Weak and strong quantum vacua in Bianchi type-I universes

Mario Castagnino
Instituto de Astronomía y Física del Espacio, Casilla de Correos 67, Sucursal 28, 1428 Buenos Aires, Argentina and Instituto de Física de Rosario (CONICET-UNR), Av. Pellegrini 250-2000 Rosario, Argentina

Francisco Diego Mazzitelli*
Instituto de Astronomía y Física del Espacio, Casilla de Correos 67, Sucursal 28, 1428 Buenos Aires, Argentina
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Using several physical criteria, we show that a reasonable quantum vacuum can be defined in Bianchi type-I universes, at the cosmological singularity (and the asymptotic far future region), provided the initial expansion would not be very violent.

INTRODUCTION

This work is devoted to the problem of the quantum vacuum definition in curved space-time and can be considered a synthesis of Refs. 1—3 (other papers on the subject are Refs. 4 to 38; see also Ref. 39 and the bibliography therein).

The only method to solve the problem seems to be to find the quantum state of curved space-time that has as many properties of the flat-space-time vacuum as possible. The flat-space-time vacuum has several properties, some of them can be generalized to curved space-time, the others cannot.

In Ref. 1 four properties of the flat vacuum are generalized to a linearly expanding Robertson-Walker universe. Two of these properties survive a further generalization (e.g., in Ref. 2 one of these properties are studied in a generic Robertson-Walker universe). These two properties are our criteria C.1 and C.2 that we study in a more general geometry, a Bianchi type-I universe. C.1 is based on the Wick trick or Euclidean form of the metric and C.2 in the addition of a term $i\epsilon$ to the squared mass. These two properties are formulated via the Feynman propagator obtained using the in and out vacua, and therefore they depend on the vacuum definition at two different times, the far future and the far past (or the singularity).

As the particle notion is observer dependent, the vacuum definition is also observer dependent, thus all these manipulations must be done in a particular and well-defined coordinate system, the one "adapted" (cf. Ref. 40) to the space-time paths of the set of chosen observers. We always choose the comoving system of coordinates, i.e., the natural generalization of the inertial system of Minkowski space to curved space. Thus, a change of system would produce a change of vacuum (in Appendix II we give a simple example).

On the other hand, in Ref. 3 two other properties are introduced: the vacuum must minimize the energy (this is our third criterion C.3) and the kernel related to the vacuum must behave like the corresponding flat-space-time kernel in the coincidence limit $x \to x'$. This last property can be formulated in a different way asking that the Cauchy data of the positive- and negative-frequency basis should be the one given by the WKB method. These properties depend on the vacuum definition at only one time—when the energy is minimized, or when the Cauchy data are given. Therefore, they are of a different kind than C.1 and C.2 that depend on the vacuum definition at two times.

The energy minimization (i.e., the Hamiltonian diagonalization) is strongly criticized in the literature (cf., e.g., Refs. 11 and 30, or 41) as a criterion to define the vacuum. In fact, there are different possible definitions of the Hamiltonian (cf. Ref. 41), the created particles could be infinite (cf. Ref. 11) and the uncertainty relation prevents an instantaneous definition of the energy (cf. Ref. 30). But the vacuum must be the minimum of something, as Hájíček pointed out (cf. Ref. 42). We shall use the energy deduced by integration from the energy-momentum tensor because it is the best candidate for the physical energy in curved space-time. Therefore, there will be no Hamiltonian-definition ambiguity (cf. discussion in Ref. 3) and we shall minimize the energy only when the uncertainty principle allows it. We shall prove that, under this requirement, the number of produced particles is finite. In this way we believe all objections are overcome.

The flat-space-time vacuum is endowed with the four introduced properties. This is also the case of all curved space-time vacua adopted unanimously by all authors as good reliable vacua: the vacuum in a static metric and the conformal massless vacuum [while the adiabatic vacuum has only the last two properties, because, being an asymptotic vacuum, it only depends on one time (cf., e.g., Ref. 39)]. Therefore, we shall conclude that a good vacuum is the one that has the four properties and we shall study different evolutions of Bianchi type-I universes to see if we can find new good vacua.

On the contrary, in zones of space-time where one or several of these properties are missing, we cannot define the vacuum and the particle notion becomes fuzzy.

We shall call a *strong vacuum* at a given time the one endowed with property C.3 and with positive- and negative-frequency basis Cauchy data given by all the terms of the WKB expansion, and a *weak vacuum* when it satisfies property C.3 and if also its Cauchy data are only given by the zeroth-order term of the WKB expansion.

We shall see that normally, when the in and out Fock bases are defined through strong vacua, properties C.1 and C.2 are satisfied and the number of the produced particles, their energy, and momentum are finite; we shall therefore conclude that the strong vacuum is a good candidate for a physical vacuum in curved space-time.

However, the weak vacuum is not as satisfactory; e.g., between two Fock bases defined through weak vacua the particle number is finite but the energy and momentum are not finite, in general. Actually, we introduce the weak vacuum because some evolution of the radius of the Robertson-Walker universe like $t^{1/2}$ or $t^{2/3}$ allows only weak vacua at its singularity.

In Sec. I we fix the notation and we comment on the different criteria that can be found in the literature to define the vacuum.

In Sec. II we study criteria C.1. and C.2, and we give sufficient conditions that warrant the applicability and equivalence of the criteria in a Bianchi type-I universe. We also study examples where the criteria do not define a unique vacuum, as well as examples where the criteria are not equivalent.

In Sec. III we compute the Cauchy data that minimize the energy in a Bianchi type-I universe. We also study in which cases the minimization can be done, i.e., when the uncertainty relation allows it.

In Sec. IV we compare the results of the previous sections with the approximate vacua computed via the WKB method, and we define the weak and strong vacua. We also study the total number of created particles and the created energy and momentum, and state several theorems.

Appendix A is a mathematical theorem.

Finally, in Appendix B we review the change of the reference system in flat space-time and see how the vacuum is modified by this change.

I. STATEMENT OF THE CRITERIA

A. General formalism

In this paper, we consider a neutral scalar field $\phi(x)$ that satisfies the Klein-Gordon equation

$$(-\nabla_\mu\nabla^\mu+m^2+\xi R)\phi(x)=0\ , \tag{1.1}$$

where ∇_μ is the covariant derivative, m is the mass, ξ is the coupling coefficient, and R is the Ricci scalar ($\mu=0,1,2,3$, $\hbar=c=1$; we are working with natural units).

We shall study the vacuum definition in Bianchi type-I metrics, i.e.,

$$ds^2=-dt^2+\sum_{j=1}^{3} a_j{}^2(t)dx_j{}^2 \tag{1.2}$$

[in the special case $a_j(t)=a(t)$ a spatially flat Robertson-Walker metric is obtained]. If we write the field as (cf. Ref. 39 for an introduction to the subject and also Ref. 41)

$$\phi(x)=\int d^3\vec{k}[a_{\vec{k}}u_{\vec{k}}(x)+a^\dagger_{\vec{k}}u^*_{\vec{k}}(x)]\ , \tag{1.3}$$

where

$$u_{\vec{k}}(x)=(2\pi)^{-3/2}e^{i\vec{k}\cdot\vec{x}}\frac{\varphi_{\vec{k}}(t)}{a(t)}\ ,$$

$$a(t)=[a_1(t)a_2(t)a_3(t)]^{1/3}$$

and we define the conformal time $\eta=\int^t dt'/a(t')$, the Klein-Gordon equation becomes

$$\varphi''_{\vec{k}}+\varphi_{\vec{k}}a^2\left[m^2+\sum_{j=1}^{3}\frac{k_j{}^2}{a_j{}^2}+(\xi-\tfrac{1}{6})+q\right]=0\ , \tag{1.4}$$

where

$$R=a^{-2}(3D'+\tfrac{3}{2}D^2+6a^2q)\ ,$$

$$D=(a^2)'a^{-2}\ ,$$

$$q=\frac{Q}{a^2}=\frac{1}{18}\sum_{i<j}(\dot{a}_ia_i{}^{-1}-\dot{a}_ja_j{}^{-1})^2\ .$$

