuration space of the top. For them the decomposition into symmetry classes is not so easy, so we shall think of k in this case as standing for (J,M,K), where K can take either sign. We expect that half-integral J's with their complications can be avoided in most model calculations, since for large J the qualitative physical difference between states with adjacent values of J is small.

The expression (12) is a solution of the field equation (8) if the operators $C_k(t)$ satisfy the coupled equations

$$\frac{d^2C_k}{d\tau^2}+\sum_{k'}\mathcal{H}_{kk'}C_{k'}=0, \tag{14}$$

where the new time coordinate τ is defined by

$$\frac{dt}{d\tau}=V(t)\equiv l_1l_2l_3, \tag{15}$$

and

$$\mathcal{H}_{kk'}(t)=\int dx\sin\theta\, w_k^*(x)[\mathcal{H}w_{k'}](x) \tag{16}$$

are the matrix elements of the operator

$$\mathcal{H}(\tau)=V^2(-{}^{(3)}\Delta+\mu^2). \tag{17}$$

(An alternative approach which does not require a change of time scale is described at the end of Sec. IV.) A given mode k is coupled to only finitely many others: those with the same values of J, M, γ, and the parity of K (if J is an integer). We do *not* require that the C_k satisfy canonical commutation relations, since we do not assign them any physical interpretation. The specification of the C's (incomplete so far) will be completed by Eq. (36) in Sec. III, where they will be used to reduce the dynamics of the field to a c-number problem. It will then be seen from Eqs. (37) and (38) that Eq. (12) is a completely general solution of the field equation.

On the other hand, if each l_a were independent of time, one would expect the eigenfunctions of the mixmaster Laplacian (10) to define modes corresponding to stable physical particles.[17] When the metric is changing in time, the notion of particle becomes ambiguous, because there is no unique way of classifying the solutions of the wave equation into positive- and negative-frequency functions (see Refs. 1 and 2). Similarly, since modes are being mixed, the separation of the field into modes becomes somewhat arbitrary. Nevertheless, it is natural to define[18] particlelike observables at each time t_0 by expanding Φ and π at that time according to

$$\Phi(x,t_0)=\sum_j (2E_j)^{-1/2}[A_j(t_0)u_j(x)+A_j^\dagger(t_0)u_j^*(x)], \tag{18a}$$

$$\pi(x,t_0)=-i(-g)^{1/2}\sum_j(\tfrac{1}{2}E_j)^{1/2}[A_j(t_0)u_j(x)-A_j^\dagger(t_0)u_j^*(x)], \tag{18b}$$

where the $u_j(x)$ are eigenfunctions of $-{}^{(3)}\Delta+\mu^2$ at t_0 with eigenvalues $E_j{}^2$. Note that the u_j and E_j are different for different t_0 (unless the metric is static). The time dependence of $A_j(t_0)$, therefore, has two sources: the Heisenberg-picture time dependence of the fields Φ and π, and the time dependence in the definition of $A_j(t_0)$ in terms of the fields at t_0. The eigenfunctions at each time t_0 should be normalized so that

$$V(t_0)\int dx\,\sin\theta\, u_j^*(x)u_{j'}(x)=\delta_{jj'}, \tag{19a}$$

$$\sum_j u_j^*(x)u_j(x')=(-g)^{-1/2}\delta^{(3)}(x-x'). \tag{19b}$$

The annihilation operators $A_j(t_0)$ and creation operators $A_j^\dagger(t_0)$ then satisfy, as a consequence of Eq. (11), the commutation relations

$$[A_j,A_{j'}]=0=[A_j^\dagger,A_{j'}^\dagger],\quad [A_j,A_{j'}^\dagger]=\delta_{jj'}. \tag{20}$$

The canonical formalism yields a Hamiltonian[19] for the field theory:

$$H(t)=\tfrac{1}{2}V(t)\int dx\,\sin\theta[(-g)^{-1}\pi^2+g^{ab}\partial_a\Phi\partial_b\Phi+\mu^2\Phi^2]. \tag{21a}$$

Substitution of Eqs. (18) gives

$$H(t_0)=\sum_j E_jA_j^\dagger(t_0)A_j(t_0)+\text{divergent } c\text{-number}. \tag{21b}$$

The quanta corresponding to the A_j may be called quasiparticles. A deeper physical study of the particle concept suggests another definition of particles (see Sec. V and Ref. 27).

