PHYSICAL REVIEW D VOLUME 29, NUMBER 8 15 APRIL 1984

Riemannian approach and cosmological singularity

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(Received 27 May 1983)

We study the definition of the Feynman propagator for a free conformally coupled scalar field on a Robertson-Walker background, as the continuation to physical space of the single propagator of a Riemannian manifold. If the space-time has a cosmological singularity, a boundary condition is proposed that leads to the definition of particle modes at the singularity.

I. INTRODUCTION

The main problems of quantum field theory on a curved background are the definition of the particle modes and the renormalization of physical quantities. The first is necessary to compute the matter creation by the gravitational field and the second is essential to calculate the back reaction and to find the cosmological evolution.

One possible way to solve the first problem is to define the propagators of the theory, and then to find which definition of particle modes they belong to. Among these propagators, the Feynman or causal propagator is useful for this task.

In flat space-time the causal propagator is the only Green's function of the theory after a Wick rotation has been performed. The Wick rotation consists of replacing the physical time by an imaginary one, so the space-time becomes Euclidean. This operation can be generalized to other metrics (cf. Refs. 1 and 2), leading to a possible definition of the propagator on the curved background. For the linearly expanding Robertson-Walker universe the causal propagator defined in this way coincides with the well-known Chitre-Hartle propagator (cf. Refs. 3 and 4).

For the application of this method it is necessary to use a scheme to make the manifold a Riemannian one, i.e., to know how the Wick rotation should be performed. In general, a given metric allows more than one such prescription, each one leading to a different particle model (cf. Ref. 5). To avoid this difficulty we will stick to Robertson-Walker metrics, in which a common scheme to make the manifold a Riemannian one can be chosen. Although covariance of the method is a point to be elucidated, this is not a definitive drawback in Robertson-Walker metrics, because one can work in the comoving reference frame that, very likely, should be endowed with special properties. Besides, the particle concept itself is certainly noncovariant (cf. Ref. 6).

In the path-integral formulation of the flat—space-time theory, the Wick rotation not only gives mathematical meaning to the path integral but also provides the right boundary conditions for the causal propagator.[7] We want to investigate whether such a recipe still works in curved space-time. In Sec. II we introduce the general formulation, and we prove that the method of defining the causal propagator through a Wick rotation works in a Robertson-Walker space without singularities. The general form of the propagator can be written in terms of the solution of the Riemannian Klein-Gordon equation that goes to zero when the conformal time reaches infinity. In Sec. III we give some examples of actual calculations.

Since exact solutions of the Klein-Gordon equation are known only for a few metrics, for a wide application of this idea it is necessary to develop approximate methods. One possibility is to make perturbative expansions around the conformally trivial coupled massless scalar field. In Sec. IV we break the conformal triviality by including the mass as perturbative parameters, and we develop the perturbative expansion as is suggested by the formulation of Sec. II. In particular, we use the perturbative series to motivate a way to handle evolution with cosmological singularities. For the possibility of breaking the conformal triviality by varying the coupling, while the field remains massless, see Ref. 8. We discuss the properties of the perturbative expansion.

In Sec. V we stress some mathematical facts about the perturbative series and apply these methods for the calculation of the particle modes to second order in the squared mass on a general Robertson-Walker metric.

II. THE RIEMANNIAN APPROACH

We will study the theory of a real scalar field on a Robertson-Walker background with flat spatial sections (cf. Ref. 6). The metric is

$$ds^2=-dt^2+A^2(t)(d\vec{x}\cdot d\vec{x}) ,$$

where t is the "physical time" and $A^2(t)$ is the "conformal factor." If we introduce the "conformal time"

$$\eta=\int^t A^{-1}(s)ds ,$$

then

$$ds^2=A^2(\eta)[-d\eta^2+(d\vec{x}\cdot d\vec{x})] .$$

For convenience, we introduce a constant λ of units

$(\text{time})^{-1}$ and numerical value 1, so

$$ds^2 = A^2(\lambda\eta)[-d\eta^2 + (d\vec{x}\cdot d\vec{x})] \ .$$

The Klein-Gordon equation for a conformally coupled field is

$$(-\nabla_i\partial^i + \tfrac{1}{6}R + m^2)\phi = 0 \ ,$$

where $R = a^{-3}(\eta)(d^2/d\eta^2)a(\eta)$ is the curvature scalar and $a(\eta) = A(\lambda\eta)$.

A particle model is a set of solutions of the Klein-Gordon equation of the form

$$\phi_{\vec{k}}(\vec{x},\eta) = \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}a(\eta)}\psi_k(\eta) \ , \quad k = |\vec{k}|$$

normalized by the equation

$$\psi_k \frac{d}{d\eta}\psi_k^* - \psi_k^* \frac{d}{d\eta}\psi_k = i \ .$$

If a particle model is known, it is possible to build a Fock basis of states and creation and annihilation operators that bear the usual commutation relations.

The Klein-Gordon equation results from the action functional

$$S[\phi] = -\tfrac{1}{2}\int d^4x\sqrt{-g(x)}[\partial_i\phi\partial^i\phi + (m^2 + \tfrac{1}{6}R)\phi^2] \ .$$

We will take the generating functional for the theory as the direct generalization of the flat space-time one,

$$\langle 0_{\text{in}} | 0_{\text{out}}\rangle|_J = W[J] = \int [\mathscr{D}\phi] e^{i(S[\phi] + \langle J,\phi\rangle)} \ ,$$

where

$$\langle J,\phi\rangle = \int d^4x\sqrt{-g(x)}J(x)\phi(x) \ ,$$

$J(x)$ is an arbitrary source, and $|0_{\text{in}}\rangle$ ($|0_{\text{out}}\rangle$) stands for the physical vacuum in the far past (future). With this assumption we are disregarding boundary-condition-fixing terms. We will find out later [Eq. (4) below] that the boundary conditions are fixed by the Wick rotation (See the Appendix).