The overdots denote t derivatives, and the primes denote η derivatives. The set $\{u_{\vec{k}}(x),u^*_{-\vec{k}}(x)\}$ is an orthonormal basis of solutions of Eq. (1.1) if the functions $\varphi_{\vec{k}}(\eta)$ satisfy the normalization condition

$$\varphi_{\vec{k}}\varphi'^*_{\vec{k}}-\varphi'_{\vec{k}}\varphi^*_{\vec{k}}=i\ . \tag{1.5}$$

The field is quantized in the usual way replacing the coefficients $a^\dagger_{\vec{k}}$ and $a_{\vec{k}}$ in (1.3) by the creation and annihilation operators which obey the commutation relations

$$[a_{\vec{k}},a^\dagger_{\vec{k}'}]=\delta(\vec{k}-\vec{k}')\ ,$$
$$[a_{\vec{k}},a_{\vec{k}'}]=[a^\dagger_{\vec{k}},a^\dagger_{\vec{k}'}]=0\ . \tag{1.6}$$

The vacuum state is defined as the one that satisfies $a_{\vec{k}}|0\rangle=0$, $\forall\vec{k}$. A basis in the state space can be constructed from the vector $|0\rangle$ and the operators $a^\dagger_{\vec{k}}$, leading to the so-called Fock representation.

Let us consider another complete orthonormal set of solutions $\{\bar{u}_{\vec{k}},\bar{u}^*_{-\vec{k}}\}$. This set defines a new vacuum state $|\bar{0}\rangle$ and a new Fock basis. The functions $u_{\vec{k}}$ and $\bar{u}_{\vec{k}}$ are related by a Bogoliubov transformation

$$u_{\vec{k}}=\alpha_{\vec{k}}\bar{u}_{\vec{k}}+\beta_{\vec{k}}\bar{u}^*_{-\vec{k}}\ , \tag{1.7}$$

and therefore

$$\varphi_{\vec{k}}=\alpha_{\vec{k}}\bar{\varphi}_{\vec{k}}+\beta_{\vec{k}}\bar{\varphi}^*_{\vec{k}}\ , \tag{1.8}$$

with

$$|\alpha_{\vec{k}}|^2-|\beta_{\vec{k}}|^2=1\ . \tag{1.9}$$

It is easy to see that the two Fock bases are different if $|\beta_{\vec{k}}|\neq0$. In this case one has $a_{\vec{k}}|\bar{0}\rangle\neq0$ (this means that $\bar{a}_{\vec{k}}\neq a_{\vec{k}}$). The expectation value of the number of particles defined by the $a_{\vec{k}}$ in the state $|\bar{0}\rangle$ is

$$N=\int d^3\vec{k}\,|\beta_{\vec{k}}|^2\ . \tag{1.10}$$

Let us now discuss in more detail the criteria to find the correct vacuum in a curved space-time.

B. Criteria for the particle model definition

As can be seen from the last section, there is an ambiguity in the vacuum definition due to the fact that there are an infinite amount of bases solutions for Eq. (1.1).

In Minkowski space, there is a natural set of modes

$$u_{\vec{k}}(x)=(2\pi)^{-3/2}e^{i\vec{k}\cdot\vec{x}}\frac{e^{-i\omega_{\vec{k}}t}}{\sqrt{2\omega_{\vec{k}}}}\ ,$$
$$\omega_{\vec{k}}=(|\vec{k}|^2+m^2)^{1/2} \qquad (1.11)$$

which makes the vacuum invariant under the action of Poincaré group. In curved space-time the Poincaré group is no longer a symmetry group of the space-time and, therefore, there is not a well-established criterion to select the $u_{\vec{k}}(x)$.

We shall study the most usual criteria that can be found in the literature on the subject.

1. Criteria based on Feynman-propagator generalization

The Feynman propagator is defined in Ref. 1 as

$$G_F(x,x')=i\langle 0_{\rm out}|0_{\rm in}\rangle^{-1}\langle 0_{\rm out}|T[\phi(x)\phi(x')]|0_{\rm in}\rangle\ , \qquad (1.12)$$

where the in and out vacua are the vacuum states at $t=0$ and $t=\infty$:

$$|0_{\rm in}\rangle=|0_{t=0}\rangle\ ,$$
$$|0_{\rm out}\rangle=|0_{t=\infty}\rangle\ ,$$

$T=$time-ordered product

and we suppose that space-time has a singularity at $t=0$.

Using Eqs. (1.3) and (1.7) we see that

$$G_F(x,x')=i\int\frac{d^3\vec{k}}{\alpha^*_{\vec{k}}}u^{\rm out}_{\vec{k}}(\vec{x},t_>)u^{*\rm in}_{\vec{k}}(\vec{x}',t_<)\ , \qquad (1.13)$$

where

$t_>=\max\{t,t'\},\ \ t_<=\min\{t,t'\}$,

$u^{\rm out}_{\vec{k}}=$particle model at $t=\infty$

$u^{\rm in}_{\vec{k}}=$particle model at $t=0$

$\alpha_{\vec{k}}=$Bogoliubov coefficient [see Eq. (1.7)] .

If $G_F(x,x')$ is known, the in-out basis can then be determined from Eq. (1.13). In Ref. 1, four criteria to generalize the Feynman propagator in an isotropic universe with linear evolution and conformal coupling ($\xi=\frac{1}{6}$) have been tested. We shall consider here two of them in more general evolutions and couplings:

(C.1) $G_F(x,x')$ is the analytic continuation of the unique Green's function of the operator $(-\nabla_\mu\nabla^\mu+m^2+\xi R)$ in the Euclidean space.

(C.2) $G_F(x,x')$ is the limit when $\epsilon\to 0^+$ of the unique Green's function of the operator $(-\nabla_\mu\nabla^\mu+m^2-i\epsilon+\xi R)$.

In Ref. 1 it is shown that both criteria work in the considered case leading to the same propagator (and so to the same in-out basis). To apply C.1 it is necessary to work with a Euclidean metric which can be obtained from the usual one (the one adapted to the comoving frame of reference) by considering $a_j(t)$ as functions of λ_t with $\lambda=1$ and doing the substitutions $t\to -it_e,\lambda\to i\lambda_e$; we then obtain

$$ds_e{}^2=dt_e{}^2+\sum_{j=1}^{3}a_j{}^2(\lambda_e t_e)dx_j{}^2 \qquad (1.14)$$

(this rule has been introduced in Ref. 2 where C.1 is generalized performing the field quantization through the Feynman path integral). To apply C.2 it was found to be necessary in Ref. 1 to add an infinitesimal imaginary part to the particle momentum for the criterion to work near the initial singularity.

In Sec. II we shall extend these results to Bianchi type-I metrics.

2. Criteria based on energy minimization

In Ref. 3 the following criterion is established to define the vacuum state at time $t=t_0$:

(C.3) The vacuum at time $t=t_0$, $|0_{t_0}\rangle$, is the state that minimizes the total energy at that time, that is to say, the one that minimizes

$$H_{(t_0)}=\int_{\Sigma_{t_0}}\langle 0_{t_0}|T_0{}^0|0_{t_0}\rangle_{\rm ren}d\sigma\ , \qquad (1.15)$$

where $T_\nu{}^\mu=$energy-momentum tensor,

$$\Sigma_{t_0}=\{x=(t,\vec{x});t=t_0\}$$
$$d\sigma=g^{1/2}(t_0\vec{x})d^3x\ ,$$

$g=\det g_{\mu 0}$ with $g_{\mu 0}$ the metric tensor .

