Scalar field in the early Universe: Coherent-state representation and thermal density matrix

Beverly K. Berger
Physics Department, Oakland University, Rochester, Michigan 48063
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A coherent-state representation valid even near the singularity is constructed for each mode of a quantized scalar field in a classical spatially homogeneous anisotropic background cosmology. The stress-energy tensor expectation values are computed in a coherent state and shown to be classical except for zero-point-energy terms. The self-consistent problem of a quantized scalar field in a changing background metric is discussed. The scalar field can also be described by a density matrix rather than a pure state. The density matrix is then used to determine expectation values. The density matrix need not be a thermal distribution although such a choice is reasonable in a realistic model. Temperature estimates are made using dimensional analysis.

I. INTRODUCTION

Recent advances in grand unified theories of strong, weak, and electromagnetic interactions have hinted that it may be possible to correlate observational data with quantum processes in the early Universe.[1,2] This has caused increasing interest in the study of quantum field theory in curved spacetime.[3] In this paper we consider a minimally coupled quantized massive scalar field in a prescribed classical background cosmological spacetime. The behavior of the classical scalar field near the cosmological singularity[4,5] is best followed quantum mechanically by constructing an (over) complete set of coherent states for each mode of the scalar field.[6,7] The coherent states are parametrized by initial conditions for the scalar field. These states become the usual minimum-uncertainty wave packets if (and only if) the time scale for the evolution of the background spacetime is much greater than the periods of oscillation of the modes of the scalar field.[8]

The coherent-state representation can be related to the N representation[4,7] so that expectation values may be easily calculated. The scalar-field stress-energy tensor expectation values can be computed in a coherent state.[9] These expectation values are shown to split into a classical term and an (infinite) vacuum fluctuation term. If the vacuum term can be regularized,[10] it is shown that it is possible to set up the self-consistent problem of a quantized scalar field in a changing classical cosmology.[11]

Observations of the cosmic microwave background indicate that the Universe is highly isotropic.[12] This high degree of isotropy may be either a consequence of very special initial conditions[13] or an inevitable result of dissipative processes in an originally chaotic Universe.[14] Ideally, the latter scenario would not require one to specify initial conditions for the Universe.

Hawking has proposed[15] a way to avoid the requirement to specify the initial conditions $p_{\vec{k}0}, q_{\vec{k}0}$ for each mode. The quantum state of the scalar field near the initial singularity is inaccessible to an observer at the present time just as the state of the quantized scalar field inside a black-hole event horizon is inaccessible to an observer at infinity.[16] Hawking's suggestion is that this ignorance of the actual state of the quantized field is best expressed by taking a random superpositon of all allowed states in the inaccessible region.[15] It is assumed that all phase information is lost so that the system can no longer be described by a pure quantum-mechanical state. It is possible, however, to construct a density matrix from which expectation values may be calculated.[7]

In this paper, we impose this "randomicity principle"[15] by superposing the coherent states in a random manner. Phase information is lost so that the scalar field is described by a density matrix rather than a pure state. The expected number of quanta at late times is the remaining free parameter for each mode. The density matrix may be used to compute interesting expectation values.

The distribution of average particle number need not be thermal although interactions (neglected in this analysis) make such a choice reasonable. If a thermal distribution is imposed, the remaining free parameter—the temperature corresponding to a chosen time or cosmological scale factor—can be fixed by dimensional analysis. A comparison with an alternative calculation which leads to a thermal distribution[17] is made.

The classical scalar field and its stress-energy tensor are introduced in Sec. II. The N representation is reviewed in Sec. III and the coherent-state representation introduced in Sec. IV. The stress-energy tensor expectation values are calculated in Sec. V and the self-consistent problem discussed in Sec. VI. The thermal density matrix is introduced in Sec. VII. An analysis to fix remaining free parameters is given in Sec. VIII. A summary is given in Sec. IX.

II. SCALAR FIELD IN CURVED SPACETIME

For convenience we consider a background cosmological metric which is spatially homogeneous, possibly anisotropic, and topologically three-torus or Euclidean. The general form for such a metric is ($\hbar = c = 1$)

$$ds^2 = -dt^2 + \sum_{i=1}^{3} a_i^2(t)(dx^i)^2 . \tag{1}$$

In this background, a minimally coupled scalar field of mass m satisfying[10]

$$(g^{\mu\nu}\nabla_\mu \nabla_\nu - m^2)\phi(x) = 0 \tag{2}$$

can be expanded in odd- and even-parity modes[4]:

$$\phi(x) = (2\pi)^{-3/2} \sum_{\vec{k}} [q_{\vec{k}}(\tau)\cos\vec{k}\cdot\vec{x} + q_{-\vec{k}}(\tau)\sin\vec{k}\cdot\vec{x}] , \tag{3}$$

where $\sum_{\vec{k}}$ is a sum over discrete modes in the three-torus model and $\int d^3\vec{k}$ in Euclidean topology. ∇_μ is the covariant derivative and $\mu = 0,1,2,3$. $g^{\mu\nu}$ is the reciprocal metric. Transformation to a new time coordinate defined by $g^{1/2}d\tau = dt$ for $g^{1/2} = a_1 a_2 a_3$ yields as an equation for the mode amplitude $q_{\vec{k}}$ (Ref. 4)

$$\frac{d^2 q_{\vec{k}}}{dt^2} + \omega_{\vec{k}}^2(\tau) q_{\vec{k}} = 0 , \tag{4a}$$

where

$$\omega_{\vec{k}}^2(\tau) = g\left(\sum_{i=1}^{3} \frac{k_i^2}{a_i^2} + m^2\right) . \tag{4b}$$