We define the Wick rotation to be the transformation

$$\eta \to -i\eta \ , \quad \lambda \to i\lambda \ ,$$

so the conformal factor is unchanged but the metric becomes positive definite. The generating functional reads

$$\langle 0_{\text{in}} | 0_{\text{out}}\rangle^R|_J = W^R[J] = \int [\mathscr{D}\phi] e^{-(S[\phi] - \langle J,\phi\rangle)} \ . \tag{1}$$

Following the flat—space-time model, we would like to reduce the generating functional to an expression quadratic in the sources.

We shift the field variable to

$$\chi(x) = \phi(x) - \int d^4y\sqrt{g(y)}J(y)G(x,y) \ ,$$

where G satisfies

$$G(x,y) = G(y,x) \tag{2}$$

and

$$(-\nabla_i\partial^i + \tfrac{1}{6}R + m^2)G(x,y) = (\sqrt{g})^{-1}\delta(x-y) \ . \tag{3}$$

In order to reach our goal, we have to impose also the boundary condition

$$n_i\sqrt{g(x)}\frac{\partial G}{\partial x_i}(x,y)\bigg|_{x\in\partial V} = 0 \quad \forall y \ , \tag{4}$$

where ∂V is the boundary of the space-time manifold and n_i is the outer normal. Then it is easy to show that if we postulate condition (4),

$$W^R[J] = W^R[0]\exp\left[\tfrac{1}{2}\int d^4x\, d^4y\sqrt{g(x)}\sqrt{g(y)}J(x)J(y)G(x,y)\right] \ . \tag{5}$$

Both Eqs. (1) and (5) are the natural generalization of the corresponding equations of flat space-time. Therefore, it seems natural to postulate condition (4) (see also the Appendix). We shall see the physical implications of this postulate in Sec. IV. Thus,

$$G(x,y) = \frac{-1}{\sqrt{g(x)}\sqrt{g(y)}}\frac{\partial^2 \ln W^R[J]}{\partial J(x)\partial J(y)} = -\frac{\langle 0_{\text{in}}|T(\phi(x)\phi(y))|0_{\text{out}}\rangle}{\langle 0_{\text{in}}|0_{\text{out}}\rangle}$$

is the Feynman (causal) propagator; T stands for chronological order.

Since the Universe is spatially flat, we can Fourier analyze G:

$$G(x,x') = (2\pi)^{-3}[a(\eta)a(\eta')]^{-1}\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}g_k(\eta,\eta') \ , \tag{6}$$

where $g_k(\eta,\eta')$ only depends on $k = |\vec{k}|$. The equation for g_k is

$$\left[-\frac{\partial^2}{\partial\eta^2} + k^2 + m^2a^2(\eta)\right]g_k(\eta,\eta') = \delta(\eta-\eta') \tag{7}$$

and the boundary condition is

$$a^3(\eta_s)\frac{\partial}{\partial\eta}\left[\frac{g_k(\eta,\eta')}{a(\eta)}\right]\bigg|_{\eta=\eta_s} = 0 \quad \forall\eta'$$

if the boundary lies at $\eta = \eta_s$.

Let us assume that η runs from $-\infty$ to $+\infty$ and that $a(\eta)$ is continuous except on a finite set and bounded on compact sets. Let H be the operator $H=-d^2/d\eta^2+m^2a^2(\eta)$. Then H is positive definite and essentially self-adjoint [H is the Hamiltonian of a nonrelativistic particle in the potential barrier $m^2a^2(\eta)$]. If φ_n are the eigenfunctions of H,

$$H\varphi_n=E_n\varphi_n\ ,\quad E_n\geq 0$$

(n may be a continuous index) then we can formally compute g_k as

$$g_k(\eta,\eta')=\sum_n \frac{\varphi_n^*(\eta)\varphi_n(\eta')}{E_n+k^2}\ .$$

This is a solution of (2), since $\sum_n\varphi_n^*(\eta)\varphi_n(\eta')=\delta(\eta-\eta')$. On more formal grounds, since $(-k^2)$ is not in the spectrum of H, then $H+k^2$ has an inverse that is a continuous operator in L^2. So, if $\sigma(\eta)\in L^2$, there exists one and only one $\rho(\eta)\in L^2$ such that

$$\sigma(\eta)=\left[-\frac{d^2}{d\eta^2}+m^2a^2(\eta)+k^2\right]\rho(\eta)\ .$$

Furthermore, $\rho(\eta)$ has two derivatives and $||\rho||_2\leq K||\sigma||_2$, where

$$||\rho||_2=\left[\int_{-\infty}^{\infty}d\eta\,|\rho(\eta)|^2\right]^{1/2}$$

and K does not depend on σ. We want to show that there exists a kernel $g_k(\eta,\eta')$ such that

$$\rho(\eta)=\int_{-\infty}^{\infty}d\eta' g_k(\eta,\eta')\sigma(\eta')$$

and that this kernel is in fact a function. First we note that if $a^2(\eta)\leq A^2$ for $|\eta|\leq\eta_0$, then

$$\left|\frac{d\rho}{d\eta}(\eta)-\frac{d\rho}{d\eta}(-\eta_0)\right|\leq\int_{-\eta_0}^{\eta}d\eta'\left|\frac{d^2\rho}{d\eta^2}\right|=\int_{-\eta_0}^{\eta}d\eta'\,|-\sigma(\eta')+[k^2+m^2a^2(\eta')]\rho(\eta')|$$
$$\leq\sqrt{2\eta_0}[1+(k^2+m^2A^2)K]||\sigma||_2$$

by the Cauchy-Schwartz inequality. Thus, if we write

$$\rho(\eta)=\rho(-\eta_0)+\frac{d\rho}{d\eta}(-\eta_0)(\eta+\eta_0)+\rho'(\eta)$$