For integral J the functions u_j are the eigenfunctions of an asymmetric top (see Refs. 12–14). The index j then stands for (J,M,γ,σ,χ), where J, M, and γ have the same significance as in the symmetric case, σ corresponds to the parity of K, and χ is an index number for the eigenvalues of ${}^{(3)}\Delta$, which takes on the same number of values as K does in the corresponding symmetric situation described above. The u_j can be expanded in terms of the w's, with coefficients which depend on time through the functions l_a:

$$u_j=V^{-1/2}\sum_k a_{kj}w_k, \tag{22}$$

where all the indices in k except K are fixed and are those of j. [The factor $V^{-1/2}$ is needed to account for the difference in the normalization conventions (13) and (19).] The a_{kj} and the associated eigenvalues $E_j{}^2$ are functions of l_1, l_2, and l_3 (and hence, of time). For further information about them, including numerical calculations, see Refs. 12–14.

The operator $A_j(t_0)$ is related by a general Bogolubov transformation (also called a linear canonical transformation or symplectic transformation) to the operators $A_{j'}(t_1)$ and $A_{j'}^\dagger(t_1)$ defined at a different time t_1. Terms in $A_j(t_0)$ involving $A^\dagger(t_1)$ operators correspond to the physical process of particle creation, to the extent that the particle interpretation of the operators is legitimate. Similarly, terms with $j'\neq j$ describe mode mixing (a scattering of the particles by the time-dependent anisotropic gravitational field). In Sec. II we shall elaborate on these general remarks, and in Sec. III the coefficients of the Bogolubov transformation in the mixmaster universe will be calculated.

II. PARTICLE CREATION, MODE MIXING, AND BOGOLUBOV TRANSFORMATIONS

For time-dependent Robertson-Walker, Kasner, and Taub universes, separation of variables in the scalar wave equation allows for mode decomposition (Refs. 2, 5, 13). However, the time dependence of the field amplitudes is not simple harmonic, as it would be in a static universe, but rather is the solution of a more general second-order differential equation of the form (14) with diagonal $\mathcal{K}_{kk'}(t)$. The positive- and negative-frequency parts of the field become mixed in the course of the evolution of the universe; creation and annihilation operators[20] at one time are linear combinations of those at a different time, so that a state in Fock space with no particles present initially has at a later time a nonzero average particle number. This is the process of particle creation. Since there is no mode coupling in universes of this class, the process is described by a diagonal Bogolubov transformation:

$$\begin{aligned}&A_k(t)=\alpha_k^*(t)A_k(t_0)+\beta_k(t)A_{-k}^\dagger(t_0),\\&|\alpha_k(t)|^2-|\beta_k(t)|^2=1.\end{aligned} \tag{23}$$

The quantity $|\beta_k(t)|^2$ gives the average number of particles present in the kth mode at time t if the state is the vacuum at t_0. If the initial state is not the vacuum, the number of particles created is increased by a factor $1+2N_k$, where N_k is the average number of particles initially present (see Ref. 2).

For a general time-dependent metric (including the mixmaster universe), the fact that the eigenfunctions of the covariant Laplacian depend on time results in mode mixing. Instead of Eq. (23) it is necessary to consider the most general linear transformation on the creation and annihilation operators of the system:

$$A_j(t)=\sum_{j'}[u_{jj'}(t)A_{j'}(t_0)+v_{jj'}(t)A_{j'}^\dagger(t_0)], \tag{24}$$

where $u_{jj'}$ and $v_{jj'}$ are complex c-number functions of time. Here, and in what follows, the indices j, j', i denote the collective quantum numbers $(J, M, \gamma, \sigma, \chi)$ of the asymmetric top eigenfunctions, and k, k', p denote the (J, M, γ, K) of the symmetric top eigenfunctions (with extensions to cover half-integral J, if needed). If at t_0 the operators $A_{j'}(t_0)$ satisfy the canonical commutation relations (20), then in order that the transformed operators $A_j(t)$ also obey these relations,