The stress-energy tensor for a scalar field is[10]

$$T_{\mu\nu} = \partial_\mu\phi\,\partial_\nu\phi - \tfrac{1}{2} g_{\mu\nu}(g^{\alpha\beta}\partial_\alpha\phi\,\partial_\beta\phi + m^2\phi^2) \tag{5}$$

for $\partial_\mu \equiv \partial/\partial x^\mu$. For the metric (1), this yields for the diagonal components[8] (using τ as time coordinate)

$$T_{00} = \frac{1}{2g}\left\{\left(\frac{\partial\phi}{\partial\tau}\right)^2 + g\left[\sum_{i=1}^{3}\frac{1}{a_i^2}(\partial_i\phi)^2 + m^2\phi^2\right]\right\} \tag{6}$$

and (for $i = 1, 2, 3$)

$$T_{ii} = (\partial_i\phi)^2 + \tfrac{1}{2} a_i^2 \left(\frac{\partial\phi}{\partial\tau}\right)^2 \frac{1}{g} - \tfrac{1}{2} a_i^2 \left[\sum_{j=1}^{3}\frac{1}{a_j^2}(\partial_j\phi)^2 + m^2\phi^2\right] . \tag{7}$$

Since the background metric is spatially homogeneous, we may require the quantum state of the system to be also spatially homogeneous.[8] Thus we need consider only the spatially homogeneous modes of expressions (6) and (7). Substitution of the expansion (3) in Eqs. (6) and (7) and $(2\pi)^{-3/2}\int d^3x$ applied to the result yields the spatially averaged components

$$\overline{T}_{00} = \frac{1}{32\pi^3 g} \sum_{\vec{k}} \left[\left(\frac{dq_{\vec{k}}}{d\tau}\right)^2 + \omega_{\vec{k}}^2(\tau) q_{\vec{k}}^2\right] \tag{8}$$

and

$$\overline{T}_{ii} = \frac{1}{32\pi^3 g} a_i^2 \sum_{\vec{k}} \left\{\left(\frac{d}{d\tau} q_{\vec{k}}\right)^2 + \left[2\frac{k_i^2}{a_i^2} g - \omega_{\vec{k}}^2(\tau)\right] q_{\vec{k}}^2\right\} \tag{9}$$

where $\sum_{\vec{k}}$ extends over both even- and odd-parity modes.

III. THE N REPRESENTATION[18]

The scalar field (3) may be quantized mode by mode by defining

$$p_{\vec{k}} \equiv \frac{dq_{\vec{k}}}{d\tau} \tag{10}$$

and imposing the usual canonical commutation relations. A complete set of orthonormal states $|n_{\vec{k}}\rangle$ can be constructed to be eigenstates of a formal number operator

$$N_{\vec{k}} \equiv A_{\vec{k}}^\dagger A_{\vec{k}} , \tag{11}$$

where

$$A_{\vec{k}} = -i\frac{d\beta_{\vec{k}}}{d\tau}(\tau) q_{\vec{k}} + i\beta_{\vec{k}}(\tau) p_{\vec{k}} . \tag{12}$$

$q_{\vec{k}}, p_{\vec{k}} = -i\partial/\partial q_{\vec{k}}$ are now operators. The c-number complex function $\beta_{\vec{k}}(\tau)$ is a solution to the classical equation (4) such that

$$\beta_{\vec{k}}^* \frac{d\beta_{\vec{k}}}{d\tau} - \beta_{\vec{k}} \frac{d}{d\tau}\beta_{\vec{k}}^* = i . \tag{13}$$

It is easily shown by differentiating Eq. (12) and using Eq. (4a) with $q_{\vec{k}}$ and $\beta_{\vec{k}}$ and Eq. (10) that $dA_{\vec{k}}/d\tau = 0$. To completely fix the representation a boundary condition must be imposed on $\beta_{\vec{k}}(\tau)$. In most models there exists a regime $\tau \approx \tau_{\rm WKB}$ defined by the WKB condition

$$\omega_{\vec{k}}^{-1}\frac{d\omega_{\vec{k}}}{d\tau} \ll \omega_{\vec{k}} , \tag{14}$$

in which we can require

$$\lim_{\tau\to\tau_{\rm WKB}} \beta_{\vec{k}}(\tau) = (2\omega_{\vec{k}})^{-1/2}\exp\left(i\int^{\tau}\omega_{\vec{k}}\,d\overline{\tau}\right) \tag{15a}$$

and

$$\lim_{\tau\to\tau_{\rm WKB}} \frac{d\beta_{\vec{k}}}{d\tau}(\tau) = i\omega_{\vec{k}}\beta_{\vec{k}}(\tau) . \tag{15b}$$

A more rigorous treatment of this type of WKB boundary condition has been given by Parker and Fulling.[8] If the scalar field is not massless ($m\neq 0$) or the topology is T^3, it is possible to choose τ_{WKB} so that Eqs. (15) are valid for all modes. If inequality (14) is valid, the formal creation and annihilation operators can be interpreted to be physical particle operators. Thus the state $|n_{\vec k}\rangle$ behaves as a harmonic-oscillator state containing $n_{\vec k}$ quanta when $\tau\approx\tau_{WKB}$. For $\tau\neq\tau_{WKB}$, the interpretation of $n_{\vec k}$ as a particle number cannot be made. Thus we shall always interpret $\langle n_{\vec k}\rangle$ to be the expected number of quanta which will be present in some state when $\tau\approx\tau_{WKB}$.

