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# Uniqueness of the propagator in spacetime with cosmological singularity

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We consider the question of the uniqueness of the Feynman propagator, or equivalently of the initial vacuum state, in a cosmological model with an initial singularity. After discussing the relationship of the propagator to positive-frequency solutions of the field equation and to physical quantities, we turn to the particular example of the linearly expanding universe. The Feynman propagator in this model was obtained by Chitre and Hartle. We show that the boundary conditions they used are not sufficient to determine the propagator uniquely. This is done by displaying a family of propagators obeying the same boundary conditions. We then explore methods of strengthening the boundary conditions by considering the temperature and chemical potential of the created particles, the massless limit of the propagator, and the square integrability of the analytically continued kernel associated with the propagator. We show that the requirement of square integrability is sufficient to determine the Feynman propagator uniquely and that the resulting propagator is that of Chitre and Hartle. We write the square-integrability condition in a way applicable to general open spacetimes. Another approach we consider is the use of conditions such as consistency with the Einstein equations to determine the temperature and chemical potential characterizing the high-momentum part of the spectrum of created particles.

## I. INTRODUCTION

Quantum field theory in curved spacetime is beset with a number of difficulties which do not appear in Minkowski space. Chief among these difficulties is that in the absence of special symmetries there is no natural definition of the vacuum state. Equivalently, one can say that there is no natural way to choose a preferred set of positive-frequency solutions of the field equation or to uniquely specify the Feynman propagator. In fact, when an "in" region and an "out" region exist in which there is sufficient symmetry to enable one to specify positive-frequency solutions, then one finds in general that a solution of the field equation which is positive frequency in the in region is a superposition of positive and negative frequencies in the out region. If the system is in the state which corresponds to the unique vacuum in the in region, then there generally are particles present in the out region. Thus, the gravitational field or the geometry of spacetime creates particles.[1,2]

When no in region having sufficient symmetry exists, as in the case of a cosmological metric having an initial singularity, one may ask if there nevertheless exists a preferred state which can serve as the in vacuum state. In this paper we will be concerned with that problem, particularly with the approach to its solution which focuses on the Feynman propagator. We make no judgment as to whether the actual universe had a cosmological singularity, but do feel that the consequences of singular as well as nonsingular models are worth investigating.

For our present purposes, it is sufficient to work with a spatially flat Robertson-Walker metric. We will first show how the Feynman propagator of a scalar field is related to the choice of an in basis of positive- and negative-frequency solutions and to observables such as the density of particles in the out region. We then turn specifically to the example of the conformally coupled scalar field in the linearly expanding universe which was considered in the important work of Chitre and Hartle.[3] They imposed boundary conditions on the kernel of the Feynman propagator by first analytically continuing to the domain in which the metric has the Riemannian signature $(+\ +\ +\ +)$ and then using a natural generalization of the Euclidean flat-spacetime boundary conditions. By exhibiting a family of propagators which satisfy those same boundary conditions, we show that they are not sufficient to determine the Feynman propagator uniquely. Finally, we consider the question of how the boundary conditions can be strengthened so as to single out one propagator. We replace the condition that in the Riemannian domain the kernel of the propagator vanishes at infinity by the condition that the kernel be square integrable. This leads *uniquely* to the propagator originally found by Chitre and Hartle. The new condition of square integrability can be written in a coordinate-independent form applicable to general open spacetimes. An alternative approach to determining a unique propagator is to use other conditions such as consistency with the Einstein equations to determine the temperature and chemical-potential parameters which characterize the spectrum of created particles.

## II. PROPAGATOR, BASIS FUNCTIONS, AND BOGOLIUBOV COEFFICIENTS

In a spatially flat Robertson-Walker universe with line element

$$ds^2 = -dt^2 + a^2(t)(dx^2+dy^2+dz^2) , \tag{2.1}$$

consider a neutral scalar field $\phi$ of mass $m$ satisfying the equation

$$(-\nabla_\mu \nabla^\mu + m^2 + \xi R)\phi(x) = 0 , \tag{2.2}$$

where $\xi$ is an arbitrary constant, $R$ is the scalar curvature, and $\nabla_\mu$ denotes the covariant derivative. One can write

$$\phi = \int d^3k [A_{\vec{k}} f_{\vec{k}}^{(+)}(x) + A^\dagger_{-\vec{k}} f_{\vec{k}}^{(-)}(x)] , \tag{2.3}$$

where

$$f_{\vec{k}}^{(+)}(x) = (2\pi)^{-3/2} \exp(i\vec{k}\cdot\vec{x})\psi_k(t) , \tag{2.4}$$

$$f_{\vec{k}}^{(-)}(x) = (2\pi)^{-3/2} \exp(i\vec{k}\cdot\vec{x})\psi_k^*(t) , \tag{2.5}$$

and $\psi_k(t)$ is a solution of

$$\left[ a^{-3}\frac{d}{dt}\left[ a^2 \frac{d}{dt}\right] + a^{-2}k^2 + m^2 + \xi R \right] \psi_k(t) = 0 . \tag{2.6}$$

It is necessary to impose the Wronskian condition

$$\psi_k^* d\psi_k/dt - \psi_k d\psi_k^*/dt = -ia^{-3} , \tag{2.7}$$

so that as a consequence of the canonical commutation relations of the field $\phi$ and its conjugate momentum the operators $A_{\vec{k}}$ and $A^\dagger_{\vec{k}}$ will satisfy the usual commutation relations for annihilation and creation operators. Defining the conserved Klein-Gordon scalar product

$$\begin{aligned}(g,h) &= -i \int_\Sigma d\Sigma_\mu (g^* \partial^\mu h - h^* \partial_\mu g) \\ &\equiv -i \int_\Sigma d\Sigma^\mu g^* \overleftrightarrow{\partial}_\mu h ,\end{aligned} \tag{2.8}$$

where $\Sigma$ is a spacelike Cauchy hypersurface, one can verify that

$$\begin{aligned}(f_{\vec{k}}^{(+)}, f_{\vec{k}'}^{(+)}) &= -(f_{\vec{k}}^{(-)}, f_{\vec{k}'}^{(-)}) = \delta(\vec{k}-\vec{k}') , \\ (f_{\vec{k}}^{(+)}, f_{\vec{k}'}^{(-)}) &= 0 .\end{aligned} \tag{2.9}$$

Using a particular solution of Eq. (2.6) subject to the Wronskian condition (2.7), one can construct the corresponding Fock basis by applying operators $A_k^\dagger$ to the vacuum state defined by $A_{\vec{k}} | 0 \rangle = 0$.

The physical interpretation of the quanta corresponding to the $A_{\vec{k}}$ depends on the choice of the $\psi_k$, or equivalently of the basis functions $f_{\vec{k}}^{(\pm)}$. When $a(t)$ is constant or slowly varying, then the basis functions can be chosen as in special relativity or by means of the WKB approximation; the corresponding quanta will then be the usual physical particles. If one has an early-time in region and a late-time out region in which $a(t)$ is constant or slowly varying, the choice of basis functions corresponding to physical particles in each of those regions is unambiguous. However, the physical basis in the in region generally does not evolve into the physically relevant basis in the out region.[1] This implies that particles are created by the expansion of the universe. As first shown in Ref. 1, the physically relevant bases at early and late times are related by a Bogoliubov transformation, and the probability for pair production can be expressed in terms of the coefficients of that transformation. A case in which the in basis does evolve into the physically relevant out basis is that of the massless conformally invariant field ($m=0$, $\xi=\frac{1}{6}$). In that case, particles are not created by the expansion of the universe and there is an unambiguous set of basis functions at all times.[1,2,4]

In a generalized sense, one can define two spacelike Cauchy hypersurfaces, such as those corresponding to different values of $t$, as the in and out regions. Except in the case when a hypersurface lies in a region where $a(t)$ is slowly varying (or when the massless conformal field is being considered), it is not clear what set of basis functions