Reference 3 deals with the spatially flat Robertson-Walker metric and, as was mentioned in that work, C.3 is equivalent to minimizing $\langle 0_{t_0}|T_0{}^0|0_{t_0}\rangle$ instead of $H(t_0)$. It was also found that the resultant vacuum diagonalizes H, that is to say

$$:H:=a^{-1}\int d^3\vec{k}\,a^\dagger_{\vec{k}}a_{\vec{k}}[m^2a^2+k^2+6\xi(1-6\xi)\dot{a}^2]^{1/2}\ , \qquad (1.16)$$

In Sec. III we shall find the vacua which minimize the energy in the anisotropic case, and we shall compare $|0_0\rangle$ and $|0_\infty\rangle$ with the ones found in Sec. II.

The energy is, of course, determined up to some uncertainty because the uncertainty principle states that

$$\Delta E\Delta t\sim 1\ .$$

In our case Δt cannot be greater than $R^{-1/2}$, the radius of curvature or, more precisely, greater than $(R_{\max})^{-1/2}=(R_{\mu\nu\lambda\rho\max})^{-1/2}$ ($R_{\mu\nu\lambda\rho}$ being the components of the curvature tensor), because only in that range can we consider the geometry more or less flat, while $\Delta E\sim\Delta\omega$. We need $\Delta\omega<\omega$ to have reliable measurement of the energy; thus, we must have

$$\omega>R^{1/2}$$

(only if this equation is fulfilled is the notion of frequency meaningful as it is also demonstrated in Ref. 42). We immediately see that there is no problem in flat space because $R=0$, or in asymptotic zones where $R\rightarrow 0$, but, as we shall see, that could also be the case in some special kinds of singularities.

3. *Adiabatic vacua*

In Ref. 43 the following argument is given to generalize the kernels $\Delta(x,x')$ and $\Delta_1(x,x')$ to curved space-time: a highly energetic particle would not "feel" the curvature effects if its wavelength is much smaller than $R_{\max}^{-1/2}$ ($R_{\max}$ being again the biggest component of the curvature tensor) and thus it must resemble a flat-space particle. Furthermore, as the high-energy behavior of a field theory is governed by the singular structure of the kernels when $x\rightarrow x'$, that structure should be reproduced by $G_1(x,x')$. It then seems reasonable to require the following condition:

$$\lim_{\substack{x\rightarrow x_0\\ x'\rightarrow x_0}} G_1^{x_0}(x,x')=\lim_{\substack{x\rightarrow x_0\\ x'\rightarrow x_0}} \sum_{n=0}^{\infty} F_n^{x_0}(x,x')\frac{\partial^n\Delta_1(s)}{(\partial m^2)^n} , \tag{1.17}$$

F being the regular functions at x_0 such that

$$F_0^{x_0}(x,x')=1,\quad F_\alpha^{x_0}(x,x')=0 \text{ if } R_{ijkl}=0 ,\qquad \alpha=1,2,\ldots$$

and s the geodesic distance between x and x'.

This condition is a relaxation of the quantum equivalence principle studied in Refs. 44—46.

In Ref. 43 it is shown that (1.17) is sufficient to define a particle model in a spatially flat Robertson-Walker metric (the proof was made, up to the second order, in a power series in H, H being the Hubble coefficient). The model obtained is

$$\varphi_{\vec{k}}^{(\eta_0)}(\eta)=\frac{e^{-i\int w_{\vec{k}}(\eta)d\eta}}{[2w_{\vec{k}}(\eta)]^{1/2}} , \tag{1.18}$$

where $w_{\vec{k}}$ is the solution of

$$w_{\vec{k}}^{\,2}+\frac{1}{2}\left[\frac{w''_{\vec{k}}}{w_{\vec{k}}}-\frac{3}{2}\frac{w'^{\,2}_{\vec{k}}}{w_{\vec{k}}^{\,2}}\right]=m^2a^2+k^2+(\xi-\tfrac{1}{6})Ra^2 , \tag{1.19}$$

computed from a WKB approximation.

On the other hand, it can be seen that this approximate solution, up to a given order, reproduces the DeWitt-Schwinger propagator up to the considered order and defines the "adiabatic vacuum" (cf. Ref. 39, Chap. 3).

In Sec. IV we shall study the agreement between the vacua defined by C.3 and these approximate solutions. We shall also see in which cases the total number of created particles, by the universe expansion, is finite.

II. STUDY OF THE CRITERIA BASED ON FEYNMAN-PROPAGATOR GENERALIZATION

A. Statement of the criteria using the in-out basis

Before we use the criteria in general evolutions we shall express them using the in-out basis. It will simplify the operations and it will allow us to deeply understand how they work.

Looking back at Eq. (1.13) and bearing in mind the derivation done in Refs. 1 and 2, we can see that it is possible to work directly with the Fourier transform of the propagator. In fact, in these papers it was demonstrated, in Robertson-Walker universe, that a good Feynman propagator can be found in all the cases such that there would exist a unique function $g_{\vec{k}}(\eta,\eta')$ solution of Eq. (1.1) (we shall write that function in the Euclidean metric in criterion C.1 or we shall add an $i\epsilon$ to its m^2 in criterion C.2) such that

$$G_F(x,x')=\int \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{x}')}}{a(\eta)a(\eta')}g_{\vec{k}}(\eta,\eta')d^3\vec{k} \tag{1.13'}$$

and such that it would not be divergent when $\eta\rightarrow\eta_{\max}$ (i.e., $t\rightarrow+\infty$) and also when $\eta\rightarrow\eta_{\min}$ (i.e., $t\rightarrow 0$) (of course, the same thing must happen with η'). $g_{\vec{k}}(\eta,\eta')$ must be continuous when $\eta=\eta'$ but it must have a jump in its first derivative there because $G_F(x,x')$ must satisfy the equation

$$(-\nabla_\mu\nabla^\mu+m^2+\xi R)G(x,x')=\delta(\vec{x}-\vec{x}')a^{-3}(t) .$$

From Eq. (1.13) we see that the properties of $g_{\vec{k}}(x,x')$ can be translated to properties of the u basis, and also that these properties are necessary, not only in Robertson-Walker universes, but also in more general cases (such as Bianchi type-I universes) if we want a finite $G_F(x,x')$. Then the criteria C.1 and C.2, translated to the in-out basis language, read as follows:

(C.1′) The out basis is the analytic continuation of the unique solution of Eq. (2.1) (see below) which does not diverge when $\eta\rightarrow\eta_{\max}$. The in basis (conjugated) is the analytic continuation of the unique solution which does not diverge when $\eta\rightarrow\eta_{\min}$. Both functions must also satisfy the normalization condition. The translation of the Klein-Gordon equation for $\varphi_{\vec{k}}(\eta)$ when the metric is the Euclidean reads

$$\varphi''_{\vec{k}}-\varphi_{\vec{k}}a^2\left[\sum_{j=1}^{3}\frac{k_j^2}{a_j^2}+m^2+(\xi-\tfrac{1}{6})R_e(\eta_e)+q_e(\eta_e)\right]=0 , \tag{2.1}$$

where

$$R_e(\eta_e)=-R(\eta_e),\quad q_e(\eta_e)=-q(\eta_e) ,$$

and a prime denotes $d/d\eta_e$. When the functions $\varphi_e^{\text{out}}(\lambda_e,\eta_e)$ and $\varphi_e^{\text{in}*}(\lambda_e,\eta_e)$ (which are the well-behaved solutions when $\eta\rightarrow\eta_{\min}$ and $\eta\rightarrow\eta_{\max}$) have been found, the out and in conjugated bases are obtained substituting $\eta_e\rightarrow i\eta$ and $\lambda_e\rightarrow -i\lambda$ in such solutions. The bases are fully determined by applying the normalization condition.