then

$$|\rho'(\eta)|\leq\int_{-\eta_0}^{\eta}d\eta'\left|\frac{d\rho}{d\eta}(\eta')-\frac{d\rho}{d\eta}(-\eta_0)\right|$$
$$\leq(2\eta_0)^{3/2}K'||\sigma||_2\ ,$$

where $K'=1+(k^2+m^2A^2)K$ only depends on η_0. If now we let σ go to zero in L^2, then $\rho(\eta')$ goes to zero uniformly in $(-\eta_0,\eta_0)$, and so ρ approaches a linear function in this interval. But, as on the other hand, ρ too goes to zero in L^2, this linear function has to be the null one. We conclude that when σ goes to zero in L^2, then $\rho(\eta)$ goes to zero for each η, i.e., the functional that carries σ on $\rho(\eta)$ is continuous for each η. But then, by Riesz's theorem, there exists an L^2 function $f_\eta(\eta')$ such that

$$\rho(\eta)=\int_{-\infty}^{\infty}d\eta' f_\eta(\eta')\sigma(\eta')\ .$$

Defining

$$g_k(\eta,\eta')=f_\eta(\eta')\ ,$$

we have shown the existence of $g_k(\eta,\eta')$. Furthermore, for each fixed η, $g_k(\eta,\eta')$ is an L^2 function, and since (7) has no L^2 homogeneous solution (because it is invertible) g_k is the only solution with that property.

Now, let us try to compute $g_k(\eta,\eta')$. Let us call h_1 and h_2 two independent homogeneous solutions of (7), such that h_1 and $dh_1/d\eta$ go to zero when η goes to $+\infty$. As the Wronskian of two solutions of (7) is constant, h_2 has to blow up at $+\infty$. But $g_k(\eta,\eta')$, which is a homogeneous solution of (7) for $\eta>\eta'$ and an L^2 function for η' fixed, cannot blow up, so

$$g_k(\eta,\eta')=f(\eta')h_1(\eta)\quad\text{if } \eta>\eta'\ .$$

As g_k is symmetric (it is the kernel of a self-adjoint operator)

$$g_k(\eta,\eta')=h_1(\eta')f(\eta)\quad\text{if } \eta<\eta'\ .$$

Thus, f is a homogeneous solution of (7), too:

$$f(\eta)=ch_1(\eta)+dh_2(\eta)\ .$$

Let us arrange h_1 and h_2 in such a way that

$$h_1\frac{d}{d\eta}h_2-h_2\frac{dh_1}{d\eta}=1\ .$$

In order to satisfy (7), $\partial g_k/\partial\eta$ must have a minus unity jump at $\eta=\eta'$ so $d=1$. At last, $g_k(\eta,\eta')$ goes to zero when η reaches $-\infty$; it follows that

$$c=-\lim_{\eta\to-\infty}\frac{h_2(\eta)}{h_1(\eta)}\ . \tag{8}$$

Thus, the general form of g_k is

$$g_k(\eta,\eta')=h_1(\eta_>)[h_2(\eta_<)+ch_1(\eta_<)]\ ,$$

where $\eta_> = \max(\eta,\eta')$, $\eta_< = \min(\eta,\eta')$. On the other hand, we can write g_k on physical space in terms of the out model (cf. Ref. 3)

$$g_k(\eta,\eta') = \psi_k(\eta_>)\left[\psi_k^*(\eta_<) + \left[\frac{C_k}{B_k}\right]^* \psi_k(\eta_<)\right],$$

where C_k and B_k are the Bogoliubov coefficients that relate the out model with the in model, $\phi_k = B_k\psi_k + C_k\psi_k^*$, and satisfy $|B_k|^2 - |C_k|^2 = 1$.

If, when continued back to physical space, h_1 and h_2 go into conjugate functions, then it is seen that h_1 goes into the out model, and that c goes into $(C_k/B_k)^*$. This and the normalization equation fix the in model. If h_1 goes into a real function, then the normalization cannot be achieved and we cannot define a particle model (cf. Ref. 4).

III. SOME EXAMPLES

In the massless case, we can choose $h_1 = (2h)^{-1/2}e^{-k\eta}$, $h_2 = (2k)^{-1/2}e^{k\eta}$. These functions meet our requirements. When we go back to physical space-time they turn into the well-known "conformal model" that is so deduced from the Wick rotation when $-\infty < \eta < \infty$.

If the space-time has an asymptotically flat out region, we can approximate the solutions of (7) by WKB solutions. Then, defining $\omega_k = [k^2 + m^2 a^2(\eta)]^{1/2}$ we see that the Euclidean solutions

$$h_1(\eta) = (2\omega_k)^{-1/2} e^{-\int^{\eta}\omega_k(\eta')d\eta'} + \cdots ,$$

$$h_2(\eta) = (2\omega_k)^{-1/2} e^{\int^{\eta}\omega_k(\eta')d\eta'} + \cdots$$

satisfy the requirements of our theory and become complex-conjugate functions when we go back to physical space, thus defining a particle model. This model coincides with the well-known adiabatic definition of the out modes. By the same reasons, our method singles out the in adiabatic modes when there is an in adiabatic zone.

The class of metrics in which η ranges from $-\infty$ to $+\infty$ also includes some singular spaces. For example, in the linearly expanding universe $[a(t) = t]$ $\eta = \ln t$, so it enters in the hypothesis of our theorem. The complete calculations, although with a different but equivalent way of defining the Wick rotation, can be seen in Refs. 3 and 4. The class of models with a cosmological singularity at $\eta = 0$ will be dealt with in Sec. IV.