$f_{\vec{k}}^{(\pm)}$, if any, correspond to the physically relevant quanta on a given hypersurface. As has been pointed out in the literature,[1,2,5,6] the concept of particle number in a strong or rapidly varying gravitational field is ill defined from an operational viewpoint. Nevertheless, one can use various mathematical criteria to attempt to single out a basis $f_{\vec{k}}^{(\pm)}$ associated with a given hypersurface, which can then be used to specify initial conditions associated with that hypersurface. A number of proposals for doing that have appeared.[7–13] The problem of finding preferred initial conditions is especially severe when one considers models with a cosmological singularity.[3,14–17]

Suppose that an in basis $f_{\vec{k}}^{(\pm)}$ has been specified as in Eqs. (2.3)–(2.9), and that an out basis $p_{\vec{k}}^{(\pm)}$ has been specified. In terms of the out basis, the field expansion is

$$\phi=\int d^2k[a_{\vec{k}}p_{\vec{k}}^{(+)}(x)+a_{-\vec{k}}^{\dagger}p_{\vec{k}}^{(-)}(x)]\ , \qquad (2.10)$$

where

$$p_{\vec{k}}^{(+)}(x)=(2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{x})\psi_k'(t)\ , \qquad (2.11)$$

$$p_{\vec{k}}^{(-)}(x)=(2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{x})\psi_k'^{*}(t)\ , \qquad (2.12)$$

and the functions $\psi_k'(t)$ obey equations analogous to (2.6) and (2.7). The out basis can be expressed in terms of the in basis by

$$\begin{aligned} p_{\vec{k}}^{(+)}&=\alpha_k^{*}f_{\vec{k}}^{(+)}-\beta_k f_{\vec{k}}^{(-)}\ ,\\ p_{\vec{k}}^{(-)}&=\alpha_k f_{\vec{k}}^{(-)}-\beta_k^{*}f_{\vec{k}}^{(+)}\ , \end{aligned} \qquad (2.13)$$

where the complex numbers $\alpha_k$, $\beta_k$ satisfy $|\alpha_k|^2-|\beta_k|^2=1$. The out creation and annihilation operators are related to the corresponding in operators by the Bogoliubov transformation

$$\begin{aligned} a_{\vec{k}}&=\alpha_k A_{\vec{k}}+\beta_k^{*}A_{-\vec{k}}^{\dagger}\ ,\\ a_{-\vec{k}}^{\dagger}&=\alpha_k^{*}A_{-\vec{k}}^{\dagger}+\beta_k A_{\vec{k}}\ . \end{aligned} \qquad (2.14)$$

The vacuum state based on the $A_{\vec{k}}$ will be denoted as $|0\ \text{in}\rangle$ and that based on the $a_{\vec{k}}$ as $|0\ \text{out}\rangle$. In many cosmological models, $a(t)$ is slowly varying in the out region so that the physically relevant choice of $p_{\vec{k}}^{(\pm)}$ and the meaning of the particles in the out region is clear. If the state of the field is $|0\ \text{in}\rangle$, then one can show that the out region contains pairs of particles of equal and opposite momenta, and that the probability of observing $n$ particles in mode $\vec{k}$ is[1,2]

$$P_n(\vec{k})=|\beta_k/\alpha_k|^{2n}|\alpha_k|^{-2}\ , \qquad (2.15)$$

where the number of particles appearing in other modes is not measured. The mean number of particles in mode $\vec{k}$ is

$$\langle N(\vec{k})\rangle=|\beta_k|^2\ . \qquad (2.16)$$

The number density of particles in the out region will be finite if and only if the quantity $\int d^3k\,|\beta_k|^2$ is finite. For simplicity, we take the state of the system to be $|0\ \text{in}\rangle$. The corresponding quantities can readily be calculated when the state of the system is not the in vacuum but some other pure or mixed state.

The Feynman propagator can be *defined* as[18,19]

$$G(x,x')=\frac{i\langle 0\ \text{out}\,|\,T[\phi(x)\phi(x')]\,|\,0\ \text{in}\rangle}{\langle 0\ \text{out}\,|\,0\ \text{in}\rangle}\ , \qquad (2.17)$$

where $T$ denotes the time-ordered product. Expressing the field operators $\phi(x)$ and $\phi(x')$ in terms of the appropriate basis functions and using Eq. (2.14), one finds

$$G(x,x')=i\int d^3k(\alpha_k^{*})^{-1}[\theta(t-t')p_{\vec{k}}^{(+)}(\vec{x},t)f_{\vec{k}}^{(+)*}(\vec{x}',t')+\theta(t'-t)p_{\vec{k}}^{(-)*}(\vec{x}',t')f_{\vec{k}}^{(-)}(\vec{x},t)]\ . \qquad (2.18)$$

Then defining[10]

$$G_{\Sigma'}h(x)\equiv-\int_{\Sigma'}d\Sigma'^{\mu}G(x,x')\overleftrightarrow{\partial}_{\mu}'h(x') \qquad (2.19)$$

$$=\begin{cases}\int d^3k(\alpha_k^{*})^{-1}p_{\vec{k}}^{(+)}(x)(f_{\vec{k}}^{(+)},h), & \text{if } x \text{ is to future of } \Sigma'\ ,\\ \int d^3k(\alpha_k^{*})^{-1}f_{\vec{k}}^{(-)}(x)(p_{\vec{k}}^{(-)},h), & \text{if } x \text{ is to past of } \Sigma'\ ,\end{cases} \qquad (2.20)$$

one readily finds that

$$\left.\begin{aligned} &G_{\Sigma'}f^{(+)}_{\vec{k}}(x)=(\alpha^*_k)^{-1}p^{(+)}_{\vec{k}}(x),\ \ G_{\Sigma'}f^{(-)}_{\vec{k}}(x)=0\ ,\\ &G_{\Sigma'}p^{(+)}_{\vec{k}}(x)=p^{(+)}_{\vec{k}}(x),\ \ G_{\Sigma'}p^{(-)}_{\vec{k}}(x)=-(\beta^*_k/\alpha^*_k)p^{(+)}_{\vec{k}}(x)\end{aligned}\right\}\ \text{if } x \text{ is to the future of } \Sigma' \tag{2.21}$$

and

$$\left.\begin{aligned} &G_{\Sigma'}f^{(+)}_{\vec{k}}(x)=-(\beta_k/\alpha^*_k)f^{(-)}_{\vec{k}}(x),\ \ G_{\Sigma'}f^{(-)}_{\vec{k}}(x)=-f^{(-)}_{\vec{k}}(x)\ ,\\ &G_{\Sigma'}p^{(+)}_{\vec{k}}(x)=0,\ \ G_{\Sigma'}p^{(-)}_{\vec{k}}(x)=-(\alpha^*_k)^{-1}f^{(-)}_{\vec{k}}(x)\end{aligned}\right\}\ \text{if } x \text{ is to the past of } \Sigma'\ . \tag{2.22}$$

It follows that, except for a factor of $(\alpha^*_k)^{-1}$, the action of $G_{\Sigma'}$ is (1) to take the positive-frequency part of the in basis $f^{(\pm)}_{\vec{k}}$ into the positive-frequency part of the out basis $p^{(\pm)}_{\vec{k}}$ when $x$ is to the future of $\Sigma'$, and (2) to take the negative-frequency part of the out basis $p^{(\pm)}_{\vec{k}}$ into the negative-frequency part of the in basis $f^{(\pm)}_{\vec{k}}$ when $x$ is to the past of $\Sigma'$. This is analogous to the action of the Feynman propagator in flat spacetime, which propagates positive frequencies into the future and negative frequencies into the past (in flat spacetime $\alpha_k=1$, $\beta_k=0$, and $p_{\vec{k}}$ and $f_{\vec{k}}$ are identical).