The vacuum $|0\rangle$ is the state annihilated by $A_{\vec k}$ for all modes $\vec k$. In this representation, the basis states are then

$$|\{n_{\vec k}\}\rangle \equiv \prod_{\vec k} |n_{\vec k}\rangle \tag{16}$$

for $\prod_{\vec k}$ a generalized product over modes and

$$|n_{\vec k}\rangle = (n_{\vec k}!)^{-1/2}\,(A_{\vec k}^{\dagger})^{n_{\vec k}}|0\rangle . \tag{17}$$

The choice $|0\rangle$ as the vacuum is somewhat arbitrary since no unique decomposition into positive- and negative-frequency modes is possible if the WKB condition (14) is violated. (See Refs. 4 and 8 for discussion of this point.)

IV. COHERENT-STATE REPRESENTATION

As an alternative to the N representation, we can construct an (over) complete normalized set $|\lambda_{\vec k}\rangle$ of coherent states for each mode.[7] This representation will be useful because it can be constructed to closely follow the classical behavior at all times. Coherent states are defined to be eigenstates of the formal annihilation operator:

$$A_{\vec k}|\lambda_{\vec k}\rangle = \lambda_{\vec k}|\lambda_{\vec k}\rangle , \tag{18}$$

where $\lambda_{\vec k}$ is a time-independent complex number and $A_{\vec k}$ is defined by Eq. (12). If the mass of the scalar field is nonzero[19] or the topology T^3 the representations are related by[7]

$$|\lambda_{\vec k}\rangle = \sum_{n_k=0}^{\infty} (n_{\vec k}!)^{-1/2}\lambda_{\vec k}^{n_{\vec k}}\exp(-|\lambda_{\vec k}|^2/2)\,|n_{\vec k}\rangle . \tag{19a}$$

The coherent states satisfy a completeness relation

$$\frac{1}{\pi}\int |\lambda_{\vec k}\rangle\langle\lambda_{\vec k}|\,d^2\lambda_{\vec k} = 1 , \tag{19b}$$

where $d^2\lambda_{\vec k} = (d\,\mathrm{Re}\lambda_{\vec k})(d\,\mathrm{Im}\lambda_{\vec k}) = |\lambda_{\vec k}|d|\lambda_{\vec k}|d\theta$ over the complex $\lambda_{\vec k}$ plane where θ is the phase of $\lambda_{\vec k}$. The states $|\lambda_{\vec k}\rangle$ are normalized to unity but not orthogonal. The set $\lambda_{\vec k}=0$ for all $\vec k$ corresponds to the vacuum $|0\rangle$. Expectation values are easily calculated using Eqs. (12), (13), (18), and (19a). In particular,

$$\langle\lambda_{\vec k}|q_{\vec k}|\lambda_{\vec k}\rangle = 2\,\mathrm{Re}(\beta_{\vec k}\lambda_{\vec k}^*) , \tag{20}$$

$$\langle\lambda_{\vec k}|p_{\vec k}|\lambda_{\vec k}\rangle = 2\,\mathrm{Re}\left(\frac{d\beta_{\vec k}}{d\tau}\lambda_{\vec k}^*\right) , \tag{21}$$

$$\langle\lambda_{\vec k}|q_{\vec k}^2|\lambda_{\vec k}\rangle = 2\,\mathrm{Re}(\beta_{\vec k}^{*2}\lambda_{\vec k}^2) + |\beta_{\vec k}|^2(2|\lambda_{\vec k}|^2+1) , \tag{22}$$

$$\langle\lambda_{\vec k}|p_{\vec k}^2|\lambda_{\vec k}\rangle = 2\,\mathrm{Re}\left[\left(\frac{d\beta_{\vec k}^*}{d\tau}\right)^2\lambda_{\vec k}^2\right] + \left|\frac{d\beta_{\vec k}}{d\tau}\right|^2(2|\lambda_{\vec k}|^2+1) , \tag{23}$$

and

$$\langle\lambda_{\vec k}|N_{\vec k}|\lambda_{\vec k}\rangle = |\lambda_{\vec k}|^2 . \tag{24}$$

It is also interesting to evaluate the uncertainties $\Delta q_{\vec k}\equiv(\langle q_{\vec k}^2\rangle-\langle q_{\vec k}\rangle^2)^{1/2}$, $\Delta p_{\vec k}\equiv(\langle p_{\vec k}^2\rangle-\langle p_{\vec k}\rangle^2)^{1/2}$ in the coherent states. We find

$$\Delta q_{\vec k} = |\beta_{\vec k}| , \tag{25a}$$

$$\Delta p_{\vec k} = |d\beta_{\vec k}/d\tau| . \tag{25b}$$

From Eqs. (15), we see that the $|\lambda_{\vec k}\rangle$ are minimum-uncertainty wave packets[20,4,7] when $\tau\approx\tau_{WKB}$. The form of Eqs. (25) also shows that quantum effects measured by $\Delta p_{\vec k}$, $\Delta q_{\vec k}$ are vacuum expectation values independent of $\lambda_{\vec k}$.