$$[A_j(t), A_{j'}(t)] = 0, \quad [A_j(t), A^\dagger_{j'}(t)] = \delta_{jj'}, \tag{25}$$

it is necessary and sufficient that the transformation coefficients satisfy the following conditions:

$$\sum_i (u_{ji}u^*_{j'i} - v_{ji}v^*_{j'i}) = \delta_{jj'}, \tag{26a}$$

$$\sum_i (u_{ji}v_{j'i} - v_{ji}u_{j'i}) = 0. \tag{26b}$$

Regarding the quantities $A_j(t)$ and $A_j(t_0)$ as the jth components of column vectors $A(t)$ and $A(t_0)$, we may write the transformation (24) in matrix notation as

$$A(t) = \underline{u}A(t_0) + \underline{v}A^\dagger(t_0), \tag{27}$$

and the conditions (26) take the form

$$\underline{u}\underline{u}^\dagger - \underline{v}\underline{v}^\dagger = 1, \quad \underline{u}\underline{\tilde{v}} - \underline{v}\underline{\tilde{u}} = 0, \tag{28}$$

where the tilde and dagger denote transposition and Hermitian conjugation, respectively. The transformation is invertible (as it will be in all the cases which arise in this paper) if and only if

$$\underline{u}^\dagger\underline{u} - \underline{\tilde{v}}\underline{v}^* = 1, \quad \underline{u}^\dagger\underline{v} - \underline{\tilde{v}}\underline{u}^* = 0, \tag{29}$$

where * denotes complex conjugation. Equations (27)–(29) define a *(general) Bogolubov transformation*.[21]

The transformation matrices $v_{jj'}(t)$ and $u_{jj'}(t)$ corresponding to the time development of a field in the mixmaster universe are not diagonal [see Eqs. (43) below]. If we start out with a pure positive-frequency wave component in a certain mode j_1, at some later time we will find a certain amount of positive- and negative-frequency waves of some other mode j_2, as well as a negative-frequency j_1 component. These effects correspond to particle creation and mode scattering, in accordance with Eq. (24).

III. CALCULATION OF THE BOGOLUBOV TRANSFORMATION

To calculate $A_j(t)$ and $A_j^\dagger(t)$, defined as in Eqs. (18), in terms of the analogous operators at another time, $A_{j'}(t_0)$ and $A^\dagger_{j'}(t_0)$—in other words, to determine the coefficients $u_{jj'}(t)$ and $v_{jj'}(t)$ of the Bogolubov transformation (24)—one may proceed in several ways. One method is to substitute Eq. (18a) into Eq. (8) to find a set of coupled differential equations satisfied by the operators A_j. These equations, however, are rather complicated.[22] We prefer to make an intermediate transformation to the operators C_k, which obey the comparatively simple equation (14). We shall go from the $A_j(t_0)$ to the $A_j(t)$ in the following steps:

$$\begin{aligned}\{A_j(t_0), A_j^\dagger(t_0)\} &\to \{\Phi(t_0), \pi(t_0)\}\\ &\to \{C_k(t_0), C_k^\dagger(t_0)\}\\ &\to \{C_k(t), \dot{C}_k(t), C_k^\dagger(t), \dot{C}_k^\dagger(t)\}\\ &\to \{\Phi(t), \pi(t)\}\\ &\to A_j(t).\end{aligned} \tag{30}$$

Here $\dot{C}_k$ is the derivative of C_k with respect to t (not τ).

First, we express $A_j(t)$ in terms of $C_k(t)$, etc. Differentiation of Eq. (12) yields for all t

$$\pi(x,t) = 2^{-1/2}(-g)^{1/2}\sum_k [\dot{C}_k(t)w_k(x) + \dot{C}_k^\dagger(t)w_k^*(x)]. \tag{31}$$

Noting from Eq. (22) that

$$\int dx \sin\theta\, u_j^*(x) w_k(x) = V^{-1/2}a^*_{kj}, \tag{32a}$$

we set

$$b_{kj} = V^{1/2}\int dx \sin\theta\, u_j^*(x)w_k^*(x) = (-1)^{\gamma+K-M}a_{(J,-M,\gamma,K),j} \quad [k \equiv (J, M, \gamma, K)]. \tag{32b}$$