Using the previous results one finds without difficulty that

$$(\beta_k/\alpha_k)^*\delta(\vec{k}-\vec{k}')=-(p^{(+)}_{\vec{k}},G_{\Sigma'}p^{(-)}_{\vec{k}'})\ . \tag{2.23}$$

This equation holds whether $\Sigma'$ is to the past or future of the spacelike hypersurface $\Sigma$ on which the scalar product is evaluated. The ratio $(\beta_k/\alpha_k)^*$ is useful because it appears in Eq. (2.15) for $P_n(\vec{k})$ and because[1,2]

$$\langle n_{\vec{k}}\text{ out}\,|\,0\text{ in}\rangle=(\beta^*_k/\alpha^*_k)^{n_{\vec{k}}}\langle 0\text{ out}\,|\,0\text{ in}\rangle\ , \tag{2.24}$$

where $|\,n_{\vec{k}}\text{ out}\rangle$ is the state with exactly $n_{\vec{k}}$ pairs present in the out region, each pair having one particle in mode $\vec{k}$ and the other in mode $-\vec{k}$. Thus, $(\beta_k/\alpha_k)^*$ is the relative amplitude for production of a pair in modes $\vec{k}$ and $-\vec{k}$. That the right-hand side of Eq. (2.23) is the relative amplitude for production of a pair can also be inferred intuitively from the corresponding Feynman diagram, as was done in Ref. 3 by Chitre and Hartle, who also gave a derivation based on quantum field theory. Note that the right-hand side of Eq. (2.23) involves only the out basis functions and the Feynman propagator $G(x,x')$. Therefore, if suitable boundary conditions which determine $G(x,x')$ can be found, then physically relevant amplitudes can be obtained without explicitly specifying the in basis $f^{(\pm)}_{\vec{k}}$. The pair-production amplitude depends on these boundary conditions (or on the choice of an in basis) and can only be said to describe the production of real particles when the proper boundary conditions are imposed.

## III. MODEL WITH COSMOLOGICAL SINGULARITY

When a cosmological singularity is present, there is in general no obvious or natural choice of in basis $f^{(\pm)}_{\vec{k}}$. The same ambiguity is evident in the choice of a Feynman propagator $G(x,x')$. This ambiguity is not entirely removed by prescriptions, such as that of DeWitt,[18,19,4] which involve writing $G(x,x')$ in the proper-time formalism and replacing $m^2$ by $m^2-i\epsilon$. The reason, as will be seen in detail at the end of Sec. IV, is that the physical spacetime manifold is rendered incomplete by the singularity so that additional boundary conditions are required. The metric of Eq. (2.1) with $a(t)=t$ (the linearly expanding universe) provides an excellent arena for investigating such questions. We proceed by writing in this section the most general form the Feynman propagator with $\xi=\frac{1}{6}$ can have in the linearly expanding universe. Then in the next two sections, we examine the effect of various possible boundary conditions in uniquely specifying $G(x,x')$.

With $a(t)=t$ and $\xi=\frac{1}{6}$, the most general solution of Eq. (2.6) is[3,20]

$$\psi_k(t)=t^{-1}[B_kH^{(1)}_{ik}(mt)+C_kH^{(2)}_{ik}(mt)]\ , \tag{3.1}$$

where $H^{(1)}_{ik}$ and $H^{(2)}_{ik}$ are the Hankel functions of the first and second kind with imaginary index $ik$, which satisfy the equation $H^{(2)*}_{ik}=\exp(-k\pi)H^{(1)}_{ik}$. The constraint on the coefficients $B_k$ and $C_k$ imposed by the Wronskian condition (2.7) is

$$|C_k|^2\exp(-k\pi)-|B_k|^2\exp(k\pi)=\pi/4\ . \tag{3.2}$$

For large $t$ ($t>>m^{-1}$), the expansion is sufficiently slow that the out basis $p_{\vec{k}}^{(\pm)}$ can be identified by using the positive-frequency WKB solution of Eq. (2.6) for $\psi_k(t)$. Using the asymptotic form of the Hankel functions of large argument, one finds that $\psi_k'(t)$ appearing in Eq. (2.11) is proportional to $H_{ik}^{(2)}(mt)$, so that the out basis is

$$p_{\vec{k}}^{(+)}(x)=\pi^{1/2}(2t)^{-1}\exp(\tfrac{1}{2}k\pi+i\phi_k)H_{ik}^{(2)}(mt)(2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{x}) \tag{3.3}$$

and

$$p_{\vec{k}}^{(-)}(x)=\pi^{1/2}(2t)^{-1}\exp(-\tfrac{1}{2}k\pi-i\phi_k)H_{ik}^{(1)}(mt)(2\pi)^{-3/2}\exp(i\vec{k}\cdot\vec{x})\ , \tag{3.4}$$

where $\phi_k$ is an arbitrary phase. The most general in basis $f_{\vec{k}}^{(\pm)}$ is given by Eqs. (2.4) and (2.5) with the $\psi_k$ of Eq. (3.1). The Bogoliubov coefficients connecting the in and out bases are then given by Eq. (2.13) as

$$\alpha_k=2\pi^{-1/2}\exp(-\tfrac{1}{2}k\pi-i\phi_k)C_k,\quad \beta_k=2\pi^{-1/2}\exp(\tfrac{1}{2}k\pi+i\phi_k)B_k\ . \tag{3.5}$$

One must require that $\int d^3k\exp(k\pi)\,|B_k|^2$ converges, and that the density of particles in the out region is finite.

The Feynman propagator corresponding to the above out basis [Eqs. (3.3) and (3.4)] and the most general in basis is given by Eq. (2.18) as

$$G(x,x')=\frac{i}{(2\pi)^3}\frac{\pi}{4tt'}\int e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}H_{ik}^{(2)}(mt_>)\left[\frac{B_k^*}{C_k^*}e^{2\pi k}H_{ik}^{(2)}(mt_<)+H_{ik}^{(1)}(mt_<)\right]d^3k\ , \tag{3.6}$$

where $t_>$ ($t_<$) is the larger (smaller) of $t$ and $t'$. Let us consider the propagators corresponding to several particular choices of the in basis.

(i) $B_k=0$. This case was considered by Nariai and Azuma.[20] (They considered propagators defined using two in vacuum states, but in this particular case $|0\ \text{in}\rangle$ is the same as $|0\ \text{out}\rangle$.) With this choice, one has $f_{\vec{k}}^{(\pm)}=p_{\vec{k}}^{(\pm)}$. It is always possible mathematically to take the in basis equal to the out basis, but for an expansion which is static at early and late times such a choice generally gives a basis which does *not* correspond to the physical basis in either the in or the out region. Therefore, taking the in basis equal to the out basis cannot be generally valid, although it may be correct for particular expansions in which no particle creation occurs. One can explicitly evaluate the Fourier integral in Eq. (3.6) with $B_k=0$ using the known properties of Hankel functions and their integrals,[21] with the result

$$G^{(0)}(x,x')=-(8\pi)^{-1}m^2r^{-1}\sinh(r)(-2m^2\sigma)^{1/2}H_1^{(2)}((-2m^2\sigma)^{1/2})\ , \tag{3.7}$$

where

$$\sigma=-2^{-1}(t^2+t'^2-2tt'\cosh r)\ , \tag{3.8}$$

where $r=|\vec{x}-\vec{x}'|$. Here $\sigma$ is half of the proper distance squared along a spacelike geodesic between $x$ and $x'$ (or minus half of the proper time squared along a timelike geodesic). The calculation leading to Eq. (3.7) is in Appendix A.

This propagator is also obtained immediately if one, as an approximation, uses only the first term of the Schwinger-DeWitt series[18] to evaluate the Feynman propagator. Similarly the Gaussian approximation to the Feynman propagator obtained through evaluation of the path integral[22] by Bekenstein and one of us (L.P.) gives this propagator. For the present metric, these approximations give an *exact* solution of the Green's-function equation.