To completely fix the coherent-state representation, we require $\langle\lambda_{\vec k}|q_{\vec k}|\lambda_{\vec k}\rangle$ to be the real solution to the classical Eq. (4) characterized by the two arbitrary constants $p_{\vec k0}, q_{\vec k0}$. This will yield $\lambda_{\vec k}$ as a function of $p_{\vec k0}, q_{\vec k0}$. The boundary condition (15) selects the appropriate exact complex solution $\beta_{\vec k}(\tau)$ to the classical equation (4).

As a typical example, we consider a cosmological model with a vanishing proper volume singularity at τ_S. In a model of this type, we expect Eq. (4b) to imply that

$$\lim_{\tau\to\tau_S}\omega_{\vec k}(\tau) = 0 . \tag{26}$$

In this case, the classical mode amplitude near τ_S can be written as

$$\lim_{\tau\to\tau_S} q_{\vec k}^{\mathrm{cl}}(\tau) = q_{\vec k0} + p_{\vec k0}\tau . \tag{27}$$

The general form for $\beta_{\vec k}(\tau)$ as $\tau\to\tau_S$ with the Wronskian (13) may be expressed as

$$\lim_{\tau\to\tau_S}\beta_{\vec k}(\tau) = e^{i\alpha}\left[b+\frac{1}{2b}(c+i)\tau\right] , \tag{28}$$

since Eq. (13) reduces the two arbitrary complex constants of the general solution to Eq. (4) to three real parameters. The form of Eq. (28) was chosen to automatically have the correct Wronskian. The parameters a, b, c are then identified when the limit as $\tau \to \tau_S$ of the solution of Eq. (4) with the correct Wronskian is taken. Thus the real numbers a, b, c are known mode-dependent parameters of the exact solutions to Eq. (4) and define the particular solution to the classical equation which satisfies the "positive-frequency" condition (15a) in the WKB limit. The coherent-state parameter $\lambda_{\vec{k}}$ can now be obtained by using Eqs. (27) and (28), respectively, in the left- and right-hand sides of Eq. (20). We find

$$\mathrm{Re}\lambda_{\vec{k}} = \frac{q_{\vec{k}0}}{2b}(c\,\sin a + \cos a) - p_{\vec{k}0}\,b\,\sin a \tag{29a}$$

and

$$\mathrm{Im}\lambda_{\vec{k}} = \frac{q_{\vec{k}0}}{2b}(-\sin a + c\,\cos a) - p_{\vec{k}0}\,b\,\cos a\,. \tag{29b}$$

From Eq. (24), this yields as the number of quanta in the state $|\lambda_{\vec{k}}\rangle$ in the limit $\tau \to \tau_{\mathrm{WKB}}$ (Ref. 21)

$$\langle\lambda_{\vec{k}}|N_{\vec{k}}|\lambda_{\vec{k}}\rangle = \frac{q_{\vec{k}0}^{\,2}}{4b^2}(c^2+1) + p_{\vec{k}0}^{\,2}b^2 - p_{\vec{k}0}q_{\vec{k}0}c\,. \tag{30}$$

The coherent-state representation presents a natural method for relating WKB behavior to singularity parameters. The procedure to obtain $\lambda_{\vec{k}}$ as a function of $p_{\vec{k}0}, q_{\vec{k}0}$ may be repeated for any dependence of $\omega_{\vec{k}}(\tau)$ or $q_{\vec{k}}^{\mathrm{cl}}(\tau)$ as $\tau \to \tau_S$ rather than Eqs. (26) and (27).

V. COHERENT-STATE STRESS-ENERGY TENSOR EXPECTATION VALUES

Expressions (22) and (23) may be used with Eqs. (8) and (9) to obtain[22] $\langle\lambda_{\vec{k}}|\overline{T}^{\vec{k}}_{00}|\lambda_{\vec{k}}\rangle$ and $\langle\lambda_{\vec{k}}|\overline{T}^{\vec{k}}_{ii}|\lambda_{\vec{k}}\rangle$, where $\overline{T}^{\vec{k}}_{00}$, $\overline{T}^{\vec{k}}_{ii}$ are the $\vec{k}$th mode pieces of $\overline{T}_{00}$ and $\overline{T}_{ii}$. We find

$$32\pi^3 g\langle\lambda_{\vec{k}}|T^{\vec{k}}_{00}|\lambda_{\vec{k}}\rangle = 2\,\mathrm{Re}\left\{\lambda_{\vec{k}}^{*2}\left[\left(\frac{d\beta_{\vec{k}}}{d\tau}\right)^2 + \omega_{\vec{k}}^{\,2}(\tau)\beta_{\vec{k}}^{\,2}\right]\right\} + (2|\lambda_{\vec{k}}|^2+1)\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \omega_{\vec{k}}^{\,2}(\tau)|\beta_{\vec{k}}|^2\right] \tag{31}$$

and

$$\frac{32\pi^3}{a_i^{\,2}} g\langle\lambda_{\vec{k}}|\overline{T}^{\vec{k}}_{ii}|\lambda_{\vec{k}}\rangle = 2\,\mathrm{Re}\left\{\lambda_{\vec{k}}^{*2}\left[\left(\frac{d\beta_{\vec{k}}}{d\tau}\right)^2 + \left(\frac{2k_i^{\,2}g}{a_i^{\,2}} - \omega_{\vec{k}}^{\,2}\right)\beta_{\vec{k}}^{\,2}\right]\right\} + (2|\lambda_{\vec{k}}|^2+1)\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \left(\frac{2k_i^{\,2}}{a_i^{\,2}}g - \omega_{\vec{k}}^{\,2}\right)|\beta_{\vec{k}}|^2\right]. \tag{32}$$