Here we have noted that our phase convention (see Ref. 16) entails

$$d^J_{KM} = d^{J*}_{KM} = d^J_{-K,-M}, \tag{33a}$$

and hence

$$w^{J*}_{KM\gamma} = (-1)^{\gamma+K-M}w^J_{K,-M\gamma}. \tag{33b}$$

We find from Eqs. (18) at time t that

$$A_j(t) = 2^{-1/2}[E_j^{1/2}\int dx(-g)^{1/2}u_j^*(x)\Phi(x,t) + iE_j^{-1/2}\int dx\, u_j^*(x)\pi(x,t)], \tag{34}$$

where E_j and u_j are those for time t. (The cancellation of terms involving $A^\dagger$ operators depends on the fact that the asymmetric top eigenfunctions u_j and $u^*_{j'}$ are orthogonal unless $E_j = E_{j'}$.) Thus Eqs. (12) and (31) at time t [with Eqs. (32)] yield

$$A_j(t) = \tfrac{1}{2}V^{1/2}\left\{E_j^{1/2}\sum_k [a^*_{kj}C_k(t) + b_{kj}C_k^\dagger(t)] + iE_j^{-1/2}\sum_k [a^*_{kj}\dot{C}_k(t) + b_{kj}\dot{C}_k^\dagger(t)]\right\}, \tag{35}$$

where V, E_j, a_{kj}, and b_{kj} are all evaluated at time t.

Next we consider the inverse of the analogous transformation at the t_0 end. It is convenient to impose the condition

$$\dot{C}_k(t_0) = -iC_k(t_0), \tag{36}$$

which we have the freedom to do, since $C_k(t)$ was not uniquely defined previously. We now have[23] from Eq. (31) at time t_0

$$\pi(x, t_0) = -i2^{-1/2}(-g)^{1/2}\sum_k [C_k(t_0)w_k(x) - C_k^\dagger(t_0)w_k^*(x)], \tag{37}$$

which with Eq. (12) is easily inverted to yield

$$\begin{aligned} C_k(t_0) &= 2^{-1/2}\left[\int dx \sin\theta w_k^*(x)\Phi(x, t_0) + iV^{-1}\int dx w_k^*(x)\pi(x, t_0)\right] \\ &= \tfrac{1}{2}V^{-1/2}\sum_j [a_{kj}(E_j^{-1/2} + E_j^{1/2})A_j(t_0) + b_{kj}(E_j^{-1/2} - E_j^{1/2})A_j^\dagger(t_0)]. \end{aligned} \tag{38}$$

In this case V, E_j, a_{kj}, and b_{kj} are evaluated at time t_0.

It remains to find the $C(t)$'s in terms of the $C(t_0)$'s. Let $h_k^{(p)}(\tau)$ be the solutions of

$$\frac{d^2h_k}{d\tau^2} + \sum_{k'}\mathcal{H}_{kk'}h_{k'} = 0, \tag{39}$$

such that

$$\begin{aligned} h_k^{(p)}(\tau_0) &= \delta_{kp}, \\ \frac{d}{d\tau}h_k^{(p)}(\tau_0) &= V\frac{d}{dt}h_k^{(p)} \\ &= -iV(t_0)\delta_{kp}, \end{aligned} \tag{40}$$

where τ_0 is the value of τ corresponding to the value t_0 of the time variable [see Eq. (15)]. (Similarly, we shall let τ_1 correspond to the time t.) Then

$$C_k(t) = \sum_p h_k^{(p)}(\tau)C_p(t_0) \tag{41}$$

(summed over all the modes coupled to k) is a solution of Eq. (14) which satisfies Eq. (36) and has the correct initial value $C_k(t_0)$ at t_0. Thus we have

$$\begin{aligned} C_k(t) &= \sum_p h_k^{(p)}(\tau_1)C_p(t_0), \\ \dot{C}_k(t) &= V^{-1}\sum_p \frac{dh_k^{(p)}}{d\tau}(\tau_1)C_p(t_0). \end{aligned} \tag{42}$$