As an example of a completely different situation, let us consider the inflationary metric $a(t) = a_0 e^{\lambda t}$. The conformal time is defined through $\eta = (-a_0\lambda)^{-1} e^{-\lambda t}$ when $t \to -\infty$, $\eta \to -\infty$, but when $t \to +\infty$, $\eta \to \eta_s = 0$, so we cannot use the results of the previous paragraph. In terms of conformal time, the conformal factor is a $(\eta) = -1/\lambda\eta$ and the scalar curvature is $R = -2\lambda^2$. In this case, the singularity is to be related to the reference frame and not to the geometry itself.

In fact, through an appropriate change of variables, the inflationary space-time can be seen as a sector of the de Sitter universe (cf. Ref. 6). This is another example showing that particle modes strongly depend upon the reference frame on which they are defined.

In the inflationary metric, Eq. (7) becomes

$$\left[-\frac{\partial^2}{\partial\eta^2} + k^2 + \frac{m^2}{\lambda^2\eta^2}\right] g_k(\eta,\eta') = \delta(\eta - \eta') .$$

If $g_k(\eta,\eta')^{1/2} f(\eta,\eta')$, it results that

$$\frac{\partial^2}{\partial\eta^2} f + \frac{1}{\eta}\frac{\partial f}{\partial\eta} - \left[k^2 + \left[\frac{m^2}{\lambda^2} + \frac{1}{4}\right]\frac{1}{\eta^2}\right] f = -\frac{\delta(\eta - \eta')}{(\eta\eta')^{1/2}} .$$

So, if $\eta \neq \eta'$, f is a Bessel function of order $\nu = (m^2/\lambda^2 + \frac{1}{4})^{1/2}$ and variable $ik\eta$. The solution that goes to zero when $\eta \to 0$ is $J_\nu(ik\eta)$, while $J_{-\nu}(ik\eta)$ blows up. The solution that remains bounded when $\eta \to -\infty$ is $H_\nu^{(2)}(ik\eta)$. Taking into account normalization conditions, we can build our candidate to the propagator as

$$g_k(\eta,\eta') = \frac{\pi}{2}(\eta\cdot\eta')^{1/2} J_\nu(ik\eta_>) H_\nu(ik\eta_<) .$$

When we return to physical space, $ik\eta$ goes into $-k\eta$ and $m^2/\lambda^2 + \frac{1}{4}$ into $\frac{1}{4} - m^2/\lambda^2$, so if $m \le \lambda/2$ the solutions are Bessel functions of real variables and orders (therefore, real functions), and we find we cannot define particle modes. If the scalar field is heavy enough $(m > \lambda/2)$ then $\nu \to i(m^2/\lambda^2 - \frac{1}{4})^{1/4}$ and we can build the particle models in and out. The Bogoliubov coefficients turn out to be

$$B_k = (1 - e^{-2\nu\pi})^{-1/2} ,$$

$$C_k = e^{-\nu\pi}(1 - e^{-2\nu\pi})^{-1/2} ; \quad \nu = \left[\frac{m^2}{\lambda^2} - \frac{1}{4}\right]^{1/2} .$$

They do not depend on k, so there is a white noise of created particles, and they blow up when the mass reaches $\lambda/2$. These unphysical results may mean that an inflationary expansion has to be quickly damped by particle-creation processes.

IV. PERTURBATIVE EVALUATION OF THE PROPAGATOR

So far we have assumed the knowledge of the exact solutions of the wave equation, but in practice this is not possible except for very few special evolutions. Actually, in the formulation of the problem that takes into account the back reaction of the created particles on the metric, the evolution is not *a priori* known, and our method can only lead to an intricate integro-differential coupled system. Thus, it is necessary to develop perturbative expansions in order to draw conclusions without an exact knowledge of the solutions of the wave equation.

In order to do so, we return to the path-integral formulation of Sec. II. We perform the trick

$$\phi(x) e^{\langle J,\phi\rangle} = \frac{1}{\sqrt{g(x)}}\frac{\partial}{\partial J(x)} e^{\langle J,\phi\rangle} .$$

On the generating function, we find

$$W[J] = \exp\left[-\left[\frac{m^2}{2}\int\frac{d^4x}{\sqrt{g(x)}}\frac{\partial^2}{\partial J(x)^2}\right]\right] W[J]\Big|_{m^2=0} .$$

The massless generating function can be handled as in Sec. II to yield

$$W[J]=W[0]\,|_{m^2=0}\exp\left[-\left[\frac{m^2}{2}\int\frac{d^4x}{\sqrt{g(x)}}\frac{\partial^2}{\partial J(x)^2}\right]\right]\exp\left[\tfrac{1}{2}\int d^4x\,d^4y\sqrt{g(x)g(y)}J(x)J(y)G_0(x,y)\right].$$

The massless source-free generating function is a constant; it can be put equal to 1 by the conformal triviality. $G_0(x,y)$ is the massless symmetric propagator that satisfies

$$(-\nabla_i\partial^i+\tfrac{1}{6}R)G_0(x,y)=\frac{\delta(x-y)}{\sqrt{g(y)}}\ ,\quad \sqrt{g(x)}n^i\frac{\partial}{\partial x^i}G_0(x,y)\Bigg|_{x\in\partial V}=0\quad\forall y\ .$$

From now on the perturbative evaluation runs as usual (cf. Ref. 9). We set

$$Z[J]=-\ln W[J]\ ,$$

where $Z[J]$ is the sum of the connected diagrams. Our "potential" $\frac{1}{2}m^2\phi^2$ is really a quadratic mass term, so the "vertex" has only two legs. The Feynman rules in coordinate space are "a line joining two points labeled x and y means $G_0(x,y)$; a vertex labeled x means $-\frac{1}{2}m^2\int d^4x\sqrt{g(x)}$."