(ii) Another Feynman propagator, considered first by Chitre and Hartle,[3] has the form

$$G^{(1)}(x,x')=i\pi(2\pi)^{-3}(2tt')^{-1}\int\exp[i\vec{k}\cdot(\vec{x}-\vec{x}')]H_{ik}^{(2)}(mt_>)J_{ik}(mt_<)d^3k\ . \tag{3.9}$$

Comparison with Eq. (3.6), using $J_{ik}=(H_{ik}^{(1)}+H_{ik}^{(2)})/2$, gives $B_k e^{2\pi k}=C_k$, and Eq. (3.2) then yields the coefficients which determine the in basis of this propagator:

$$B_k=\tfrac{1}{2}\sqrt{\pi}\,e^{-k\pi/2}(e^{2k\pi}-1)^{-1/2}e^{i\phi_k'}\ , \tag{3.10}$$

$$C_k=\tfrac{1}{2}\sqrt{\pi}\,e^{3k\pi/2}(e^{2k\pi}-1)^{-1/2}e^{i\phi_k'}\ , \tag{3.11}$$

where $\phi_k'$ is an arbitrary phase. The corresponding Bogoliubov coefficients are

$$\alpha_k=e^{k\pi}(e^{2k\pi}-1)^{-1/2}e^{-i(\phi_k-\phi_k')}\ , \tag{3.12}$$

$$\beta_k=(e^{2k\pi}-1)^{-1/2}e^{-i(\phi_k+\phi_k')}\ . \tag{3.13}$$

These give with Eqs. (2.15) and (2.16) the probability of detecting $n$ particles in mode $k$ at late times as

$$p_n(\vec{k})=e^{-2\pi nk}(1-e^{-2\pi k})\ , \tag{3.14}$$

and the average number in mode $\vec{k}$ as

$$\langle N(\vec{k})\rangle=(e^{2\pi k}-1)^{-1}\ . \tag{3.15}$$

The physical momentum is $k/a(t)$. Therefore, when the momentum is sufficiently large that the mass can be neglected, the spectrum, as pointed out by Chitre and Hartle,[3] resembles that of black-body radiation of temperature

$$T=[k_B\pi a(t)]^{-1}\ , \tag{3.16}$$

where $k_B$ is the Boltzmann constant.

(iii) Consider now the family of propagators which have the form

$$G^{(\Lambda)}(x,x')=G^{(0)}(x,x')+\frac{i}{(2\pi)^3}\frac{\pi}{4tt'}\int e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\Lambda H_{ik}^{(2)}(mt_<)H_{ik}^{(2)}(mt_>)d^3k\ , \tag{3.17}$$

where $\Lambda$ is a complex function of $k$ and $m$. The last term is a solution of the homogeneous field equation (2.2) with $\xi=\frac{1}{6}$. In the particular cases $\Lambda=0$ and $\Lambda=1$, Eq. (3.17) gives the propagators of Eq. (3.7) and Eq. (3.9), respectively. One finds that the coefficients which determine the in basis are

$$B_k=(\sqrt{\pi}/4)e^{-\pi k+i\phi_k'}(|\Lambda|^{-2}e^{2\pi k}-1)^{-1}\ , \tag{3.18}$$

$$C_k=(\Lambda^*)^{-1}e^{2\pi k}B_k\ . \tag{3.19}$$

Then Eqs. (3.5), (2.15), and (2.16) yield

$$P_n(\vec{k})=|\Lambda|^{2n}e^{-2\pi nk}(1-|\Lambda|^2e^{-2\pi k}) \tag{3.20}$$

and

$$\langle N(\vec{k})\rangle=(|\Lambda|^{-2}e^{2\pi k}-1)^{-1}\ . \tag{3.21}$$

The quantity $\Lambda(k,m)$ can be chosen to correspond to any desired probability distribution of particles present at late times. If one takes

$$|\Lambda|^{-2}=\zeta e^{(\gamma-2\pi)k}\ , \tag{3.22}$$

with $\zeta$ and $\gamma$ independent of $k$, then for momenta large with respect to the mass the distribution will be thermal, with temperature

$$T=[k_B\gamma a(t)]^{-1} \tag{3.23}$$

and chemical potential

$$\mu=-[\gamma a(t)]^{-1}\ln\zeta\ . \tag{3.24}$$

The possibility of a nonzero chemical potential has been discussed in the literature.[23,24] For completeness, we note that because the particles of each created pair are correlated the distribution of particles at high momenta is truly thermal only if we assume that those correlations have been destroyed by other interactions or are not measurable.

## IV. BOUNDARY CONDITIONS AND FEYNMAN PROPAGATORS

In order to make physical predictions about such quantities as the particle density at late times, one must distinguish between the various in bases and propagators discussed in the previous section by imposing boundary conditions. Let us first consider the boundary conditions imposed by Chitre and Hartle.[3] In the Schwinger-DeWitt[18,19,4] representation of the Feynman propagator,

$$G(x,x')=i\int_0^\infty\langle x,s\,|\,x',0\rangle e^{-im^2s}ds\ , \tag{4.1}$$

where $m^2$ is taken to have an infinitesimal negative imaginary part. The kernel $\langle x,s\,|\,x',0\rangle$ is a solution of the Schrödinger equation

$$i\frac{\partial}{\partial s}\langle x,s\,|\,x',0\rangle=(-\nabla_\mu\nabla^\mu+\tfrac{1}{6}R)\langle x,s\,|\,x',0\rangle \tag{4.2}$$

of a fictitious particle moving on a curved four-dimensional hypersurface (coordinates $x^\mu$) with a scalar "time" coordinate $s$. We will use the conventions of Ref. 4, in which the propagator and kernel are scalars rather than scalar densities. The kernel satisfies the boundary condition

$$\lim_{s\to 0}\langle x,s\,|\,x',0\rangle=[-g(x)]^{-1/2}\delta(x,x') , \tag{4.3}$$

and can be regarded as the probability amplitude for the fictitious particle to propagate from $x'^\mu$ at time 0 to $x^\mu$ at time $s$. Because the physical spacetime is bounded by the singularity, one requires further boundary conditions to determine $\langle x,s\,|\,x',0\rangle$.

Motivated by the path-integral representation of the kernel, Chitre and Hartle rotate the coordinates $x^\mu$ by an angle $\pi/2$ in the complex plane and write $t=i\lambda$, $x^i=i\chi^i$, to obtain the Riemannian metric $\gamma_{\mu\nu}$ defined by the line element obtained from Eq. (2.1) with $a=t$:

$$dl^2=d\lambda^2+\lambda^2[(d\chi^1)^2+(d\chi^2)^2+(d\chi^3)^2] . \tag{4.4}$$

They also rotate $s$ in the complex plane by $-\pi/2$, writing $s=-i\Omega$, so that the analytically continued kernel (with $\lambda\equiv\chi^0$), $\langle\chi,\Omega\,|\,\chi',0\rangle$, satisfies the equation

$$\frac{\partial}{\partial\Omega}\langle\chi,\Omega\,|\,\chi',0\rangle=(\tilde\nabla_\mu\tilde\nabla^\mu-\tfrac{1}{6}\tilde R)\langle\chi,\Omega\,|\,\chi',0\rangle , \tag{4.5}$$

where $\tilde\nabla_\mu\tilde\nabla^\mu$ is the covariant Laplacian formed from the metric $\gamma_{\mu\nu}$ and coordinates $\chi^\mu$, and $\tilde R$ is the scalar curvature of the four-dimensional space described by Eq. (4.4). The boundary condition (4.3) is replaced by

$$\lim_{\Omega\to 0}\langle\chi,\Omega\,|\,\chi',0\rangle=\eta\gamma^{-1/2}\delta(\chi,\chi') , \tag{4.6}$$

where $\eta$ is a possible phase which can appear due to the rotations in the complex plane and $\gamma$ is the determinant of the metric $\gamma_{\mu\nu}$. The kernel $\langle x,s\,|\,x',0\rangle$ is obtained from $\langle\chi,\Omega\,|\,\chi',0\rangle$ by analytic continuation.