Finally, combining Eqs. (35), (42), and (38), we obtain the coefficients of the Bogolubov transformation:

$$u_{jj'} = \frac{1}{4}\left[\frac{V(t)}{V(t_0)}\right]^{1/2}\sum_{k,p}[a_{kj}^*a_{pj'}(E_j^{1/2}h_k^{(p)} + E_j^{-1/2}\dot{h}_k^{(p)})(E_{j'}^{-1/2} + E_{j'}^{1/2}) + b_{kj}b_{pj'}^*(E_j^{1/2}h_k^{(p)*} + E_j^{-1/2}\dot{h}_k^{(p)*})(E_{j'}^{-1/2} - E_{j'}^{1/2})], \tag{43a}$$

$$v_{jj'} = \frac{1}{4}\left[\frac{V(t)}{V(t_0)}\right]^{1/2}\sum_{k,p}[a_{kj}^*b_{pj}(E_j^{1/2}h_k^{(p)} + E_j^{-1/2}\dot{h}_k^{(p)})(E_{j'}^{-1/2} - E_{j'}^{1/2}) + b_{kj}a_{pj'}^*(E_j^{1/2}h_k^{(p)*} + E_j^{-1/2}\dot{h}_k^{(p)*})(E_{j'}^{-1/2} + E_{j'}^{1/2})]. \tag{43b}$$

Here quantities with indices j and j' are evaluated at times t and t_0, respectively; also, $h_k^{(p)}$ and its derivative are evaluated at τ_1, and the time differentiation in $\dot{h}_k^{(p)}$ is with respect to t. The physical significance of these transformation coefficients has been discussed in Sec. II.

IV. CONFORMAL COUPLING

The equation of a conformally coupled scalar field is

$$(g^{\mu\nu}\nabla_\mu\nabla_\nu - \mu^2 - \tfrac{1}{6}R)\Phi = 0, \tag{44}$$

where the scalar curvature[24] of the mixmaster space-time is

$$\begin{aligned} R &= {}^{(4)}R \\ &= 2\left(\sum_a \frac{\ddot{l}_a}{l_a} + \frac{\dot{l}_1\dot{l}_2}{l_1l_2} + \frac{\dot{l}_2\dot{l}_3}{l_2l_3} + \frac{\dot{l}_1\dot{l}_3}{l_1l_3}\right) \\ &\quad - V^{-2}[l_1^4 + l_2^4 + l_3^4 - \tfrac{1}{2}(l_1^2 + l_2^2 + l_3^2)^2]. \end{aligned} \tag{45}$$

The first term has the form of ${}^{(4)}R$ for a Kasner universe, and the second term is the three-dimensional scalar curvature, ${}^{(3)}R$, of the mixmaster space. Equation (8) is replaced by

$$\ddot{\Phi} + 2\Gamma\dot{\Phi} - {}^{(3)}\Delta\Phi + (\mu^2 + \tfrac{1}{6}R)\Phi = 0. \tag{46}$$

The damping of anisotropy in the expansion rates should be most evident in the case of conformal coupling, since it is in that case that isotropy tends to reduce the particle production.

The eigenfunctions of $-{}^{(3)}\Delta + \mu^2 + \frac{1}{6}R$ are the same as those of $-{}^{(3)}\Delta + \mu^2$, with different eigenvalues, $E_j^2 + \frac{1}{6}R$. We shall show that the field equation (46) can be reduced, like Eq. (8), to a system of coupled equations of the form (14), with different coefficients in place of $\mathcal{H}_{kk'}$. Therefore, the entire calculation of Sec. III applies to the conformal theory, except for minor changes which will be clearly indicated in the following discussion.

There are several transformations which can be used to remove the $\dot{\Phi}$ term from Eq. (46), arriving at equations like Eq. (14). First, using the variable τ of Eq. (15), one obtains much as before

$$V^{-2}\frac{\partial^2\Phi}{\partial\tau^2}-{}^{(3)}\Delta\Phi+(\mu^2+\tfrac{1}{6}R)\Phi=0\,, \tag{47}$$

and hence Eq. (14) with

$$\mathcal{H}(\tau)=V^2(-{}^{(3)}\Delta+\mu^2+\tfrac{1}{6}R)\,. \tag{48}$$

With this operator $\mathcal{H}$ in Eq. (16) and with E_j replaced by $(E_j{}^2+\frac{1}{6}R)^{1/2}$, Sec. III applies.