(C.2′) $\varphi_{\vec{k}}^{\text{in}*}$ ($\varphi_{\vec{k}}^{\text{out}}$) is the limit when $\epsilon \to 0^+$ of the unique solution of Eq. (2.2) (see below) which do not diverge when $\eta \to \eta_{\min}$ ($\eta \to \eta_{\max}$). Equation (1.4) with $m^2 - i\epsilon$ and $k_j{}^2 - i\epsilon$ instead of m^2 and $k_j{}^2$, respectively, is

$$\varphi''_{\vec{k}} + \varphi_{\vec{k}} a^2 \left[m^2 - i\epsilon + \sum_{j=1}^{3} \frac{k_j{}^2 - i\epsilon}{q_j{}^2} + (\xi - \tfrac{1}{6})R + q \right] = 0 \ . \tag{2.2}$$

The in-out bases are again fully determined by the normalization condition.

These criteria will work in all cases when they fix a unique in and out basis and these bases can be normalized. It is easy to show that both criteria work when the metric is the Minkowski metric giving the usual orthonormal positive- and negative-frequency basis.

B. Application to Bianchi type-I metrics

In this section we shall apply the criteria C.1′ and C.2′ to metrics like

$$ds^2 = -dt^2 + \sum_{j=1}^{3} a_j{}^2(\lambda t) dx_j{}^2 \ .$$

We shall find sufficient conditions on the functions $a_j(t)$ for both criteria to work and to be equivalent. On the other hand, we shall show examples where they do not work and others where they are not equivalent.

First we shall study the case $a_j(t) = a(t)$ (Robertson-Walker metric) and later the general case. As we have seen, the existence of a unique (unless a multiplicative constant) well-behaved solution is necessary when $\eta \to \eta_{\min}$ and $\eta \to \eta_{\max}$ of Eq. (2.1) and (2.2) for the criteria to select the in-out bases uniquely.

To study the asymptotic behavior of solutions of Eqs. (2.1) and (2.2) we use the following theorem, which is an extension of theorems 2.1 and 2.2 in Chap. 6 of Ref. 47 and it can be demonstrated using the theorem 10.2 of the quoted reference.

(T.1) In a given finite or infinite interval (b_1, b_2) let $f(x)$ be a twice continuously differentiable function with $R_e f(x) \neq 0$, $g(x)$ a continuous function and

$$V_{b_j,x} = \left| \int_{b_j}^{x} \left| f^{-1/4} \frac{d^2 f^{-1/4}}{dx^2} - g f^{-1/2} \right| dx \right|_{\substack{j=1,2 \\ b_1 < x < b_2}} \ .$$

Then, in the interval, the differential equation

$$\frac{d^2\varphi}{dx^2} = (f + g)\varphi$$

has two twice continuously differentiable solutions

$$\varphi_1(x) = f^{-1/4} \exp\left[\int f^{1/2} dx \right] [1 + \epsilon_1(x)] \ ,$$

$$\varphi_2(x) = f^{-1/4} \exp\left[-\int f^{1/2} dx \right] [1 + \epsilon_2(x)]$$

such that

$$|\epsilon_j(x)| \ , \left| f^{-1/2} \frac{d\epsilon_j}{dx} \right| \leq \exp(V_{b_j,x}) - 1, \quad j = 1,2$$

provided that $V_{b_j,x} < \infty$, $j = 1,2$.

1. Application of the criteria to Robertson-Walker universes with initial singularity

a. Sufficient conditions for the applicability and equivalence of the methods. The methods based on criteria C.1′ and C.2′ select in-out bases and are equivalent if $a(t)$ satisfies the following conditions (we shall suppose conformal coupling, that is to say, $\xi = \frac{1}{6}$).

1. $a(t)$ is a twice continuously differentiable function, except eventually, in a finite number of points.
2. $a(0) = 0$, $\lim_{t \to \infty} a(t) = a_0 \leq \infty$.
3. $\int_{t_0}^{\infty} \left[\left| \frac{\dot{a}}{a} \right| + \left| \frac{\dot{a}}{a} \right|^2 \right] dt < \infty$

for some t_0 and $R \underset{t\to\infty}{\longrightarrow} 0$.

4. $\int_{t_0}^{t} \frac{dt'}{a(t')} \underset{t\to 0}{\longrightarrow} -\infty$

for some t_0 (i.e., $\eta_{\min} = -\infty$).

In fact, Eqs. (2.1) and (2.2) read

$$\varphi''_{\vec{k}} - (\mu^2 a^2 + u^2)\varphi_{\vec{k}} = 0 \ , \tag{2.3}$$

where

$$\mu^2 = m^2 \ ,$$
$$u^2 = k^2 \ ,$$

for Eq. (2.1) and

$$\mu^2 = i\epsilon - m^2 \ ,$$
$$u^2 = i\epsilon - k^2 \ ,$$

for Eq. (2.2) where the primes in these two equations denote, respectively, $d/d\eta_e$ and $d/d\eta$.

To study the behavior of the solutions near the initial singularity ($t \to 0$, i.e., $\eta \to -\infty$) we can use T.1 with $f = u^2$, $g = \mu^2 a^2$, $b_1 = -\infty$, $b_2 =$arbitrary [smaller than the first point of discontinuity of $\ddot{a}(t)$]. If the criteria C.1′ and C.2′ are applied, it can easily be shown that the basis selected is the solution of Klein-Gordon equation whose asymptotic behavior near the initial singularity is

$$\varphi_{\vec{k}}^{\text{in}}(\eta) \underset{\eta \to -\infty}{\simeq} \frac{e^{-ik\eta}}{\sqrt{2k}} \ . \tag{2.4}$$

In the same way, taking $f = u^2 + \mu^2 a^2$, $g = 0$, $b_1 =$arbitrary [larger than the first point of discontinuity of $\ddot{a}(t)$], $b_2 = \eta_{\max}$, it can be seen that the out basis chosen by the criteria is the solution of Klein-Gordon equation with the asymptotic behavior

$$\varphi_{\vec{k}}^{\text{out}} \underset{\eta \to \eta_{\max}}{\simeq} \frac{\exp\left[-i \int (m^2 a^2 + k^2)^{1/2} d\eta \right]}{[2(m^2 a^2 + k^2)^{1/2}]^{1/2}} \ . \tag{2.5}$$

b. Extension to the case $\eta_{\min} = 0$. If condition 4 of II B 1 a is not fulfilled, the criteria C.1′ and C.2′ do not work near the initial singularity because $t = 0$ is a regular point of Eq. (2.3) and then all solutions are well behaved there. However, the in basis can be obtained using the following trick: let $A(\eta)$ be a function defined as

$$A(\eta)=\begin{cases}0, & \eta<0,\\ a(\eta), & \eta\geq 0.\end{cases} \tag{2.6}$$

Then C.1′ and C.2′ work and select the basis

$$\psi_{\vec{k}}^{\text{in}}=\begin{cases}\dfrac{e^{-ik\eta}}{\sqrt{2k}}, & \eta\leq 0\\ \alpha_{\vec{k}}\varphi_{\vec{k}}^{\text{out}}+\beta_{\vec{k}}\varphi_{\vec{k}}^{\text{out}*}, & \eta>0\end{cases}$$
$$\psi_{\vec{k}}^{\text{out}}=\begin{cases}\dfrac{1}{\sqrt{2k}}(\alpha'_{\vec{k}}e^{-ik\eta}+\beta'_{k}e^{ik\eta}), & \eta\leq 0\\ \varphi_{k}^{\text{out}}(\eta), & \eta>0\end{cases} \tag{2.7}$$