From the uncertainties $\Delta q_{\vec{k}}$, $\Delta p_{\vec{k}}$ given by Eq. (25), it is clear that only the vacuum terms in the expectation values (22) and (23) do not appear in $\langle q_{\vec{k}}\rangle^2$ or $\langle p_{\vec{k}}\rangle^2$ for coherent states. Since $\langle q_{\vec{k}}\rangle$ and thus $\langle p_{\vec{k}}\rangle$ have been constructed to follow the classical behavior of the field amplitude and $\overline{T}^{\vec{k}}_{\mu\nu}$ contains only terms of the form $p_{\vec{k}}^{\,2}$ or $q_{\vec{k}}^{\,2}$ [see Eqs. (8) and (9)], only the zero-point-energy terms in $\langle\overline{T}^{\vec{k}}_{\mu\nu}\rangle$ in a coherent state cannot be obtained by treating $\overline{T}^{\vec{k}}_{\mu\nu}$ as a classical quantity. As is well known,[22] the vacuum expectation values are the vacuum energy density

$$\rho_0 \equiv -\langle 0|\overline{T}_0^{\,0}|0\rangle = \frac{1}{32\pi^3 g}\sum_{\vec{k}}\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \omega_{\vec{k}}^{\,2}(\tau)|\beta_{\vec{k}}|^2\right] \tag{33}$$

and anisotropic pressure

$$P_{i0} \equiv \langle 0|\overline{T}_i^{\,i}|0\rangle = \frac{1}{32\pi^3 g}\sum_{\vec{k}}\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \left(\frac{2k_i^{\,2}g}{a_i^{\,2}} - \omega_{\vec{k}}^{\,2}\right)|\beta_{\vec{k}}|^2\right]. \tag{34}$$

The $\lambda_{\vec{k}}$, or equivalently $p_{\vec{k}0}, q_{\vec{k}0}$, may be chosen so that the classical stress-energy tensor expectation values are finite if $\tau \neq \tau_S$. Only the vacuum expectation values must be regularized. Thus we may express the stress-energy tensor expectation values in any coherent state

$$|\{\lambda_{\vec{k}}\}\rangle \equiv \prod_{\vec{k}}|\lambda_{\vec{k}}\rangle \tag{35}$$

to be

$$\rho = \rho_0 + \rho^{\mathrm{cl}}, \quad P_i = P_{i0} + P_i^{\mathrm{cl}} \tag{36}$$

for

$$\rho^{\mathrm{cl}} = \frac{1}{16\pi^3 g}\sum_{\vec{k}}\left(\mathrm{Re}\left\{\lambda_{\vec{k}}^{*2}\left[\left(\frac{d\beta_{\vec{k}}}{d\tau}\right)^2 + \omega_{\vec{k}}^{\,2}\beta_{\vec{k}}^{\,2}\right]\right\} + |\lambda_{\vec{k}}|^2\left(\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \omega_{\vec{k}}^{\,2}|\beta_{\vec{k}}|^2\right)\right) \tag{37}$$

the classical energy density and

$$P_i^{\mathrm{cl}} = \frac{1}{16\pi^3 g}\sum_{\vec{k}}\left(\mathrm{Re}\left\{\lambda_{\vec{k}}^{*2}\left[\left(\frac{d\beta_{\vec{k}}}{d\tau}\right)^2 + \left(\frac{2k_i^{\,2}g}{a_i^{\,2}} - \omega_{\vec{k}}^{\,2}\right)\beta_{\vec{k}}^{\,2}\right]\right\} + |\lambda_{\vec{k}}|^2\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \left(\frac{2k_i^{\,2}g}{a_i^{\,2}} - \omega_{\vec{k}}^{\,2}\right)|\beta_{\vec{k}}|^2\right]\right) \tag{38}$$

the classical anisotropic pressure. The term classical is used because in fact Eqs. (37) and (38) are equivalent to

$$\rho^{\mathrm{cl}} = \overline{T}_{00} = -(\overline{T}_0{}^0)\,, \tag{39a}$$

$$P_i^{\mathrm{cl}} = a_i{}^{-2}\overline{T}_{ii} = (\overline{T}_i{}^i)\,, \tag{39b}$$

where $\overline{T}_{00}$, $\overline{T}_{ii}$ are from Eqs. (8) and (9) with $q_{\vec{k}}$ interpreted to be the classical solution to Eq. (4). [Indices are raised and lowered with the metric (1).] That is—if rather than a quantized scalar field, we treated the classical scalar field, defined $\lambda_{\vec{k}}$ and $\beta_{\vec{k}}$ as we have before, and used Eqs. (20) and (21) with the expectation values replaced by classical variables $q_{\vec{k}}, p_{\vec{k}}$ to express $q_{\vec{k}}, p_{\vec{k}}$ in terms of $\lambda_{\vec{k}}$ and $\beta_{\vec{k}}$, then $\overline{T}^{\vec{k}}_{\mu\nu}$ from Eqs. (8) and (9) considered to be a classical quantity could be written in terms of $\lambda_{\vec{k}}$ and $\beta_{\vec{k}}$. This procedure would yield expressions (37)–(39). This almost classical behavior of $\langle T^{\vec{k}}_{\mu\nu}\rangle$ is special to coherent states and is due to the presence of only vacuum terms in the uncertainties given by Eq. (25).