In attempting to uniquely specify $\langle\chi,\Omega,\,|\,\chi',0\rangle$ they impose the following two boundary conditions[3]:

(i) For small values of $\Omega$ and for $\chi,\chi'$ connected by only one geodesic,

$$\langle\chi,\Omega\,|\,\chi',0\rangle\underset{\Omega\to 0}{\sim}\eta(4\pi\Omega)^{-2}\tilde\Delta^{1/2}(\chi,\chi')\times\exp\left[-\frac{\tilde\sigma(\chi,\chi')}{2\Omega}\right] , \tag{4.7}$$

where $\tilde\Delta$ is defined in terms of the Van Vleck–Morette determinant as

$$\tilde\Delta(\chi,\chi')=[\gamma(\chi)\gamma(\chi')]^{-1/2}\times\mathrm{Det}(\partial^2\tilde\sigma/\partial\chi^\alpha\partial\chi'^\beta) . \tag{4.8}$$

Here $\tilde\sigma(\chi,\chi')$ is half the proper distance squared along the geodesic joining $\chi$ and $\chi'$. For the metric under consideration[3]

$$\tilde\sigma=(\lambda^2+\lambda'^2-2\lambda\lambda'\cos\rho)/2 \tag{4.9}$$

and

$$\tilde\Delta=\rho^{-2}\sin^2\rho , \tag{4.10}$$

where $\rho=|\chi-\chi'|$. In the original spacetime, $\sigma$ is given by Eq. (3.8) and

$$\Delta(x,x')=-\,|g(x)g(x')|^{-1/2}\times\mathrm{Det}(-\partial^2\sigma/\partial x^\alpha\partial x'^\beta) \tag{4.11}$$

is given by

$$\Delta=r^{-2}\sinh^2 r , \tag{4.12}$$

where $r=|\vec{x}-\vec{x}'|$.

(ii) As the separation between $\chi$ and $\chi'$ approaches infinity

$$\langle\chi,\Omega\,|\,\chi',0\rangle\to 0 . \tag{4.13}$$

Using the boundary conditions of Eqs. (4.7) and (4.13), they[3] arrive at the propagator $G^{(1)}$ of Eq. (3.9). We now show that the analytic continuation of the kernel corresponding to the propagator $G^{(0)}$ of Eq. (3.7) also satisfies the boundary conditions of Eqs. (4.7) and (4.13), so that those boundary conditions are not sufficient to uniquely determine the Feynman propagator.

The propagator $G^{(0)}(x,x')$ of Eq. (3.7) can be written in the form of Eq. (4.1) with the kernel[18,22]

$$\langle x,s\,|\,x',0\rangle^{(0)}=\frac{-i}{(4\pi s)^2}\Delta^{1/2}(x,x')\times\exp\left[i\frac{\sigma(x,x')}{2s}\right] , \tag{4.14}$$

as can be verified by direct integration. Here $\sigma$ and $\Delta$ are given by Eqs. (3.8) and (4.12), respectively. In Appendix B we show explicitly that this kernel is an *exact* solution of the Schrödinger equation (4.2) for the metric of Eq. (2.1). The analytic continuation of Eq. (4.14) which satisfies Eq. (4.5) is

$$\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)} = \frac{i}{(4\pi\Omega)^2}\tilde{\Delta}^{1/2}(\mathcal{X},\mathcal{X}') \times \exp\left[-\frac{\tilde{\sigma}(\mathcal{X},\mathcal{X}')}{2\Omega}\right], \quad (4.15)$$

where $\tilde{\sigma}$ and $\tilde{\Delta}$ are given by Eqs. (4.9) and (4.10), respectively. This kernel obviously satisfies the boundary condition of Eq. (4.7). Furthermore, $\tilde{\sigma}$ or $\tilde{\Delta}^{-1}$ becomes large as the separation between $\mathcal{X}$ and $\mathcal{X}'$ increases, so that $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)}$ approaches zero in accordance with Eq. (4.13). Thus $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)}$ satisfies both conditions. Analytically continuing it back to Eq. (4.14) using $\Omega = is$, $\lambda = -it$, and $\rho = -ir$, and substituting into Eq. (4.1), one obtains the propagator $G^{(0)}(x,x')$.

Chitre and Hartle[3] find that the analytic continuation of the kernel $\langle x,s \mid x',0\rangle^{(1)}$ corresponding to the propagator $G^{(1)}(x,x')$ of Eq. (3.9) is

$$\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(1)} = \langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)} + Q(\mathcal{X},\mathcal{X}',\Omega), \quad (4.16)$$

where

$$Q(\mathcal{X},\mathcal{X}',\Omega) = \frac{i\exp[-(\lambda^2+\lambda'^2)/4\Omega]}{(2\pi)^3 2\Omega\lambda\lambda'\rho}\int_{-\infty}^{\infty} d\psi \exp\left[-\frac{\lambda\lambda'\cosh\psi}{2\Omega}\right] \times \left\{\frac{1}{[\psi+i(\pi-\rho)]^2} - \frac{1}{[\psi+i(\pi+\rho)]^2}\right\}. \quad (4.17)$$

They show that the kernel $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(1)}$ satisfies both boundary conditions Eqs. (4.7) and (4.13). Therefore, both of the kernels $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)}$ and $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(1)}$ [which lead to the propagators $G^{(0)}(x,x')$ and $G^{(1)}(x,x')$, respectively] satisfy the boundary conditions imposed in Ref. 3, so that those boundary conditions do not uniquely determine the Feynman propagator.

One can in fact find a family of kernels which satisfy those boundary conditions. Because both $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)}$ and $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(1)}$ are solutions of the analytically continued Schrödinger equation (4.5), it follows that $Q(\mathcal{X},\mathcal{X}',\Omega)$ is also a solution. Introducing the parameter $\Lambda$, one then obtains the family of solutions

$$\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(\Lambda)} = \langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)} + \Lambda Q(\mathcal{X},\mathcal{X}',\Omega), \quad (4.18)$$

every member of which satisfies the boundary conditions of Eqs. (4.7) and (4.13). When these kernels are analytically continued and substituted into Eq. (4.1), they yield the family of propagators $G^{(\Lambda)}(x,x')$ of Eq. (3.17) with $\Lambda$ independent of $k$. Choosing $\Lambda$ independent of $k$ corresponds to Eq. (3.22) with $\gamma = 2\pi$. Therefore, each member of this class of Feynman propagators corresponds to a distribution of particles at late times which is thermal at high momenta and characterized by temperature

$$T = [k_B 2\pi a(t)]^{-1} \quad (4.19)$$

and chemical potential

$$\mu = [\pi a(t)]^{-1}\ln|\Lambda| . \quad (4.20)$$

Let us examine more closely the boundary conditions that are satisfied by the kernels $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(0)}$ and $\langle \mathcal{X},\Omega \mid \mathcal{X}',0\rangle^{(1)}$ by taking the limit of each of them as $\Omega$ approaches zero through positive values. The boundary values of each kernel in the $\Omega = 0$ hypersurface completely determines it as a solution of Eq. (4.5) for $\Omega > 0$ [alternatively, one could do the same analysis with the original Schrödinger equation (4.2) and the kernels defined on the physical spacetime]. However, it is necessary to include the boundary values corresponding to nonphysical values of the analytically continued time variables $\lambda$ and $\lambda'$. As $\Omega$ increases, the effect of the boundary conditions in the nonphysical region propagate or diffuse into the physical region and influence the form of the kernels in the physical region. As we shall see, the boundary conditions at $\Omega = 0$ of both kernels [and hence of the entire class in Eq. (4.18)] are the same in the physical region, but differ in the nonphysical region. The physical region is the region in which

$\lambda$ (and $\lambda'$) is greater than zero.[3] That is because times to the future of the cosmological singularity ($t>0$) were rotated by $\pi/2$ in the complex plane, corresponding to positive values of $\lambda$.