(the coefficients $\alpha_{\vec{k}}$, $\beta_{\vec{k}}$, $\alpha'_{\vec{k}}$, and $\beta'_{\vec{k}}$ are such that $\psi_{\vec{k}}^{\text{in-out}}$ and their derivatives are continuous in $\eta=0$). We can easily verify that the particle creation between $t=0$ and $t=\infty$ is

$$|\beta_{\vec{k}}|^2=\frac{1}{2k}[\,|\varphi_{\vec{k}}^{\text{out}}(0)|^2+k^2|\varphi_{\vec{k}}^{\text{out}}(0)|^2-k]\ . \tag{2.8}$$

The extension (2.6) has been used and commented on in Ref. 2. It is justified because all physical quantities are given by integrals with respect to $\sqrt{g}\,d^4x$ so the fictitious region introduces neither an extra contribution nor antiphysical consequences. On the other hand, the result obtained is physically desirable because the physical momentum of the particles is $\vec{k}/a$; then, near the initial singularity, they are ultrarelativistic and therefore they must behave like massless ones. This behavior is, in fact, shown by Eq. (2.4).

c. Remarks. As we have already mentioned, in Ref. 1 it was found necessary to add an infinitesimal imaginary part to the particle momentum in order that C.2′ works near the initial singularity in the case $a(t)=t$. It is easy to see that this condition is essential in all cases if we want C.2′ to work in this region; if we do not add such an imaginary part then the asymptotic behavior of the solutions is

$$\varphi(\eta)\underset{\eta\to\eta_{\min}}{\simeq}Ae^{ik\eta}+Be^{-ik\eta}$$

and therefore C.2′ does not select the in basis because all solutions are well behaved when $t\to 0$.

The condition 3 is fulfilled if $a(t)=t^\alpha$ for $t>t_0$ and $\alpha>0$. For higher increasing evolutions, which do not satisfy this condition (i.e., for evolutions such that H would not vanish when $t\to\infty$) the criteria do not necessarily work. For example:

(i) if $a(t)=e^{\lambda t}$ for $t>t_0$ and $\lambda\ll 1$, C.1′ selects out bases but C.2′ does not.

(ii) if $a(t)=e^{\lambda t}$ for $t>t_0$ and $\lambda>2m$, C.2′ does not work while C.1′ select a function as out bases. Nevertheless, this function is real and it cannot be normalized.

The results that we found here can be easily extended to the case $\xi\neq\frac{1}{6}$: in order that C.1′ and C.2′ select univocally the in basis it is sufficient to add the following condition:

5. $\int_0^\epsilon Ra\,dt<\infty$

for some ϵ.

If $a(t)=t^\alpha$ for $t>t_0$, this condition is satisfied if $\alpha>1$ (and in the special case $\alpha=\frac{1}{2}$). The criteria work in the out region without additional requirements.

If condition 5 is not fulfilled, then there are cases in which C.1′ and C.2′ do not work. For example, if $a(t)=t$, $m=0$, $\xi<\frac{1}{6}$, the criteria do not select the in basis for $k<(1-6\xi)^{1/2}$.

2. *Application of the criteria to Bianchi type-I universes with initial singularity*

a. Sufficient conditions for the applicability and equivalence of the methods. The methods select in-out bases and are equivalent if the functions $a_j(t)$ satisfy the following conditions (we assume conformal coupling $\xi=\frac{1}{6}$):

(1) $a_j(t)$, $j=1,2,3$ are twice continuously differentiable functions except, eventually, in a finite number of points.

(2) $a_j(0)=0$, $a_j(t)\underset{t\to\infty}{\longrightarrow}a_{j0}$, $a_{j0}\leq\infty$, $j=1,2,3$.

(3) R and q vanish when $t\to\infty$, so that

$$\int_{t_0}^{\infty}\left[\left|\frac{\ddot{a}_j}{a_j}\right|+\left[\frac{\dot{a}_j}{a_j}\right]^2\right]dt<\infty$$

for some t_0, $j=1,2,3$.

(4) $\int_0^\epsilon a_j\left[\frac{\dot{a}_1}{a_1}\right]^2dt<\infty$

for some $\epsilon>0$, $j=1,2,3$, $a_1(t)$ being the smallest radius when $t\to 0$, that is to say

$$a_1(t)\leq a_2(t)\leq a_3(t)\ \text{ for }\ t\to 0\ .$$

(5) The functions $\dot{a}_j$ and $\ddot{a}_j$ do not oscillate around $t=0$. Equations (2.1) and (2.2) are, in this case,

$$\varphi''_{\vec{k}}-a^2\varphi_{\vec{k}}\left[\mu^2+\sum_{j=1}^{3}\frac{u_j^2}{a_j^2}-q_*\right]=0\ , \tag{2.9}$$

where

$$\mu^2=m^2\ ,$$
$$u_j^2=k_j^2\ ,$$
$$q_*=-q(\eta_e)\ ,$$

for Eq. (2.1), and

$$\mu^2=i\epsilon-m^2\ ,$$
$$u_j^2=i\epsilon-k_j^2\ ,$$
$$q_*=q(\eta)\ ,$$

for Eq. (2.2) where the primes in these two equations denote, respectively, $d/d\eta_e$ and $d/d\eta$. We can verify, in the same way as we did in II B 1 a that C.1′ and C.2′ select the solutions of the Klein-Gordon equation with the following asymptotic behavior:

$$\text{in basis } \varphi^{\text{in}}_{\vec{k}} \underset{t\to 0}{\simeq} \frac{\exp\left[-i\int f_{\vec{k}}\,d\eta\right]}{\sqrt{2f_{\vec{k}}}}\,, \quad \text{with } f_{\vec{k}} = \left[\sum_{j=1}^{3} a^2\frac{k_j^2}{a_j^2}\right]^{1/2} . \tag{2.10}$$

$$\text{out basis } \varphi^{\text{out}}_{\vec{k}} \underset{t\to\infty}{\simeq} \frac{\exp\left[-i\int (m^2a^2+f_{\vec{k}}^{\,2})^{1/2}\right]}{[2(m^2a^2+f_{\vec{k}}^{\,2})^{1/2}]^{1/2}} . \tag{2.11}$$

b. Remarks. Condition (4) is fulfilled if $a_j(t)=t^{\alpha_j}$ with $\alpha_j>1$. It is interesting to remark the analogy between the isotropic case with $\xi\neq\frac{1}{6}$ and the anisotropic case (cf. II B 1 c). The results of II B 2 a can be extended to the case of nonconformal coupling, requiring that

(5) $\int_0^{\epsilon} Ra_j dt < \infty$ for some $\epsilon>0$, $j=1,2,3$.

III. VACUA DEFINED BY THE FIELD ENERGY MINIMIZATION

A. Application to Bianchi type I metrics

As we have pointed out in I B 2, it is reasonable to define the vacuum state at time $t=t_0$, $|0_{t_0}\rangle$, as the one which minimizes the expectation value of the $T_0{}^0$ component of the energy-momentum tensor (due to the spatial homogeneity this is equivalent to minimize the total field energy).

In Ref. 3, the boundary conditions that must satisfy the particle model, at $t=t_0$, to minimize the total energy at that time, were found in the isotropic case. Here we extend these results to the anisotropic case.