The only connected graphs are the vacuum loops and the two-point functions. The integral corresponding to the vacuum loop of nth order is

$$A_n=\int d^4x_1\sqrt{g(x_1)}\cdots d^4x_n\sqrt{g(x_n)}G_0(x_1,x_2)\cdots G_0(x_{n-1},x_n)G_0(x_n,x_1)\ .$$

For the two-point function of nth order

$$B_n(x,y)=\int d^4x_1\sqrt{g(x_1)}\cdots d^4x_n\sqrt{g(x_n)}G_0(x,x_1)\cdots G_0(x_n,y)\ .$$

The weights are $-k^{-1}2^{k-1}$ for A_k and 2^k for B_k (cf. Ref. 8), so the final result is

$$Z[J]=Z[0]\,|_{m^2=0}+\tfrac{1}{2}\sum_{j=1}^{\infty}\frac{(-m^2)^j}{j}A_j-\tfrac{1}{2}\sum_{j=0}^{\infty}(-m^2)^j\langle\langle B_j(1,2),J(1)\rangle,J(2)\rangle\ ,$$

where $Z[0]\,|_{m^2=0}$ can be set equal to zero. The propagator is

$$G(x,y)=\frac{-1}{\sqrt{g(x)}\sqrt{g(y)}}\frac{\partial^2 Z[J]}{\partial J(x)\partial J(y)}\Bigg|_{J=0}=\sum_{j=0}^{\infty}(-m^2)^jB_j(x,y)\ . \tag{9}$$

From its definition $B_0(x,y)=G_0(x,y)$ and

$$B_j(x,y)=\int d^4x_1\sqrt{g(x_1)}G_0(x,x_1)B_{j-1}(x_1,y)\ ,\quad j\geq 1 \tag{10}$$

we have

$$(-\nabla_i\partial^i+\tfrac{1}{6}R)B_j(x,y)=B_{j-1}(x,y)\ ,\quad j\geq 1\ .$$

Differentiating under the summation sign, we can see that $G(x,y)$ satisfies the massive Klein-Gordon equation and the boundary condition. Finally, we note that

$$A_j=\int d^4x\sqrt{g(x)}B_{j-1}(x,x)\ .$$

Thus,

$$\frac{\partial Z[0]}{\partial m^2}=-\tfrac{1}{2}\sum_{j=1}^{\infty}(-m^2)^{j-1}A_j=-\tfrac{1}{2}\int d^4x\sqrt{g(x)}G(x,x)\ .$$

As we saw in Sec. III, if η runs from $-\infty$ to $+\infty$, the apparatus of Sec. II leads to the usually accepted massless propagator, which is conformal to flat-space massless D_F:

$$G_0(x,x')=\frac{-1}{a(\eta)a(\eta')}\int\frac{d^3k}{(2\pi)^3}\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}\,')}}{2k}e^{-k(\eta_>-\eta_<)}=\frac{1}{a(\eta)a(\eta')}\frac{1}{(\eta-\eta')^2+(\vec{x}-\vec{x}\,')^2}\ . \tag{11}$$

The recurrence relation (10) defines the following B_j's. If there is a cosmological singularity ($0\leq\eta\leq\infty$), after applying the methods of Sec. II there remains an unknown constant α_k,

$$G_0(x,x')=\frac{-1}{a(\eta)a(\eta')}\int\frac{d^3k}{(2\pi)^3}\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}\,')}}{2k}(e^{-k(\eta_>-\eta_<)}+\alpha_ke^{-k(\eta+\eta')})\ ,$$

because we cannot use the condition that $g_k(\eta,\eta')\rightarrow 0$

when $\eta \to -\infty$. If we recall the boundary condition (4) we get

$$\lim_{\eta\to 0^+}\left[\left[ka^2-\frac{1}{2}\frac{da^2}{d\eta}\right]-\alpha_k\left[ka^2+\frac{1}{2}\frac{da^2}{d\eta}\right]\right]=0 .$$

The different possibilities are the following:

(a) If a^2 goes to zero but $da^2/d\eta$ does not, then the solution is $\alpha_k=-1$. But this implies that the Bogoliubov coefficients B_k and C_k are both infinite, because α_k is the analytical continuation of $(C_k/B_k)^*$ and $|B_k|^2-|C_k|^2=1$.

(b) The same holds if $da^2/d\eta$ goes to zero but a^2 does not.

(c) If both a^2 and $da^2/d\eta$ have nonzero limits, then

$$\alpha_k=\frac{ka^2(0)-\frac{1}{2}\dot{a}^2(0)}{ka^2(0)+\frac{1}{2}\dot{a}^2(0)}\to 1$$

when $k\to\infty$, leading to an ultraviolet catastrophe. The fulfillment of our program has led us to particle models that are different from the conformal one, but also to unphysical results. The boundary condition (4) may be wrong or else a universe that appears from nothing with a finite radius or finite expansion rate is by itself unphysical.

(d) In the remaining case, both a^2 and $\dot{a}^2$ go to zero, the boundary condition is trivial, and α_k remains unknown.

One way to eliminate this ambiguity is to add to physical space-time a fictitious zone where $a^2(\eta)=0$, $-\infty<\eta<0$. Then we are back in the singularity-free case and as we saw in Sec. III we can use conformal triviality to put $\alpha_k=0$. Since all physical quantities are expressed in terms of integrals over the invariant measure $d^4x\sqrt{g(x)}$, this fictitious zone does not lead to unphysical results, and the inverse conformal factors that appear in the propagator are easily handled.

On the other hand, since the mass does not appear in the Klein-Gordon equation in the added region, and the particle models are continuous, the massive-particle model approaches the massless one as the singularity. This is a desirable physical result, since in this "hot" singularity model particles must behave as ultrarelativistic ones near the singularity, and so their masses are to be neglected. Besides, it agrees with other well-known criteria, for example, Hamiltonian diagonalization at the singularity (cf. Refs. 10 and 11).