First consider $\langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(0)}$. As $\Omega\to 0$ through positive values, the kernel is negligible except for $\tilde{\sigma}$ small. As $\mathcal{X}$ approaches $\mathcal{X}'$, the quantity $\tilde{\Delta}$ approaches unity, and using the Gaussian representation of the $\delta$ function, one obtains

$$\lim_{\Omega\to 0^+} \langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(0)} = i\lambda^{-3}\delta(\vec{\mathcal{X}}-\vec{\mathcal{X}}')\delta(\lambda-\lambda') , \tag{4.21}$$

where the factor of $\lambda^{-3}=\gamma^{-1/2}$, as in Eq. (4.6). The first term of $\langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(1)}$ in Eq. (4.16) of course satisfies this boundary condition. The second term $Q$ is defined in the physical region, where $\lambda\lambda'>0$, by Eq. (4.17). For small positive values of $\Omega$ one can evaluate the integral in Eq. (4.17) by the method of steepest descent, with the result that

$$Q \underset{\Omega\to 0^+}{\sim} -i\pi^{-1}(\rho^2-\pi^2)^{-2}(\lambda\lambda')^{-3/2}(4\pi\Omega)^{-1/2} \times \exp\left[-\frac{(\lambda+\lambda')^2}{4\Omega}\right] . \tag{4.22}$$

This expression can be analytically continued to define $Q$ throughout the entire $(\lambda,\lambda')$ plane for small positive $\Omega$. Using the Gaussian representation of the Dirac $\delta$-function, one obtains the boundary value that

$$\lim_{\Omega\to 0^+} Q = -i\pi^{-1}(\rho^2-\pi^2)^{-2}(\lambda\lambda')^{-3/2}\delta(\lambda+\lambda') . \tag{4.23}$$

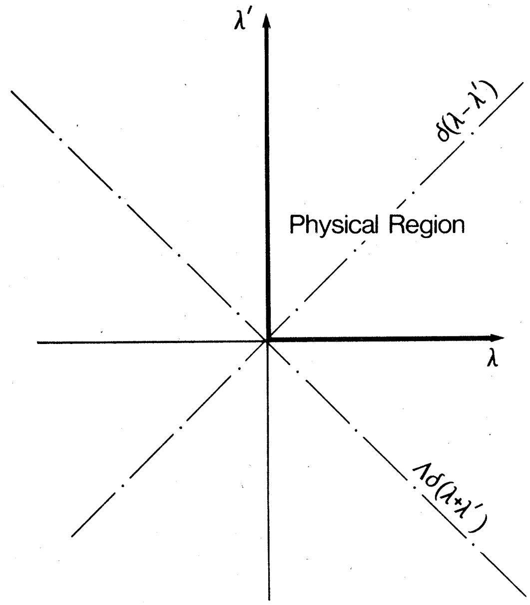


FIG. 1. Initial data for kernels (4.18) in the extended region.

Thus, $\langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(1)}$ satisfies the boundary condition

$$\lim_{\Omega\to 0^+} \langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(1)} = i\lambda^{-3}\delta(\vec{\mathcal{X}}-\vec{\mathcal{X}}')\delta(\lambda-\lambda') - i\pi^{-1}(\rho^2-\pi^2)^{-2}(\lambda\lambda')^{-3/2}\delta(\lambda+\lambda') , \tag{4.24}$$

where $\rho=|\vec{\mathcal{X}}-\vec{\mathcal{X}}'|$. This same result can also be obtained by starting with the representation of $\langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(1)}$ in terms of the Bessel function $I_\kappa(\lambda\lambda'/2\Omega)$ which is well defined for all $\lambda$ and $\lambda'$ [Ref. 3, Eq. (3.11)] and using the large-argument asymptotic expansion of $I_\kappa$. For the class of kernels defined in Eq. (4.18), the boundary condition is the same as Eq. (4.24) with the second term on the right multiplied by $\Lambda$. The boundary condition at $\Omega=0$ on $\langle \mathcal{X},\Omega\,|\,\mathcal{X}',0\rangle^{(\Lambda)}$ is schematically illustrated in Fig. 1 for the $\lambda,\lambda'$ plane.

The second term of Eq.(4.24) vanishes in the physical region, so that the kernels obey the same boundary conditions there. However, in the nonphysical region, the kernels have different boundary values along the line $\lambda+\lambda'=0$. As $\Omega$ increases, this difference eventually propagates into the physical region. It is now clear why direct evaluation of the path integral in Ref. 22 gives $\langle x,s\,|\,x',0\rangle^{(0)}$ and not $\langle x,s\,|\,x',0\rangle^{(1)}$. In that reference, a general spacetime was considered and the boundary condition of Eq. (4.3) was imposed for *all* values of the spacetime variables, thereby excluding solutions such as $\langle x,s\,|\,x'0\rangle^{(1)}$. That boundary condition seems appropriate in the absence of boundaries such as are implied by the presence of a cosmological singularity. When such a singularity is present one may want to impose further boundary conditions on $G(x,x')$ near the singularity (i.e., when $t$ or $t'$ vanishes). That can be done by imposing conditions on the kernel along the boundary of the physical region (Fig. 1) for all non-negative values of $\Omega$ (or $s$), or equivalently by imposing appropriate conditions on the kernel at $\Omega=0$ in the nonphysical region as described above.

## V. OTHER POSSIBLE BOUNDARY CONDITIONS

In this section we consider three methods by means of which one may attempt to specify the Feynman propagator uniquely. The methods involve the rate at which the kernel $\langle \chi,\Omega \mid \chi',0\rangle$ vanishes as the separation of the two points approaches infinity, the massless limit of the kernel, and specification of a thermal distribution of created particles, respectively.

From Eq. (4.15), one sees that for large $\rho$ the kernel $\langle \chi,\Omega \mid \chi',0\rangle^{(0)}$ vanishes as $\rho^{-1}\sin\rho$. Therefore, $\int \mid \langle \chi,\Omega \mid \chi',0\rangle^{(0)} \mid^2 d^3\chi$ does *not* converge, and the kernel $\langle \chi,\Omega \mid \chi',0\rangle^{(0)}$ has no Fourier transform. (Its Fourier transform is a distribution but not a function.) That is why that kernel was not obtained by the method of Ref. 3, which made use of Fourier expansion in plane waves $\exp[i\vec{\kappa}\cdot(\vec{\chi}-\vec{\chi}')]$. One can therefore use the square integrability of the kernel or the existence of its Fourier transform as an additional criterion, which at least in the present case is met by only one kernel.

To show that only one kernel has a Fourier transform on the Riemannian domain, we start with Eq. (3.6), the most general form of the Feynman propagator. Using the relationship between Hankel and Bessel functions, one can write that expression as

$$G(x,x')=\frac{i\pi}{(2\pi)^3 2tt'}\int e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\left[\left[\frac{e^{2\pi k}B_k^*}{C_k^*}-1\right](e^{2\pi k}-1)^{-1}H_{-ik}^{(2)}(mt_>)J_{-ik}(mt_<)+e^{2\pi k}(e^{2\pi k}-1)^{-1}\left[1-\frac{B_k^*}{C_k^*}\right]H_{ik}^{(2)}(mt_>)J_{ik}(mt_<)\right]d^3k\ . \tag{5.1}$$

Making use of representations of products of Bessel and Hankel functions (Ref. 21, p. 439), one can write Eq. (5.1) in the form of Eq. (4.1) with the kernel given by

$$\langle x,s \mid x',0\rangle=i\exp\left[\frac{t^2+t'^2}{4is}\right][2tt'(2\pi)^3 s]^{-1}\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\left[(1-e^{-2\pi k})^{-1}\left[1-\frac{B_k^*}{C_k^*}\right]I_{ik}\left[\frac{itt'}{2s}\right]+\left[\frac{e^{2\pi k}B_k^*}{C_k^*}-1\right](e^{2\pi k}-1)^{-1}I_{-ik}\left[\frac{itt'}{2s}\right]\right]. \tag{5.2}$$

Analytically continuing this kernel in the manner of Chitre and Hartle by writing $s=-i\Omega$, $t=i\lambda$, $\vec{x}=i\vec{\chi}$, $\vec{k}=-i\vec{\kappa}$, one finds that the second term in the kernel $\langle \chi,\Omega \mid \chi',0\rangle$ obtained from Eq. (5.2) involves the function $I_{-\kappa}(\lambda\lambda'/2\Omega)$, where $\kappa>0$. However, from the integral representation of $I_\nu(z)$ given in Ref. 21, p. 181, it is clear that the term involving $I_{-\kappa}(\lambda\lambda'/2\Omega)$ is divergent. Therefore, the kernel has a well-defined Fourier transform in the Riemannian domain if and only if $C_k^*=e^{2\pi k}B_k^*$. This condition is the one which gives the propagator $G^{(1)}(x,x')$ as discussed in connection with Eq. (3.9). In that case Eq. (5.2) reduces to

$$\langle x,s \mid x',0\rangle^{(1)}=\frac{i}{(2\pi)^3 2tt's}\exp\left[\frac{t^2+t'^2}{4is}\right]\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}I_{ik}\left[\frac{itt'}{2s}\right] \tag{5.3}$$

in agreement with the kernel found by Chitre and Hartle.