On the other hand, following Ref. 5, one can write

$$\frac{dt}{d\eta}=v\equiv V^{1/3}, \quad \chi=v\Phi\,. \tag{49}$$

The equation becomes

$$\frac{\partial^2\chi}{\partial\eta^2}+v^2[-{}^{(3)}\Delta+\mu^2+\tfrac{1}{6}R-v^{-3}v'']\chi=0\,, \tag{50}$$

where a prime indicates differentiation with respect to η. Writing in analogy to Eq. (12)

$$\chi(x,t)=2^{-1/2}\sum_k[G_k(t)w_k(x)+G_k^\dagger(t)w_k^*(x)]\,, \tag{51}$$

we obtain in place of Eq. (14)

$$\frac{\partial^2 G_k}{\partial\eta^2}+\sum_{k'}[(\Omega^2)_{kk'}+Q\delta_{kk'}]G_{k'}=0\,, \tag{52}$$

where (in notation adapted from Ref. 5)

$$\Omega^2=v^2(-{}^{(3)}\Delta+\mu^2)\,, \tag{53}$$

$$\begin{aligned}Q(\eta)&=\tfrac{1}{6}v^2R-v^{-1}v''\\&=\frac{1}{18}\left[\left(\frac{l_1'}{l_1}-\frac{l_2'}{l_2}\right)^2+\left(\frac{l_2'}{l_2}-\frac{l_3'}{l_3}\right)^2+\left(\frac{l_3'}{l_3}-\frac{l_1'}{l_1}\right)^2\right]\\&\quad-\tfrac{1}{6}v^{-4}[l_1{}^4+l_2{}^4+l_3{}^4-\tfrac{1}{2}(l_1{}^2+l_2{}^2+l_3{}^2)^2]\,.\end{aligned} \tag{54}$$

In the formulas of Sec. III, therefore, $\mathcal{H}_{kk'}$ is to be replaced by $(\Omega^2)_{kk'}+Q\delta_{kk'}$, and E_j by $(E_j{}^2+\frac{1}{6}R)^{1/2}$. Moreover, the factor $[V(t)/V(t_0)]^{1/2}$ in Eqs. (43) must be replaced by $[V(t)/V(t_0)]^{1/6}$. The advantage of Eqs. (52)–(54) is that Q does not involve second-order η derivatives.

The first term in Eq. (54) (involving derivatives of the l's) matches the result of Zel'dovich and Starobinsky for the Kasner universe.[25] The second term represents the effect of three-space curvature. The primary sources of different behavior of the system in the mixmaster case, as compared with Kasner, will be the off-diagonal matrix elements of Ω^2, and the additional term in Q.

For completeness, we remark that an alternative approach to the theory of minimal coupling is also available. Let

$$F_k(t)=V^{1/2}C_k(t) \tag{55}$$

and retain the original time coordinate t. One obtains as the analogue of Eq. (14)

$$\frac{d^2F_k}{dt^2}-(\Gamma^2+\dot{\Gamma})F_k+\sum_{k'}M_{kk'}F_{k'}=0\,, \tag{56}$$

where the $M_{kk'}$ are matrix elements of $-{}^{(3)}\Delta+\mu^2$. The $\frac{1}{6}R$ term could be added to this operator for conformal coupling. In this case Sec. III is modified by replacing $\mathcal{H}_{kk'}$ with $M_{kk'}-(\Gamma^2+\dot{\Gamma})\delta_{kk'}$, and the factor $[V(t)/V(t_0)]^{1/2}$ does not appear in Eqs. (43). We prefer the approach presented in Sec. I, because (for minimal coupling) the operator $\mathcal{H}$ [Eq. (17)] has a simple form and is positive definite, a feature which simplifies asymptotic analysis.

V. DISCUSSION

In this paper we considered the quantum theory of a scalar field in a mixmaster universe, as part of an investigation of the question of anisotropy damping caused by particle creation and mode mixing. It is next necessary to construct the energy-momentum tensor, the expectation value of which acts as the source of the gravitational field.[26] The energy-momentum tensor is thus the primary physical quantity. The introduction of suitable creation and annihilation operators is useful, nevertheless, in renormalization of the energy-momentum tensor and in the specification of state vectors.