Furthermore, to set $\alpha_k=0$ it is necessary to avoid creation of particles in the conformally invariant massless theory, an effect that is usually believed not to occur (cf. Ref. 12). Then the massless propagator reduces to the conformal one (11), which satisfies the boundary condition

$$\frac{\partial}{\partial\eta}a(\eta)G_0(x,x')\Big|_{\eta=0}=\int d^3y\, Y(\vec{x}-\vec{y})G_0(y,x') ,$$

where $y=(0,\vec{y})$ and

$$Y(\vec{x})=\int\frac{d^3k}{(2\pi)^3}e^{i\vec{k}\cdot\vec{x}}k .$$

Differentiating under the integral sign we can see that this boundary condition is shared by all B_j's and thus for the massive propagator itself. If, as in Sec. II,

$$G(x,x')=\int\frac{d^3k}{(2\pi)^3}\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}}{a(\eta)a(\eta')}h_1(\eta_>)\times[h_2(\eta_<)+d_kh_1(\eta_<)] ,$$

it follows that

$$\frac{dh_2}{d\eta}(0)+d_k\frac{dh_1}{d\eta}(0)=k[h_2(0)+d_kh_1(0)] .$$

If we solve this equation for d_k and go back to physical space, we can write the Bogoliubov coefficients in terms of the out model ψ_k, which is the analytic continuation of h_1, as

$$B_k=(2k)^{-1/2}[k\psi_k^*(0)-i\dot{\psi}_k^*(0)] ,$$

$$C_k=(-1)(2k)^{-1/2}[k\psi_k(0)-i\dot{\psi}_k(0)] .$$

Thus, the in model is

$$\phi_k(\eta)=\frac{1}{\sqrt{2k}}\{[k\psi_k^*(0)-i\dot{\psi}_k^*(0)]\psi_k(\eta)-[k\psi_k(0)-i\dot{\psi}_k(0)]\psi_k^*(\eta)\} .$$

The Cauchy data for the in model at the singularity are the massless ones:

$$\phi_k(0)=\frac{1}{\sqrt{2k}} ,\quad \dot{\phi}_k(0)=-i\left[\frac{k}{2}\right]^{1/2} .$$

From now on, we will handle the cosmological singular spaces as singularity-free ones with $a(\eta)=0$ for $-\infty<\eta<0$. This ensures, through the calculations of Sec. II, that the massless model is the conformal one and avoids the introduction of a boundary condition at the singularity. As a last remark, we note that for $a(\eta)=\eta^\delta$, $a^2(0)=0$ and $\dot{a}^2(0)=0$ if $\delta>\frac{1}{2}$. In terms of physical time t, this means $a(t)\sim t^\epsilon$ with $\epsilon>\frac{1}{3}$. So the radiation-dominated universe $(\epsilon=\frac{1}{2})$ and the matter-dominated universe $(\epsilon=\frac{2}{3})$ fall into class (d) above.

V. CLOSE STUDY OF THE PERTURBATION SERIES

The first striking fact about the perturbation series (9) is that all its terms are infinite, even in flat space-time. In fact, since flat space D_F vanishes as x^{-2}, the integrand for flat space B_1 vanishes as $D_F{}^2\sim x^{-4}$, thus the integral over all space-time is logarithmically divergent.

To find out the meaning of this fact we formally Fourier transform Δ_F, D_F, and the B_j's. The Fourier transform of D_F is $+k^{-2}$: as the recurrence relation (10) dictates that B_j is the convolution of D_F and B_{j-1}, the Fourier transform of B_j is the product of the transforms, and so $(+k^{-2})^{j+1}$. Finally, the complete Fourier transform of Δ_F is, by the perturbative expansion,

$$\sum_{j=0}^{\infty}(-m^2)^j/k^{2(j+1)} .$$

If $k^2>m^2$ the series converges to

$$(k^2)^{-1}(1+m^2/k^2)^{-1} .$$

Therefore, we see that the built-in infrared divergence is completely fictitious, since the result can be easily converted into the right Fourier transform $(m^2+k^2)^{-1}$, which has no singularity.

So we realize that we must rely not on the direct development (9) but on its Fourier transform. As in general space-times we have no temporal translational invariance, we do not work with the complete Fourier transform but with the partial one (6). Writing

$$B_j(x,x')=\int \frac{d^3k}{(2\pi)^3}\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}}{a(\eta)a(\eta')}\left[\frac{1}{2k}\right]^{j+1} b_k^{(j)}(\eta,\eta') ,$$

then

$$g_k(\eta,\eta')=\frac{1}{2k}\sum_{j=0}^{\infty}\left[\frac{-m^2}{2k}\right]^j b_k^{(j)}(\eta,\eta')$$

with

$$b_k^{(0)}(\eta,\eta')=e^{-k(\eta_>-\eta_<)}$$

and

$$b_k^{(j)}(\eta,\eta')=\int_{-\infty}^{\infty} d\xi\, a^2(\xi) b_k^{(j-1)}(\xi,\eta')e^{-k|\eta-\xi|} , \quad j\geq 1 .$$

It is clear that all $b_k^{(j)}$'s are real and positive. If the function $a^2(\eta)$ is polynomially bounded, all $b_k^{(j)}$'s are in fact fast decreasing, since $b_k^{(0)}$ is, and the operations of multiplying by a polynomially bounded function and taking convolution with $e^{-k|\eta|}$ preserve this fast- decreasing character. $b_k^{(0)}$ is continuous but not differentiable; differentiating under the integral sign we see that

$$\left[-\frac{\partial^2}{\partial\eta^2}+k^2\right] b_k^{(j)}(\eta,\eta')=(2k)b_k^{(j-1)}(\eta,\eta')a^2(\eta) , \quad j\geq 1 .$$