VI. REMARKS ON THE SELF-CONSISTENT PROBLEM

If we can assume that the scalar field is in a coherent state, the self-consistent problem—inclusion of the effect of the scalar field on the classical background cosmology (1)—can be formulated. We must solve[11] (using the conventions of Ref. 23 with $G=1$)

$$G_{\mu\nu} = 8\pi\langle\{\lambda_{\vec{k}}\}|T_{\mu\nu}|\{\lambda_{\vec{k}}\}\rangle\,, \tag{40}$$

where $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R$ is the Einstein tensor formed from the metric (1) and $|\{\lambda_{\vec{k}}\}\rangle$ is a coherent state. In terms of the original time coordinate (overdot$=d/dt$) Eqs. (40) become[24]

$$\frac{\dot a_1\dot a_2}{a_1a_2} + \frac{\dot a_1\dot a_3}{a_1a_3} + \frac{\dot a_2\dot a_3}{a_2a_3} = 8\pi(\rho^{\mathrm{cl}} + \rho_0^{\mathrm{reg}}) \tag{41}$$

and

$$-\frac{\ddot a_2}{a_2} - \frac{\ddot a_3}{a_3} - \frac{\dot a_2\dot a_3}{a_2a_3} = 8\pi(P_1^{\mathrm{cl}} + P_{10}^{\mathrm{reg}}) \tag{42}$$

with permuted expressions for the 2 and 3 components. The stress-energy terms ρ^{cl}, P_i^{cl} are [see Eq. (39)] from Eqs. (8) and (9) with $q_{\vec{k}}$ classical and ρ_0^{reg}, P_{i0}^{reg} are suitably regularized expressions obtained from Eqs. (33) and (34). The condition that $\nabla_\mu\langle T^\mu_\nu\rangle = 0$ imposes the additional requirement that

$$\dot\rho + \sum_{i=1}^{3}(a_i)^{-1}\dot a_i(\rho + P_i) = 0\,. \tag{43}$$

The regularized vacuum expectation values have been catalogued for several interesting background cosmologies.[25] If the set of initial conditions $p_{\vec{k}0}, q_{\vec{k}0}$ for the classical energy density and anisotropic pressure is chosen conveniently, a self-consistent solution may be obtained by solving Eqs. (4), (39), and (41)–(43) with the prescribed ρ_0^{reg}, P_0^{reg} as a function of the background metric.[26] Performance of this calculation for various backgrounds and choices of classical scalar fields will be left to a later paper.

We note that to use a scalar field in a coherent state to calculate quantum effects leading to singularity avoidance[3,9] may yield ambiguous results. This is due to the fact that the energy conditions required by the singularity theorems are violated by a classical scalar field of mass m if the Universe scale factor is smaller than the Compton wavelength associated with the mass m.[27]

VII. CONSTRUCTION OF THE DENSITY MATRIX AND EXPECTATION VALUES

To avoid specification of $p_{\vec{k}0}, q_{\vec{k}0}$ or equivalently $\lambda_{\vec{k}}$, we recognize that any state of the scalar field may be constructed by superposing the $|\lambda_{\vec{k}}\rangle$. Since the actual $\lambda_{\vec{k}}$ values required at the singularity are not known, we may assume a Gaussian distribution of $\lambda_{\vec{k}}$ values. We may assume that the state of the system is

$$|\;\rangle_{\vec{k}} = \int d^2\lambda_{\vec{k}}\,\alpha(\lambda_{\vec{k}})|\lambda_{\vec{k}}\rangle\,. \tag{44}$$

According to the "randomicity principle," however, phase information for the amplitude $\alpha(\lambda_{\vec{k}})$ cannot be determined. Thus only $|\alpha(\lambda_{\vec{k}})|^2$ may be specified. This allows construction of a density matrix

$$\rho_{\vec{k}} \equiv |\;\rangle_{\vec{k}\,\vec{k}}\langle\;| = \int d^2\lambda_{\vec{k}}|\alpha(\lambda_{\vec{k}})|^2|\lambda_{\vec{k}}\rangle\langle\lambda_{\vec{k}}|\,, \tag{45a}$$

where we have assumed that the random-phase approximation replaces

$$\int d^2\lambda_{\vec{k}}\int d^2\lambda'_{\vec{k}}\alpha^*(\lambda'_{\vec{k}})\alpha(\lambda_{\vec{k}})|\lambda_{\vec{k}}\rangle\langle\lambda'_{\vec{k}}|$$

with

$$\int d^2\lambda_{\vec{k}}\int d^2\lambda'_{\vec{k}}\delta(\lambda'_{\vec{k}} - \lambda_{\vec{k}})\alpha^*(\lambda'_{\vec{k}})\alpha(\lambda_{\vec{k}})|\lambda_{\vec{k}}\rangle\langle\lambda'_{\vec{k}}|\,.$$

The diagonal matrix elements of the density matrix are $|\alpha(\lambda_{\vec{k}})|^2|\lambda_{\vec{k}}\rangle\langle\lambda_{\vec{k}}|$ for each value $\lambda_{\vec{k}}$. We then require a Gaussian

$$|\alpha(\lambda_{\vec{k}})|^2 = \frac{1}{\pi\langle n_{\vec{k}}\rangle}e^{-|\lambda_{\vec{k}}|^2/\langle n_{\vec{k}}\rangle}\,, \tag{45b}$$

where $\langle n_{\vec{k}}\rangle$ is the expected value of $A^\dagger_{\vec{k}}A_{\vec{k}}$.[7] [In quantum optics, the density matrix (45) can arise when an oscillator is excited by incoherent sources.[7]] Since from Sec. IV the $|\lambda_{\vec{k}}\rangle$ have unit norm, Eqs. (45) imply that

$$\mathrm{tr}\rho_{\vec{k}} \equiv 2\pi \int_0^\infty |\lambda_{\vec{k}}|d|\lambda_{\vec{k}}||\alpha(\lambda_{\vec{k}})|^2\langle\lambda_{\vec{k}}|\lambda_{\vec{k}}\rangle\langle\lambda_{\vec{k}}|\lambda_{\vec{k}}\rangle = 1 .$$