The $T_0{}^0$ component of the energy-momentum tensor is [Ref. 41, Eq. (2.4)],

$$\begin{aligned}2a^4T_0{}^0 &= \chi'^2+(6\xi-1)\dot a(\chi\chi'+\chi'\chi)+a^2\sum_{j=1}^{3}a_j^{-2}(\partial_j\chi)^2\\ &\quad +[m^2a^2+(1-6\xi)\dot a^2-6\xi Q]\chi^2\\ &\quad -4\xi a^2\sum_{j=1}^{a}a_j^{-2}\partial_j(\chi\partial_j\chi)\,,\end{aligned} \tag{3.1}$$

where

$$\chi(\eta,\vec{x})=a(\eta)\int[a_{\vec{k}}u_{\vec{k}}(\eta,\vec{x})+a^{\dagger}_{\vec{k}}u^{*}_{\vec{k}}(\eta,\vec{x})]d^3\vec{k}\,,$$

$$u_{\vec{k}}(\eta,\vec{x})=(2\pi)^{-3/2}e^{i\vec{k}\cdot\vec{x}}\frac{\varphi_{\vec{k}}(\eta)}{a(\eta)} .$$

Thus, the expectation value of $T_0{}^0$ in the vacuum state reads

$$\begin{aligned}\langle 0|T_0{}^0|0\rangle=\frac{1}{16\pi^3a^4}\int d^3k\Bigg[&\varphi'_{\vec{k}}\varphi'^{*}_{\vec{k}}+\dot a(6\xi-1)(\varphi_{\vec{k}}\varphi'^{*}_{\vec{k}}+\varphi'_{\vec{k}}\varphi^{*}_{\vec{k}})+\varphi_{\vec{k}}\varphi^{*}_{\vec{k}}[m^2a^2+(1-6\xi)\dot a^2-6\xi Q]\\ &+a^2\sum_{j=1}^{3}\frac{k_j^2}{a_j^2}\varphi_{\vec{k}}\varphi^{*}_{\vec{k}}\Bigg] .\end{aligned} \tag{3.2}$$

If we write for each fixed η

$$\begin{aligned}\varphi_{\vec{k}}(\eta)&=(2w_{\vec{k}})^{-1/2}e^{-i\varphi}\,,\\ \varphi'_{\vec{k}}(\eta)&=-\varphi_{\vec{k}}\left[iw_{\vec{k}}+\frac{1}{2}\frac{w'_{\vec{k}}}{w_{\vec{k}}}\right]\end{aligned} \tag{3.3}$$

($w_{\vec{k}}$ and $w'_{\vec{k}}$ are arbitrary and real functions) the values of $w_{\vec{k}}$ and $w'_{\vec{k}}$ which minimize the field energy at each time are

$$\begin{aligned}w^{MV}_{\vec{k}}&=\left[m^2a^2+a^2\sum_{j=1}^{3}\frac{k_j^2}{a_j^2}-6\xi(6\xi-1)\dot a^2-6\xi Q\right]^{1/2},\\ w'^{MV}_{\vec{k}}&=2\dot a(6\xi-1)w^{MV}_{\vec{k}} .\end{aligned} \tag{3.4}$$

That is to say, the particle model at $\eta=\eta_0$ is given by the function $\varphi^{(\eta_0)}_{\vec{k}}(\eta)$ which is a solution of the Klein-Gordon equation and it has the Cauchy data (3.3) with $w_{\vec{k}}$ and $w'_{\vec{k}}$ given by (3.4).

One can easily verify that in this case

$$:H_{(t_0)}:=a^{-1}\int a^{\dagger}_{\vec{k}}a_{\vec{k}}w^{MV}_{\vec{k}}(t_0)d^3\vec{k} . \tag{3.5}$$

Therefore, the results obtained also diagonalize the total field energy at that time [under this prescription, Eqs. (3.4) were found in Ref. 41 in the special case $\xi=\frac{1}{6}$].

1. Comparison with the vacua obtained in Sec. II. Cases where the field energy cannot be minimized

To derive Eq. (3.4), we have assumed that $w_{\vec{k}}$ and $w'_{\vec{k}}$ are real quantities. This condition is necessary for the basis to be normalizable and for the energy to be an Hermitian operator.

This is the case if we have the following: (i) Minimal coupling ($\xi=0$). (ii) Isotropic metric with conformal coupling ($\xi=\frac{1}{6}$, $Q=0$). If these conditions are not fulfilled, it could not, in general, be possible to minimize Eq. (3.5) for real values of $w^{MV}_{\vec{k}}$, $\forall\vec{k}$. It is interesting to note that $w^{MV}_{\vec{k}}\in\mathrm{R}$ if the particle energy

$$\left[m^2+\sum_{j=1}^{3} k_j{}^2/a_j{}^2\right]^{1/2}$$

is greater than

$$[6\xi q+6\xi(6\xi-1)H^2]^{1/2}$$

and this is the case if the particle wavelength is much smaller than $(R_{\mu\nu\sigma\lambda\max})^{-1/2}$ or $R_{\max}^{-1/2}$, i.e., the notion of frequency is meaningful as it is discussed in Sec. I B 2 ($R_{\mu\nu\sigma\lambda}$ being the curvature tensor).

If we require $w_{\vec{k}}^{MV}(t)\in R$ for $\vec{k}\neq 0$ in a Bianchi type-I metric with conformal coupling we must have at $t_0=0$,

$$a_j{}^2(0)q(0)=0$$

and at $0<t_0\leq\infty$,

$$m^2>q(t_0)\ ,$$

while, in a Robertson-Walker metric with $\xi\notin[0,\frac{1}{6}]$, at $t_0=0$,

$$\dot{a}(0)=0$$

and at $0<t_0\leq\infty$,

$$m^2>6\xi(6\xi-1)H^2(t_0)\ .$$

From this equation we can conclude that if evolutions like $a_j(t)=t^{\alpha_j}$ are considered, then the necessary conditions to minimize the field energy at $t_0=0$ and $t_0=\infty$ agree with the ones required in Sec. II to apply criteria C.1′ and C.2′ (except the isotropic case with $\xi\in[0,\frac{1}{6}]$).

Using the asymptotic behaviors of the in-out bases selected in Sec. II we can show that the vacua obtained there minimizes the energy near the initial singularity and in the out region ($t\to\infty$), respectively.

2. *Remarks*

If criteria C.1′ and C.2′ work, but the conditions stated in Sec. II are not satisfied, then, not necessarily the energy can be minimized. For example, $a(t)=t$, $m=0$, $\xi>\frac{1}{6}$. In this case C.1′ and C.2′ select the in basis but the energy cannot be minimized at $t_0=0$ when

$$k^2<6\xi(6\xi-1)\ .$$

If C.1′ and C.2′ do not work, the condition $w_{\vec{k}}\in R$ is not sufficient for C.3 to work. For example, $a(t)=e^{\lambda t}$, $\xi=\frac{1}{6}$, $0<m<\lambda/2$ or $a(t)=t$, $0\leq\xi<\frac{1}{6}$. Here in both cases one has $w_{\vec{k}}^{MV}\in R$. However, C.3 does not work at $t_0=\infty$ in the first example and at $t_0=0$ in the second one. The vacua produced by C.3 does not always lead to a finite particle creation (cf. Ref. 41). In the next section we shall study this problem in more detail.