Thus, $b_k^{(j)}$ has $(2j)$ continuous derivatives, if $a^2(\eta)$ is infinitely differentiable. If $a^2(\eta)$ is bounded, the series converges uniformly for large enough k. Indeed, if $a^2(\eta)\leq A^2$, $\forall\eta$, then

$$|b_k^{(j)}(\eta,\eta')| \leq \frac{2A^2}{k}\max_{\eta,\eta'} |b_k^{(j-1)}(\eta,\eta')| \leq \left[\frac{2A^2}{k}\right]^j$$

because $|b_k^{(0)}|\leq 1$, so the series converges for $k^2>m^2A^2$. As the derivatives converge uniformly too, it can be shown that the sum satisfies Eq. (7), and as the solution is unique, this means that the series converges to $g_k(\eta,\eta')$. The way to the particle models is now straightforward. First one must compute g_k up to the desired order in m^2. Then one must continue back to physical space-time and rearrange terms as in Ref. 3. The results up to second order are as follows.

(a) Out model:

$$\psi_k(\eta)=\frac{e^{i(m^2/2k)F(\eta)}}{\sqrt{2k}}\left\{e^{-ik\eta}\left[1-\left[\frac{im^2}{2k}\right]K(\eta)\right]+e^{ik\eta}\left[\left[\frac{im^2}{2k}\right]L(\eta)+\left[\frac{im^2}{2k}\right]^2 M(\eta)\right]\right\} ,$$

where

$$F(\eta)=\int_\eta^\infty ds\, a^2(s) , \quad K(\eta)=\int_\eta^\infty ds\, a^2(s)e^{2iks}\int_\eta^\infty dr\, a^2(r)e^{-2ikr} ,$$

$$L(\eta)=-\int_\eta^\infty ds\, a^2(s)e^{-2iks} , \quad M(\eta)=2\int_\eta^\infty ds\, a^2(s)\int_s^\infty dr\, a^2(r)e^{-2ikr} .$$

The integrals are to be understood as the analytical continuation of the Riemannian ones. On the other hand, since $F(\eta)$ contributes only as a phase, this integral does not need to be extended up to $+\infty$.

(b) In model:

$$\phi_k(\eta)=e^{-i(m^4/4k^2)\varphi}\frac{e^{i(m^2/2k)F(\eta)}}{\sqrt{2k}}\left\{e^{-ik\eta}\left[1-\left[\frac{im^2}{2k}\right]^2 N^*(\eta)\right]+e^{ik\eta}\left[\left[\frac{im^2}{2k}\right]\phi^*(\eta)+\left[\frac{im^2}{2k}\right]^2 P^*(\eta)\right]\right\} ,$$

where

$$\varphi=\int_0^\infty du(\sin 2ku)\int_{-\infty}^\infty dv\, a^2(v)a^2(v-u) ,$$

$$F(\eta)=\int_\eta^\infty ds\, a^2(s) ,$$

$$N(\eta)=\int_{-\infty}^\eta ds\, a^2(s)e^{-2iks}\int_{-\infty}^s dr\, a^2(s)e^{2ikr} ,$$

$$\phi(\eta)=\int_{-\infty}^\eta ds\, a^2(s)e^{2iks} ,$$

$$P(\eta)=2\int_{-\infty}^\eta ds\, a^2(s)\int_{-\infty}^s dr\, a^2(r)e^{2ikr} .$$

(c) Bogoliubov coefficients:

$$B_k=1-\frac{1}{2}\left[\frac{im^2}{2k}\right]^2\left|\int_{-\infty}^\infty ds\, a^2(s)e^{-2iks}\right|^2 ,$$

$$C_k=\left[\frac{im^2}{2k}\right]\int_{-\infty}^\infty ds\, a^2(s)e^{-2iks}+2\left[\frac{im^2}{2k}\right]^2\int_{-\infty}^\infty ds\, a^2(s)\int_{-\infty}^s dr\, a^2(r)e^{-2ikr}$$

(cf. Ref. 10).

VI. FINAL REMARKS

The definition of asymptotic particle modes in Robertson-Walker universes through the Wick rotation is applicable in most physically interesting evolutions. Furthermore, it satisfies the best-known criteria for the definition of a particle model; for example, it agrees with WKB definitions of positive frequency if there are asymptotically flat regions, it diagonalizes the metric Hamiltonian at the singularity, and it preserves the conformal triviality of the massless model.

Our perturbative expansion is complementary to the well-known Schwinger-DeWitt one (cf. Ref. 6), since this is well defined for large masses, and ours for small ones. Its mathematical foundations are clear (see Ref. 2) and can be extended to more general situations, including for example, nonzero-spatial-curvature or anisotropic models. (For a Riemannian scheme and solutions of the Klein-Gordon equation in Bianchi type-1 universes see Ref. 5.)

This method furnishes only asymptotic in and out states. Even if other schemes (i.e., Hamiltonian diagonalization or adiabatic modes) lead to the definition of intermediate models, the physical interpretation of these modes is under discussion (cf. Ref. 13).

The main drawback of this model is that it is written in a highly noncovariant way. This is the price to be paid for mathematical simplicity. As we said in the Introduction, the covariance of the theory is to be elucidated (cf. Ref. 5).

Even if this prescription is accepted as a good definition of particle modes, it stands still the more interesting problem of back reaction. To handle this, it is necessary to have first a sound renormalization method for the energy-momentum tensor (cf. Ref. 6). We are continuing our research on these lines.