We would like to express the requirement of square integrability in a way which can be applied to more general metrics and which is independent of the choice of coordinates. Let $\gamma_{\mu\nu}$ denote a Riemannian metric on a manifold $M'$ which can be regarded as an analytic continuation of the original spacetime. Let $\langle \chi,\Omega \mid \chi',0\rangle$ represent the analytic continuation of the kernel to $M'$ with coordinates denoted by $\chi$. The proposed boundary condition is that

$$\int \mid \langle \chi,\Omega \mid \chi',0\rangle \mid^2 \gamma^{1/2}d^4\chi \text{ is convergent}\ . \tag{5.4}$$

This is to hold for each value of $\chi'$ for which the kernel is well defined. Here $\gamma$ is the determinant of the Riemannian metric. (It may also be necessary to ignore divergences which may appear from interior points of integration.) In addition, one would of course impose the boundary condition of Eq (4.7) in the domain corresponding to the physically allowed values of the coordinates. For the metric of Eq. (4.4) the kernel $\langle \chi,\Omega \mid \chi',0\rangle^{(1)}$ of Chitre and Hartle is uniquely determined by Eqs. (4.7) and (5.4). In that case, the factor $\gamma^{1/2}=\lambda^3$ ensures that the integration over $\lambda$ is convergent, and one may carry out the integrations either over the physical domain or over all values of the coordinates without alternating the result. In general, the least stringent condition is to carry out the integrations in Eq. (5.4) only over the physical domain (unless other examples should show that the stronger condition is necessary).

Next consider the Feynman propagator of the massless field. For the massless conformal field in an isotropically expanding universe, there is a natural way to define the positive-frequency solutions of the wave equation.[1] For the metric of Eq. (2.1) and wave equation (2.2) with $\xi=\frac{1}{6}$ and $m=0$, the positive-frequency solutions have the form of Eq. (2.4) with

$$\psi_k(t)=\frac{a(t)^{-3/2}}{[2\omega(t)]^{1/2}}\exp\left[-i\int^t\omega(t')dt'\right], \tag{5.5}$$

where $\omega(t)=k/a(t)$. With $a(t)=t$ this reduces to

$$\psi_k=t^{-1}(2k)^{-1/2}\exp(-ik\ln t) \tag{5.6}$$

to within an arbitrary phase. In this case there is no particle creation or mixing of positive and negative frequencies by the expansion. Hence $p_{\vec{k}}^{(\pm)}=f_{\vec{k}}^{(\pm)}$ and $\alpha_k=1$, so that Eq. (2.18) gives the Feynman propagator as

$$G(x,x')=i(2\pi)^{-3}\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}\times(2ktt')^{-1}(t_</t_>)^{ik}\,. \tag{5.7}$$

Performing the integration, one obtains the distribution

$$G(x,x')=(4\pi tt')^{-1}[\delta(r^2-\ln^2 t/t')+i\pi^{-1}(r^2-\ln^2 t/t')^{-1}]\,. \tag{5.8}$$

(If one writes $\tau=\ln t$, then it is clear that the metric, the positive-frequency basis functions, and the Feynman propagator are conformally related to those in Minkowski spacetime.) It is natural to impose the boundary condition that in the limit as $m\to 0$ the Feynman propagator of the conformally coupled field should have the form of Eq. (5.7) or Eq. (5.8).

Chitre and Hartle showed in Ref. 3 that the massless limit of the propagator $G^{(1)}(x,x')$ is indeed of the form of Eq. (5.7). On the other hand, one can show that $G^{(0)}(x,x')$ does not approach the form of Eq. (5.7) or Eq. (5.8) in the massless limit. Therefore, the above boundary condition at $m=0$ does prefer $G^{(1)}$ over $G^{(0)}$. However, that boundary condition is *not* sufficient to uniquely determine the Feynman propagator when $m$ does not vanish. We show that by exhibiting a set of propagators which have the same massless limit as $G^{(1)}$ but differ from $G^{(1)}$ when the mass is not zero. The propagators $G^{(\Lambda)}$ of Eq. (3.17) which correspond to the kernels of Eq. (4.18), will all have the same massless limit as $G^{(1)}$ if $\Lambda$ is taken to be a function of $m$ such that $\lim_{m\to 0}\Lambda(m)=1$. Therefore, we can choose $\Lambda$ such that $\lim_{m\to 0}G^{(\Lambda)}=\lim_{m\to 0}G^{(1)}$ but $G^{(\Lambda)}\neq G^{(1)}$ for $m\neq 0$.

A third way in which one can attempt to single out the Feynman propagator is to impose the boundary condition that the probability distribution of created particles for large momenta be thermal with a specified temperature $T$ and chemical potential $\mu$. Then the propagator would be that of Eq. (3.17) with $\Lambda$ determined to within an arbitrary phase by Eqs. (3.22)–(3.24). The values of $T$ and $\mu$ would have to come from other considerations, as for example, dimensional arguments or consistency with the Einstein equations as in Refs. 25 and 2. In those references, it was shown that for a wide class of models without a cosmological singularity an analysis based on in and out regions gave a spectrum which at high momenta was thermal. The present boundary condition would be a way of generalizing that result to models with a cosmological singularity. In order to make use of the Einstein equations one would of course have to work with a general function $a(t)$ as in Sec. II. This boundary condition is also applicable to spatially closed universes and does not require that the line element be continued to the Riemannian domain.

Of the three possible boundary conditions considered here, the most natural way of strengthening the boundary conditions on the analytically continued kernel is the postulate of square integrability. It is quite interesting that the simple vanishing of the kernel which yields a unique propagator in flat spacetime is not sufficient in curved spacetime.

The conjecture that for a general open spactime the boundary conditions of Eqs. (4.6) and (5.4) imposed in the physical region are sufficient to determine a unique propagator remains to be proved.

In this paper, we used the relation between in and out basis functions and Feynman propagators to write down the most general expression for the Feynman propagator in the linearly expanding universe. We then proved that the direct generalization by Chitre and Hartle of the boundary conditions used in flat spacetime actually admits a large class of propagators. Each of these propagators can be characterized by a temperature and a chemical potential. Several alternative boundary conditions were considered for singling out the Feynman propagator. One possible approach is to determine the above temperature and chemical potentials by other considerations, such as the requirement of consistency with the Einstein equations. Another approach is to strengthen the boundary conditions on the analytically continued kernel by requiring that it be square integrable. That condition is sufficient in the present model to determine the propagator uniquely.