IV. ADIABATIC VACUA

A. The vacuum definition and the WKB approximation

As we have pointed out in I B 3, if we require that the generalization of $\Delta_1(x,x')$ to curved space-time $[G_1(x,x')]$ copies the same singularities of the $\Delta_1(x,x')$ [Eq. (17), Sec. I B 3] the particle model obtained is

$$\varphi_{\vec{k}}^{(\eta_0)}(\eta)=\frac{\exp\left[-i\int w_{\vec{k}}(\eta)d\eta\right]}{[2w_{\vec{k}}(\eta)]^{1/2}}\ , \tag{4.1}$$

where $w_{\vec{k}}$ is the solution of

$$w_{\vec{k}}{}^2+\frac{1}{2}\left[\frac{w''_{\vec{k}}}{w_{\vec{k}}}-\frac{3}{2}\frac{w'_{\vec{k}}{}^2}{w_{\vec{k}}{}^2}\right]=\omega_{\vec{k}}{}^2+(\xi-\tfrac{1}{6})Ra^2+Q\ , \tag{4.2}$$

computed from the power series

$$w_{\vec{k}}=\omega_{\vec{k}}\sum_{i=0}^{\infty}\frac{\Omega^{(i)}}{\omega_k^{2i}},\ \ \omega_{\vec{k}}{}^2=m^2a^2+a^2\sum_{j=1}^{3}k_j{}^2/a_j{}^2 \tag{4.3}$$

(that is to say, a WKB approximation). This has been studied in Refs. 3 and 43 in a Robertson-Walker universe. On the other hand, if one computes the kernels G_1 or G_f with the approximate solution up to a fixed order, then the kernels obtained reproduce the DeWitt-Schwinger propagator up to the considered order (Ref. 39, Chap. 3).

Keeping this in mind, it is interesting to investigate when the vacua defined by C.3 agree with this approximate vacua and what the order of coincidence is. We can classify the vacua defined by C.3 as follows:

Weak vacuum[48,49] (at $t=t_0$) is the one where the Cauchy data which minimize the field energy agree with the Cauchy data of the WKB approximation of zeroth order.

Strong vacuum (at $t=t_0$) is the one where the agreement takes place at all orders of $1/w_k$. In this case the vacuum has two important properties, it minimizes the energy, and its kernels copy the singularities of the corresponding flat-space-time kernels (it is the "good vacuum" in Ref. 3).

B. Cases where a weak vacuum exists

According to the definition given above, the weak particle model at $\eta=\eta_0$ is given by the exact solution of Klein-Gordon equation which has, at $\eta=\eta_0$, the Cauchy data of the WKB approximation of order 0 if, in addition, it minimizes the field energy at that time. This function is

$$\varphi_{\vec{k}}^{(\eta_0)}(\eta)=\frac{\exp\left[-i\int\omega_{\vec{k}}d\eta\right]}{\sqrt{2\omega_{\vec{k}}}}[1+\epsilon_k^{(\eta_0)}(\eta)]\ , \tag{4.4}$$

and its derivative

$$\varphi_{\vec{k}}^{\prime(\eta_0)}(\eta)=-i\left[\frac{\omega_{\vec{k}}}{2}\right]^{1/2}\exp\left[-i\int\omega_{\vec{k}}d\eta\right]\left[1+\epsilon_{\vec{k}}^{(\eta_0)}(\eta)+i\frac{\epsilon'^{(\eta_0)}}{\omega_{\vec{k}}}-\frac{i\omega'_{\vec{k}}}{2\omega_{\vec{k}}{}^2}\right]\ , \tag{4.5}$$

where

$$\epsilon^{(\eta_0)}_{\vec k}(\eta_0)=\epsilon'^{(\eta_0)}_{\vec k}(\eta_0)/\omega_{\vec k}(\eta_0)=0 .$$

The existence of such function is justified by T.1 (under some conditions at $\eta=\eta_{\min}$ and $\eta=\eta_{\max}$ that we shall specify below). The Cauchy data of this function at $\eta=\eta_0$ are given by

$$\varphi^{(\eta_0)}_{\vec k}(\eta_0)=\frac{e^{-i\varphi}}{\sqrt{2w_{\vec k}}} ,$$
$$\varphi'^{(\eta_0)}_{\vec k}(\eta_0)=-\varphi_{\vec k}\left[iw_{\vec k}+\frac{w'_{\vec k}}{2w_{\vec k}}\right] , \qquad (4.6)$$

where

$$w_{\vec k}=\omega_{\vec k},\quad w'_{\vec k}=\omega'_{\vec k} .$$

To make these Cauchy data minimize the field energy we must have

$$\omega_{\vec k}=w^{MV}_{\vec k} ,$$
$$\frac{\omega'_{\vec k}}{\omega_{\vec k}^{2}}=\frac{w'^{MV}_{\vec k}}{(w^{MV}_{\vec k})^2} . \qquad (4.7)$$

Consequently, in order for the vacuum at η_0 to be weak we must have the following:

(a) The hypothesis of T.1 must be satisfied, that is to say, $a_j(t)$ are twice continuously differentiable functions, $j=1,2,3$ and $V_{\xi_0\eta}(F)<\infty$ where η is a point in the neighborhood of η, and

$$F=\int[\omega_{\vec k}^{-1/2}(\omega_{\vec k}^{-1/2})''-\omega_{\vec k}^{-1}(Q+(\xi-\tfrac{1}{6})Ra^2)]d\eta .$$

(b) Equations (4.7) must be fulfilled.

C. Cases where strong vacuum exists

To study in which situations the vacua are strong we must solve Eq. (2.2) with a power series like (4.3), where

$$\omega_{\vec k}^{2}=m^2a^2+a^2\sum_{j=1}^{3}\frac{k_j^2}{a_j^2}=m^2a^2+k^2b^2 .$$

If this is done the $\Omega^{(i)}$ can be recurrently calculated; for example, we have

$$\Omega^{(0)}=1 ,$$
$$\Omega^{(1)}=\tfrac{1}{2}\left[(\xi-\tfrac{1}{6})Ra^2+Q+\tfrac{1}{4}\left[\frac{b'}{b}\right]^2-\tfrac{1}{2}\left[\frac{b'}{b}\right]'\right] . \qquad (4.8)$$

It can be shown by a complete induction that the function $\Omega^{(i)}$ has the following behavior when the evolution is $a_j(t)=t^{\alpha_j}$ near the singularity and in the out region

$$\frac{\Omega^{(i)}}{\omega^{2i}_{\vec k}}\underset{t\to\infty}{\longrightarrow}0,\quad i\geq 1$$

$$\frac{\Omega^{(i)}}{\omega^{2i}_{k}}\underset{t\to 0}{\sim}\begin{cases} t^{2[1+i(\alpha-1)]}, & \text{for } i>1 \\ & \text{if the metric is isotropic and } \xi=\tfrac{1}{6}; \\ t^{2i(\alpha_{jm}-1)}, & \text{for } i\geq 0 \\ & \text{when the metric is not isotropic,} \\ & \text{for arbitrary } \xi; \\ & \alpha_{jm}=\text{smallest index such that } k_j\neq 0 . \end{cases}$$

Using these results and the conditions found in Sec. IV B we can classify the vacua defined by C.3 as follows:

$$\text{Robertson-Walker}\ \ \xi=\tfrac{1}{6}\begin{cases} t_0=0,\quad a(t)=t^{\alpha}\begin{cases}\alpha>\tfrac{1}{3}\to\text{weak vacuum}\\ \alpha\geq 1\to\text{strong vacuum}\end{cases}\\ 0<t_0<\infty,\quad \begin{cases}\dot a(t_0)=0\to\text{weak vacuum}\\ \left.\begin{array}{l}\dot a(t)=0,\quad t\in(t_0-\epsilon,t_0+\epsilon)\\ \text{or}\\ \left.\dfrac{d^na}{dt^n}\right|_{t_0}=0\quad\forall n\end{array}\right\}\to\text{strong vacuum}\end{cases}\\ t_0=\infty,\quad a(t)=t^{\alpha},\quad \alpha>0\to\text{strong vacuum}\end{cases}$$

$$\begin{array}{c}\text{Bianchi type-I}\\ \text{arbitrary } \xi\\ j=1,2,3.\end{array}\begin{cases} t_0=0,\quad a_j(t)=t^{\alpha_j}\to\alpha_j>1\to\text{strong vacuum}\\ 0<t_0<\infty,\quad \begin{cases}\dot a_j(t_0)=0\to\text{weak vacuum}\\ \left.\begin{array}{l}\dot a_j(t)=0,\quad t\in(t_0-\epsilon,t_0+\epsilon)\\ \text{or}\\ \left.\dfrac{d^na_j}{dt^n}\right|_{t_0}=0\quad\forall n\end{array}\right\}\to\text{strong vacuum}\end{cases}\\ t_0=\infty,\quad a_j(t)=t^{\alpha_j}\to\alpha_j>0\to\text{strong vacuum} .\end{cases}$$

(we have not imposed the condition of Sec. I B 2 here.)