APPENDIX

If the path integral

$$\int [\mathscr{D}\phi] e^{i(S[\phi]+\langle J,\phi\rangle)} ,$$

over all configurations of fields with boundary conditions

$$\phi(\vec{x},t)=\varphi(\vec{x}) , \quad \phi(\vec{x},t')=\varphi'(\vec{x}) ,$$

is understood as the transition amplitude between states of well-defined field variables from time t to time t', then the generating functional should be written

$$W[J]=\langle 0(t) \mid 0(t')\rangle = \int [\mathscr{D}\varphi][\mathscr{D}\varphi_1] \int_{\substack{\phi(\vec{x},t)=\varphi(\vec{x}) \\ \phi(\vec{x},t')=\varphi_1(\vec{x})}} [\mathscr{D}\phi] e^{i(S[\phi]+\langle J,\phi\rangle)} \langle 0(t) \mid \varphi(t)\rangle \langle \varphi_1(t') \mid 0(t')\rangle , \tag{A1}$$

where $\mid 0(t)\rangle$ is the vacuum at time t and $\mid \varphi(t)\rangle$ is the common eigenvector of the operators $\{\phi(\bar{x},t),\bar{x}\in \mathrm{R}^3\}$ satisfying

$$\phi(\bar{x},t) \mid \varphi(t)\rangle = \varphi(\bar{x}) \mid \varphi(t)\rangle .$$

Such a state exists since $\{\phi(\bar{x},t \mid ,\bar{x}\in \mathrm{R}^3\}$ are commuting observables. Furthermore two states defined by different functions φ and ψ are orthogonal,

$$\langle \varphi(t) \mid \psi(t)\rangle = \delta(\varphi-\psi) ,$$

where the δ symbol means that, for any suitable functional $J[\phi]$,

$$\int [\mathscr{D}\varphi] J[\varphi] \delta \mid \varphi \mid = J[0] .$$

Finally the $\mid \varphi\rangle$ states are complete, meaning that

$$\int [\mathscr{D}\varphi] \mid \varphi(t)\rangle\langle\varphi(t)\mid = \mathbb{1} ,$$

where $\mathbb{1}$ is the identity operator in the Hilbert space of physical states.

To compute the bracket $\langle 0(t) \mid \varphi(b)\rangle$, we recall that it is annihilated by any destruction operator $a_{\vec{k}}$. The $a_{\vec{k}}$ are written in terms of the field variables as

$$a_{\vec{k}} = (F^{+}_{\vec{k}},\phi) = -i \int d^3x \sqrt{-g} \left[\frac{\partial F^{+*}_{\vec{k}}(\vec{x},t)}{\partial t} \phi(\vec{x},b) - F^{+*}_{\vec{k}}(\vec{x},t) \frac{\partial \phi(\vec{x},t)}{\partial t} \right] ,$$

where (,) is the Klein-Gordon inner product (cf. Ref. 6) and $\{F^{+}_{\vec{k}}\}$ is the positive-frequency part of the particle model at time t. So we have the functional equation

$$a_{\vec{k}} \mid 0(t)\rangle = \int [\mathscr{D}\varphi](-i) \int d^3x \sqrt{-g} \left[\frac{\partial F^{*+}_{\vec{k}}}{\partial t} \phi(\vec{x},t) - F^{+*}_{\vec{k}} \frac{\partial \phi(\vec{x},t)}{\partial t} \right] \mid \varphi(t)\rangle\langle\varphi(t)\mid 0(t)\rangle = 0 . \tag{A2}$$

The action of the operator $\partial\phi/\partial t$ on the ket $\mid \varphi(t)\rangle$ is defined through

$$\left\langle x \left| \frac{\partial \phi}{\partial t}(\vec{x},t) \right| \varphi(t) \right\rangle = \frac{i}{\sqrt{-g}} \frac{\partial}{\partial \varphi(\bar{x})} \langle x \mid \varphi(t)\rangle$$

(where the derivative is a functional one) for any bra $\langle x\,|$. In this way we recover the commutation relation

$$\left[\phi(\vec{x},t),\frac{\partial\phi}{\partial t}(\vec{x}\,',t)\right]=\frac{i}{\sqrt{-g}}\delta(\vec{x}-\vec{x}\,')\ .$$

Integrating by parts in (A2) and using the independence of the $|\,\varphi\rangle$ kets, we are left with

$$\int d^3x\left[(-i)\sqrt{-g}\,\frac{\partial F^{+*}_{\vec{k}}(\vec{x},t)}{\partial t}\varphi(\vec{x})+F^{+*}_{\vec{k}}(\vec{x},t)\frac{\partial}{\partial\varphi(\vec{x})}\right]\langle\varphi(t)\,|\,0(t)\rangle=0\ ,\quad \forall\vec{k},\varphi(\vec{x})\ , \tag{A3}$$

whose solution is

$$\langle\varphi(t)\,|\,0(t)\rangle=\exp\left[-\tfrac{1}{2}\int d^3x\,d^3y\,\varphi(\vec{x})\varphi(\vec{y})H^t(\vec{x}-\vec{y})\right] \tag{A4}$$

with

$$H^t(\vec{x}-\vec{y})=\int\frac{d^3k}{(2\pi)^3}e^{i\vec{k}\cdot(\vec{x}-\vec{y})}(-i)\sqrt{-g(t)}\times\frac{d}{dt}\ln f_k^*(t)\ ,$$

where $f_k(t)$ is the temporal part of the particle model:

$$F^{\pm}_{\vec{k}}(\vec{x},t)=\frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}}f_k(t)\ .$$

If we use (A4) in (A1), we will see that the complete generating functional includes boundary-condition-fixing terms that depend on the particle models at times t and t'. In this work we set $t=0$ or $t=-\infty$ and $t'=+\infty$.

In the flat—space-time theory, after the Wick rotation is performed only field configurations with finite Euclidean action contribute to the path integral. Since these configurations go to zero at $\pm\infty$, the brackets in (A4) have value one and can thus be omitted. The Feynman propagator is defined as the only Euclidean Green's function that is finite at $\pm\infty$ (cf. Refs. 3 and 7).

In this work we study what models result if this method is translated to the curved background.

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