Instantaneous diagonalization of the Hamiltonian was used here as the basis for defining creation and annihilation operators. Recent work[27] on the analogous theory of a quantized scalar field in a Robertson-Walker universe suggests that a different definition is more useful and natural in connection with renormalization of the energy-momentum tensor and specification of state. The operators so defined correspond to physical particles for large momenta or slow expansion rates, in which cases the concept of physical particle is meaningful. The generalization of that approach to the mixmaster geometry is under study. The techniques of the present paper and the results regarding the existence of particle creation and mode mixing will almost certainly remain valid, even though we anticipate that the definition of particle operators and the corresponding Bogolubov transformation will be somewhat modified. To complete the determination of the renormalized energy-momentum tensor, furthermore, it is necessary to analyze the asymptotic behavior at large E_j of the Bogolubov coefficients. While these questions are under investigation, we plan to study anisotropy damping in universes of the Kasner or Taub type, for which the problem of coupled modes does not arise. We intend then to continue with the mixmaster problem.

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[9]In this paper we use the metric signature $(-+++)$. Also, we set $\hbar = c = 1$. Indices μ, ν, ... range from 0 to 3; a, b ... range from 1 to 3.

[10]A three-dimensional space with the topology of the three-sphere, considered as a differentiable manifold, can be identified with the group SU(2) (see, e.g., the first paper of Ref. 15). The latter is in two-to-one correspondence with SO(3), the three-dimensional rotation group, which is also the manifold of possible orientations of a rigid body (asymmetric top). The group $G \equiv SU(2) \otimes SU(2)$ acts on SU(2) itself by left and right multiplication: $(A, B) \in G$ corresponds to the mapping $U \rightarrow AUB^{-1}$, all $U \in SU(2)$. Under the identification of SU(2) with the sphere, G is seen to be homomorphic to SO(4), the connected part of the isometry group of a metric three-sphere. The left multiplications form the subgroup of isometries which remain when one passes to a mixmaster space (which has the topology of a true three-sphere but not its metric). Under the further identification with the states of a top, these preserved symmetries correspond to ordinary rotations in space, while the broken ones (the right multiplications) are rotations about axes fixed in the body. One of the latter operations is not a symmetry unless its axis is an axis of symmetry of the body.

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[19]H, the Hamiltonian of the field theory, must not be confused with $-{}^{(3)}\Delta + \mu^2$, the Hamiltonian of the asymmetric top (plus a constant). In the static situation the latter may be regarded as the square of the Hamiltonian describing a single particle before second quantization (see Ref. 17).

[20]These may be defined in various ways for mathematical convenience, and correspond to quanta which do not necessarily coincide with physical particles, except in the static limit. However, an identification of physical particle operators in the high-momentum limit leads to renormalization of the energy-momentum tensor (see Ref. 27).

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[23]Note that Eqs. (36) and (37) hold only at time t_0. The asymmetry between t_0 and t is introduced purely for calculational convenience. Note also that Eqs. (37) and (12) do not imply Eq. (36), since the w_j^*, as a set, are not linearly independent of the w_j.

[24]The sign conventions adopted here are such that $R=+6[\ddot{a}/a+(\dot{a}/a)^2]$ for a spatially flat Robertson-Walker space-time with radius function $a(t)$. The definition of R in terms of the metric $g_{\mu\nu}$ coincides with that of Ref. 5. [taken from L. D. Landau and E. M. Lifshitz, *The Classical Theory of Fields* (Addison-Wesley, Reading, Mass., 1951)]. However, because the sign of our metric [Eq. (3)] is opposite to that of Ref. 5, expressions for R in terms of parameters such as $a(t)$ or the $l_a(t)$ are also opposite in sign. Hence the relative sign of μ^2 and $\frac{1}{6}R$ in Eq. (44), unlike Ref. 5, agrees with that in most American literature on the conformally coupled scalar field [C. G. Callan, Jr., S. Coleman, and R. Jackiw, Ann. Phys. (N.Y.) 59, 42 (1970); L. Parker, Phys. Rev. D 7, 976 (1973)], although our metric is opposite in sign.

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