The coherent state for the scalar field is the product over modes of the coherent state for each mode. We assume the modes to be noninteracting so that the density matrix for the field is just the product of the density matrices for each mode.[7] Thus we find for the scalar field a density matrix

$$\rho = \int \left(\prod_{\vec{k}} \frac{d^2\lambda_{\vec{k}}}{\pi\langle n_{\vec{k}}\rangle}\right) \exp\left(-\sum_{\vec{k}} \frac{|\lambda_{\vec{k}}|^2}{\langle n_{\vec{k}}\rangle}\right) |\{\lambda_{\vec{k}}\}\rangle\langle\{\lambda_{\vec{k}}\}| , \quad (46)$$

where

$$|\{\lambda_{\vec{k}}\}\rangle \equiv \prod_{\vec{k}} |\lambda_{\vec{k}}\rangle .$$

The density matrix (46) may be used to evaluate expectation values through[7]

$$\langle A\rangle = \mathrm{tr}\rho A , \quad (47)$$

where $\langle A\rangle$ is the expectation value of any operator A. If it is convenient, the mode $\vec{k}$ portion of ρ from Eq. (45) may be used to find $\langle A_{\vec{k}}\rangle$. It is easy to show that

$$\langle N_{\vec{k}}\rangle = \mathrm{tr}\rho_{\vec{k}} A_{\vec{k}}^\dagger A_{\vec{k}} = \langle n_{\vec{k}}\rangle \quad (48)$$

so that the formulation is consistent. Using the density matrix as in Eq. (47) for the stress-tensor expectation values yields

$$\begin{aligned}\langle T^{\vec{k}}_{\mu\nu}\rangle &= \mathrm{tr}\, T^{\vec{k}}_{\mu\nu}\rho_{\vec{k}} \\ &= \int d^2\lambda_{\vec{k}} |\alpha(\lambda_{\vec{k}})|^2 \langle\lambda_{\vec{k}}|T^{\vec{k}}_{\mu\nu}|\lambda_{\vec{k}}\rangle , \end{aligned} \quad (49)$$

where $|\alpha(\lambda_{\vec{k}})|^2$ is given by Eq. (45b) and the coherent-state expectation values are to be found from Eqs. (31) and (32). Since $d^2\lambda_{\vec{k}} = |\lambda_{\vec{k}}|d|\lambda_{\vec{k}}|d\phi_{\vec{k}}$ for $\lambda_{\vec{k}} = |\lambda_{\vec{k}}|e^{i\phi_{\vec{k}}}$, the terms in braces in expectations (31) and (32) do not contribute to the expectation value (49). Since $\langle\lambda_{\vec{k}}|N_{\vec{k}}|\lambda_{\vec{k}}\rangle = |\lambda_{\vec{k}}|^2$ and $\mathrm{tr}\rho_{\vec{k}} = 1$, we find easily that

$$\langle T^{\vec{k}}_{00}\rangle = \frac{1}{32\pi^3 g}(2\langle n_{\vec{k}}\rangle + 1)\left[\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \omega_{\vec{k}}^2(\tau)|\beta_{\vec{k}}|^2\right] \quad (50)$$

and

$$\langle T^{\vec{k}}_{ii}\rangle = \frac{a_i^{\,2}}{32\pi^3 g}(2\langle n_{\vec{k}}\rangle + 1)\left\{\left|\frac{d\beta_{\vec{k}}}{d\tau}\right|^2 + \left[\frac{2k_i^{\,2}}{a_i^{\,2}}g - \omega_{\vec{k}}^2(\tau)\right]|\beta_{\vec{k}}|^2\right\} . \quad (51)$$

We have previously argued[4] that the interpretation of $\langle n_{\vec{k}}\rangle$ as a particle number is valid only in a WKB regime defined by $\omega_{\vec{k}}^{-1}d\omega_{\vec{k}}/d\tau \ll \omega_{\vec{k}}$. This condition will be valid for mode proper wavelengths smaller than the Hubble radius.[3] In such a regime (say for $\tau \approx \tau_{\mathrm{WKB}}$) we require the WKB limit Eqs. (15) for $\beta_{\vec{k}}$. Now evaluate Eqs. (50) and (51) in the WKB limit so that $\langle n_{\vec{k}}\rangle$ can have its usual interpretation. We find

$$\lim_{\tau\to\tau_{\mathrm{WKB}}} \langle T^{\vec{k}}_{00}\rangle = \frac{1}{16\pi^3 g}(\langle n_{\vec{k}}\rangle + \tfrac{1}{2})\omega_{\vec{k}} \quad (52)$$

and

$$\lim_{\tau\to\tau_{\mathrm{WKB}}} \langle T^{\vec{k}}_{ii}\rangle = \frac{k_i^{\,2}}{16\pi^3\omega_{\vec{k}}}(\langle n_{\vec{k}}\rangle + \tfrac{1}{2}) . \quad (53)$$