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## APPENDIX A

Let us consider the propagator $G^0(x,x')$ given by the Fourier integral

$$G^{(0)}(x,x')=\frac{i}{(2\pi)^3}\frac{\pi}{4tt'}\int d^3k\, e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}H_{ik}^{(2)}(mt_>)H_{ik}^{(1)}(mt_<)\ . \tag{A1}$$

Integration over the angles gives

$$G^{(0)}(x,x')=-\frac{i}{16\pi tt'r}\frac{\partial}{\partial r}\int_0^\infty dk[e^{-ikr}H_{ik}^{(2)}(mt_>)H_{ik}^{(1)}(mt_<)+e^{ikr}H_{ik}^{(2)}(mt_>)H_{ik}^{(1)}(mt_<)]\ . \tag{A2}$$

Using the symmetry of the product of the Hankel functions under the replacement $k\to -k$ one obtains

$$G^0(x,x')=-\frac{i}{16\pi tt'r}\frac{\partial}{\partial r}\int_{-\infty}^{+\infty} e^{-ikr}H_{ik}^{(2)}(mt_>)H_{ik}^{(1)}(mt_<)dk\ . \tag{A3}$$

The Hankel functions $H_{ik}^{(2)}(mt_>)$ and $H_{ik}^{(1)}(mt_<)$ can be represented by the following expressions (see Ref. 21, p. 180):

$$H_{ik}^{(1)}(mt_<)=(\pi i)^{-1}e^{\pi k/2}\int_{-\infty}^{+\infty} e^{imt_<\cosh w-ikw}dw \tag{A4}$$

and

$$H_{ik}^{(2)}(mt_>)=-(\pi i)^{-1}e^{-\pi k/2}\int_{-\infty}^{+\infty} e^{-imt_>\cosh v-ikv}dv\ . \tag{A5}$$

Inserting the latter integral representations into Eq. (A3) and changing the order of integrations, one obtains

$$G^{(0)}(x,x')=-\frac{i}{8\pi^2 tt'r}\frac{\partial}{\partial r}\int_{-\infty}^{+\infty} e^{-im[t\cosh v-t'\cosh(r+v)]}dv\ . \tag{A6}$$

Evaluation of the above integral depends on the sign of the parameter $\sigma$, given by Eq. (3.8). When the points $x$ and $x'$ are connected by a timelike geodesic, i.e.,

$$-2\sigma\equiv t^2+t'^2-2tt'\cosh r>0\ , \tag{A7}$$

one obtains

$$t\cosh v - t'\cosh(r+v) = \sqrt{-2\sigma}\cosh(v-w)\ , \tag{A8}$$

along with

$$\tanh w = \frac{t'\sinh r}{t - t'\cosh r}\ . \tag{A9}$$

In the opposite case, i.e., when $-2\sigma<0$, one obtains

$$t\cosh v - t'\cosh(r+v) = \sqrt{2\sigma}\sinh(w'-v)\ , \tag{A10}$$

where

$$\tanh w' = \frac{t - t'\cosh r}{t'\sinh r}\ . \tag{A11}$$

Accordingly we can rewrite Eq. (A6) either as

$$G^0(x,x') = -\frac{i}{8\pi^2 tt'r}\frac{\partial}{\partial r}\int_{-\infty}^{+\infty} e^{-im\sqrt{-2\sigma}\cosh v'}dv' \quad \text{for } \sigma<0\ , \tag{A12}$$

or as

$$G^0(x,x') = -\frac{i}{8\pi^2 tt'r}\frac{\partial}{\partial r}\int_{-\infty}^{+\infty} e^{im\sqrt{2\sigma}\sinh v'}dv' \quad \text{for } \sigma>0\ . \tag{A13}$$

Using the integral representations of the Hankel functions of real $[H_0^{(2)}(x)]$ and imaginary $[K_0(x)]$ arguments as given in Ref. 17, pp. 180 and 183,

$$H_0^{(2)}((-2m^2\sigma)^{1/2}) = -\frac{1}{\pi i}\int_{-\infty}^{+\infty} e^{-i(-2m^2\sigma)^{1/2}\cosh v'}dv'\ , \tag{A14}$$

$$K_0((2m^2\sigma)^{1/2}) = \tfrac{1}{2}\int_{-\infty}^{+\infty} e^{+i(2m^2\sigma)^{1/2}\sinh hv'}dv'\ , \tag{A15}$$

one finds

$$\begin{aligned} G^0(x,x') &= -\frac{1}{8\pi tt'r}\frac{\partial}{\partial r}H_0^{(2)}((-2m^2\sigma)^{1/2}) \\ &= -\frac{m^2}{8\pi}\frac{\sinh r}{r}\frac{H_1^{(2)}((-2m^2\sigma)^{1/2})}{(-2m^2\sigma)^{1/2}}\ , \quad \sigma<0 \end{aligned} \tag{A16}$$

and

$$\begin{aligned} G^0(x,x') &= -\frac{i}{4\pi^2 tt'r}\frac{\partial}{\partial r}K_0((2m^2\sigma)^{1/2}) \\ &= \frac{im^2}{4\pi^2}\frac{\sinh r}{r}\frac{K_1((2m^2\sigma)^{1/2})}{(2m^2\sigma)^{1/2}}\ , \quad \sigma>0\ . \end{aligned} \tag{A17}$$

Using now the relationship between functions $K_1(x)$ and $H_1^{(2)}(x)$ (Ref. 26, p 375),

$$K_1(x) = -\tfrac{1}{2}\pi H_1^{(2)}(-ix)\ , \tag{A18}$$

Eq. (A17) can be rewritten as

$$G^0(x,x') = -\frac{m^2}{8\pi}\frac{\sinh r}{r}\frac{H_1^{(2)}[-i(2m^2\sigma)^{1/2}]}{[-i(2m^2\sigma)^{1/2}]} = -\frac{m^2}{8\pi}\frac{\sinh r}{r}\frac{H_1^{(2)}((-2m^2\sigma)^{1/2})}{(-2m^2\sigma)^{1/2}}\ . \tag{A19}$$

In the latter expression we explicitly used the fact that $H_1^{(2)}(z)$ tends to zero as $|z|\to\infty$ only when $-\pi<\arg z<0$.

Therefore, for both signs of the parameter $\sigma$ the propagator $G^0(x,x')$ can be written as

$$G^0(x,x') = -\frac{m^2}{8\pi}\frac{\sinh r}{r}\frac{H_1^{(2)}((-2m^2\sigma)^{1/2})}{(-2m^2\sigma)^{1/2}}\ . \tag{A20}$$

## APPENDIX B

Let us prove that the kernel $\langle x,s\,|\,x',0\rangle^{(0)}$ given by Eqs. (4.14), (4.12), and (3.8) is an exact solution of the Schrödinger equation (4.2), i.e.,

$$i\frac{\partial}{\partial s}\langle x,s\,|\,x',0\rangle^{(0)}=(-\nabla_\mu\nabla^\mu+\tfrac{1}{6}R)\langle x,s\,|\,x',0\rangle^{(0)}\;. \tag{B1}$$

In the case of the Robertson-Walker universe (2.1) the Ricci scalar $R$ is equal to $6/t^2$. Therefore, Eq. (B1) can be written explicitly as

$$i\frac{\partial}{\partial s}\langle x,s\,|\,x',0\rangle^{(0)}=\left[\frac{1}{t^3}\frac{\partial}{\partial t}\left[t^3\frac{\partial}{\partial t}\right]-\frac{1}{t^2}\nabla^2+\frac{1}{t^2}\right]\langle x,s\,|\,x',0\rangle^{(0)}\;. \tag{B2}$$

Here $\nabla^2$ is the three-dimensional Laplacian.

The left-hand side of Eq. (B2) gives

$$i\frac{\partial}{\partial s}\langle x,s\,|\,x',0\rangle^{(0)}=\left[\frac{\sigma}{2s^2}-\frac{2i}{s}\right]\langle x,s\,|\,x',0\rangle\;. \tag{B3}$$

The time-derivative part of Eq. (B2) is found to be

$$\frac{1}{t^3}\frac{\partial}{\partial t}\left[t^3\frac{\partial}{\partial t}\right]\langle x,s\,|\,x',0\rangle^{(0)}=\left[\left[-\frac{2i}{s}+\frac{\sigma}{2s^2}\right]-\frac{t^2\sinh^2 r}{4s^2}+\frac{3i}{2s}\frac{t'}{t}\cosh r\right]\langle x,s\,|\,x',0\rangle\;, \tag{B4}$$

whereas the Laplacian part of Eq. (B2) is equal to

$$-\frac{1}{t^2}\nabla^2\langle x,s\,|\,x',0\rangle^{(0)}=\frac{1}{t^2}\left[1-\frac{t^2t'^2\sinh^2 r}{4s^2}+\frac{3itt'\cosh r}{2s}\right]. \tag{B5}$$

Substituting Eqs. (B3)—(B5) into Eq. (B2) leads to an identity.

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