Using the definition (4b) for $\omega_{\vec{k}}$ and the metric (1), it is clear that the trace of $\langle T^{\vec{k}}_{\mu\nu}\rangle$ is formally zero for a massless scalar field. Of course, regularization of the vacuum stress-energy term may yield a trace anomaly.[3]

VIII. A THERMAL DISTRIBUTION

Let us rewrite Eq. (52) using the definition (4b) for $\omega_{\vec{k}}$. Let us further define the energy density ϵ to be $\sum_{\vec{k}}\langle(-T_0^{0\vec{k}})\rangle$ where $\sum_{\vec{k}}$ is either a sum over discrete modes for T^3 topology or $\int d\vec{k}$ for E^3 topology. Thus

$$\epsilon = \frac{1}{16\pi^3 g^{1/2}} \sum_{\vec{k}} (\langle n_{\vec{k}}\rangle + \tfrac{1}{2})\left(\sum_{i=1}^{3}\frac{k_i^{\,2}}{a_i^{\,2}} + m^2\right)^{1/2} . \quad (54)$$

Thermodynamical considerations may be invoked to prescribe $\langle n_{\vec{k}}\rangle$.

For an anisotropically expanding Universe containing only noninteracting scalar quanta, there is no reason to assume that the system is in thermal equilibrium.[28] In a realistic model, however, other fields and interactions are present so that a temperature should be definable. In fact, inclusion of "back reaction" of the field quanta on the metric[14] may argue for thermalization as well as isotropization. Let us attempt to define a reasonable thermal distribution. A similar analysis has been given by Parker (Ref. 17).

First assume that only the "classical" $\langle n_{\vec{k}}\rangle$ participates in the thermal distribution since the zero-point-energy (vacuum) contribution is determined uniquely and separately by regularization.[3] Let us further assume that a self-consistent calculation has been performed[29] leading in the WKB regime to a background metric which is isotropic: $a_1 = a_2 = a_3 = a$. With these assumptions, the energy density (54) becomes

$$\epsilon = \frac{1}{2(2\pi)^3}\frac{1}{a^3}\sum_{\vec{k}} \langle n_{\vec{k}}\rangle\left(\frac{k^2}{a^2} + m^2\right)^{1/2} , \quad (55)$$

where $k^2 = \sum_{i=1}^{3} k_i^{\,2}$. Now let us consider the temperature to be sufficiently high that the quanta are relativistic so m may be neglected. Then

$$\langle n_{\vec{k}} \rangle = (e^{k/aT} - 1)^{-1} \tag{56}$$

for a temperature (in energy units)

$$T = T_c a_c / a \,. \tag{57}$$

We may interpret k/a to be the proper wave number for the mode $\vec{k}$. This yields $\langle n_{\vec{k}} \rangle$ which is time independent although the energy density (55) does decrease during the expansion (as a^{-4} for the relativistic limit and as a^{-3} for the nonrelativistic limit).

We have now reduced the specification of the scalar field to the parameter $T_c a_c$. In the standard cosmological models,[30] one associates the Planck temperature $T_{\text{Pl}} \equiv (c^3\hbar/G)^{1/2}$ with the Planck time $t_{\text{Pl}} \equiv (G\hbar/c^5)^{1/2}$. If we then choose $T_c = T_{\text{Pl}}$, k/a_c becomes the proper wave number for the mode $\vec{k}$ at the Planck time. From Eq. (58) we see that this also implies the association of the observed present blackbody temperature with the present proper wave number.[31]

XI. DISCUSSION

An overcomplete set of coherent states can be constructed for each mode of a scalar field in a background anisotropic cosmology. In the WKB regime, $\tau \approx \tau_{\text{WKB}}$, these states become minimum-uncertainty wave packets.[20]

The coherent-state representation becomes useful when a particular complex eigenvalue $\lambda_{\vec{k}}$ is associated with parameters $p_{\vec{k}0}, q_{\vec{k}0}$ of the classical solution for the mode amplitude. The expectation values of $q_{\vec{k}}, p_{\vec{k}}$ in the coherent states are just the classical solutions. Quantum effects appear only in zero-point-energy terms. In a self-consistent "back-reaction" calculation, assumption of a coherent state for the scalar field allows the stress-energy tensor expectation values to be treated as a superposition of classical and regularized vacuum terms.

By starting with the coherent-state representation one can naturally incorporate our ignorance of the state of a quantized field near the cosmological singularity. Invoking a randomicity principle leads to a density matrix (rather than pure state) for the quantized field. The density matrix used is the same as that for a scalar field excited by incoherent sources.[7]

The density matrix need not be a thermal distribution, although arguments with regarded to neglected interactions and back reaction suggest that such a distribution might not be unreasonable. In this regard, we cite a calculation by Parker[17] in which a thermal distribution is obtained by evaluating $\langle n_{\vec{k}} \rangle$ at late times for a scalar field initially in the vacuum state in a universe whose scale factor smoothly approaches a constant rather than a singularity. (The initial vacuum state is of course defined in such a model.) The resultant thermal distribution is quite general for models of this class.[17] The temperature parameter (analogous to $T_c a_c$) depends on the constant approached by the scale factor.[17] Such behavior by the scale factor might be reasonable in cosmological models which exhibit a bounce. Calculations indicate that (in a closed universe) such a bounce could occur for a model containing a scalar field of mass m when the cosmological scale factor is on the order of the Compton wavelength $1/m$.[32]

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