It is interesting to note that, for the studied evolutions, the necessary conditions for the vacuum to be strong are sufficient to apply C.1′ and C.2′ (cf. Sec. II) (the isotropic case with conformal coupling is an exception, but if we do not perform the extension of Sec. II B 1 b then we find the same result).

D. Dependence of $|\beta_k|$ with k

Here we shall study under which conditions the total number of created particles, by the universe expansion, is finite. We consider, by simplicity, only the case in which the evolution ceases at a given instant.[50] Let

$$\varphi''_{\vec{k}}+\varphi_{\vec{k}}(k^2 p+q)=0 , \qquad (4.9)$$

where p and g do not depend on k and are constant for $\eta>\eta_0$ (p must be a positive twice continuous differentiable function and g a continuous function).

Let $z=\int^{\eta} p^{1/2} d\eta$ and suppose that

(i) $\int_{z_{\min}}^{z_1} |\psi(v)|\,dv<\infty$ for some $z_1>z_0$,

(ii) $\int_{z_{\min}}^{z} e^{-2ikv}\psi(v)dv \underset{k\to\infty}{\sim} O(k^{-1})$,

where

$$\psi=-gp^{-1}+p^{-3/4}(p^{-1/4})'' ,$$

then the following solutions of Eq. (4.9):

$$\varphi_k^{\rm in}(z)=(2kp^{1/2})^{-1/2}e^{-ikz}[1+h_k(z)] ,$$

$$h_k(z_{\min})=\left.\frac{h'_k(z)}{p_{(z)}^{1/2}}\right|_{z_{\min}} ,$$

$$\varphi_k^{\rm out}(z)=\frac{e^{-i[k^2p(\eta_0)+g(\eta_0)]^{1/2}\eta}}{\{2[k^2p(\eta_0)+g(\eta_0)]^{1/2}\}^{1/2}},\quad \eta>\eta_0 ,$$

are connected by a Bogoliubov transformation such that $|\beta_k|=O(k^{-2})$.

We prove this theorem in Appendix A. If it is applied to the evolutions with which we are concerned then we can check that the total particle creation between $t=0$ and $t=\infty$ is finite, if the evolution ceases for $\eta>\eta_0$ and has the following behavior near the initial singularity

Robertson Walker $\xi=\frac{1}{6}$,

$a(t)$ arbitrary

Robertson Walker $\xi\neq\frac{1}{6}$,

$a(t)=t^{\alpha},\alpha>1$

Bianchi type-I arbitrary ξ,

$a_j(t)=t^{\alpha_j},\alpha_j>1$, $j=1,2,3$.

The same result can be generalized for the particle creation between two intermediate times requiring the vacua at those times (t_1 and t_2) to be weak. This can be seen using Eq. (1.41) of Ref. 42 with $u=k$,

$$p=\frac{m^2a^2}{k^2}+a^2\sum_{j=1}^{3}\frac{\beta_j^2}{\alpha_j^2}\quad (k\beta_j=k_j)$$

which reads

$$|\beta_{\vec{k}}|=O(k^{-2})+O\left[\frac{\omega'_{\vec{k}}}{\omega_{\vec{k}}^2}(t_1)\right]+O\left[\frac{\omega'_{\vec{k}}}{\omega_{\vec{k}}^2}(t_2)\right] . \qquad (4.10)$$

Since at t_1 and t_2 the vacua are weak, then $\omega'_{\vec{k}}(t_1)=\omega'_{\vec{k}}(t_2)=0$ and consequently $|\beta_{\vec{k}}|=O(k^{-2})$.

Also, if both intermediate times have strong vacua, not only is the created particle number finite, but also $|\beta_{\vec{k}}|\to 0$ faster than any power of k when $k\to\infty$. That is evident because there is only one WKB expansion (4.3) and both vacua have a $W_{\vec{k}}$ that fulfills this expansion, therefore their difference can only be nonanalytical in k, and must vanish faster than any power of k. In this case we could eventually find a spectrum like $|\beta_{\vec{k}}|\sim e^{-k}$ or a blackbody radiation behavior. Thus, the energy, and the momentum of the created particles that can be computed via integrals like $\int |\beta_k|^2 k\, d^3\vec{k}$ are also finite. As it is physically reasonable that also these magnitudes would be finite we conclude that the strong vacuum is the really good one.

V. CONCLUSIONS

If we require the considered criteria to be compatible, then we can conclude that there are reasonable particle models in asymptotic and static periods (this has been extensively studied in the literature) and we can add, as a result of this paper, that we also have a good model (the strong) in the general case of a Bianchi type-I metric at the initial singularity if the expansion is not very violent. This is the case if $a_j(t)=t^{\alpha_j}$ with $\alpha_j>1$.

These conditions can be relaxed in the special case of an isotropic metric with conformal coupling: we have a weak vacua at the initial singularity if $a^2\dot{a}\underset{t\to 0}{\to}0$ [if $a(t)=t^{\alpha}$ then it must be $\alpha>\frac{1}{3}$].

The condition found in the general case ($\alpha_j>1$) can be physically interpreted. If $a_j(t)=t^{\alpha_j}$ then $\dot{a}_j(t)=\alpha_j t^{\alpha_j-1}$. Consequently the condition found agrees with $\lim_{t\to 0}\dot{a}_j<\infty$ except the limit case $\alpha_j=1$. This seems reasonable: the methods work at the initial singularity if the initial expansion velocity is finite. Although we loose the classical evolutions $t^{1/2}$ and $t^{2/3}$, we must remember that the cosmologic solution will contain the so-called "back reaction" phenomenon, so the quoted evolutions can be the asymptotic states when $t\to\infty$ but they surely do not describe the early state of the universe.

On the other hand, the condition $\alpha_j>1$ agrees with the one quoted in Sec. I B 2: $\omega>(R_{\mu\nu\lambda\rho_{\max}})^{1/2}$ ($R_{\mu\nu\lambda\rho_{\max}}$ being the biggest component of the curvature tensor and ω the particle frequency) as can be easily shown. Thus, the notion of frequency and energy are meaningful, as a result of the uncertainty relation, at the singularity (or at least as a limit when $t\to 0$).

Therefore, we arrive at a very clear notion of strong vacuum; it is the one that minimizes the energy when energy is well defined. This happens in flat space-time, or when $R \to 0$ in the out asymptotic region, but now we can see that it could happen equally well in the in region for certain evolutions.

The matter present in the universe near the initial singularity should be represented with a more complete model than the neutral scalar field ϕ (for example, with a grand-unified model). In addition, the gravitational field must be quantized there. However, it is possible that the theorems proved here could remain valid (appropriately modified) in more complicated models.

This work leaves opened this line of research: to try to generalize the vacua introduced above to more realistic universe models, then if this is possible, an important cosmologic problem, the particle notion at the initial singularity could be solved.

APPENDIX A

Here we prove the theorem quoted in Sec. IV D. Theorem 2.2, Chap. 6, Ref. 47, states the existence of the solution

$$\varphi_k^{\rm in}(z)=(2kp^{1/2})^{-1/2}e^{-ikz}[1+h_k(z)] \ , \quad (A1)$$

with

$$|h_k(z)| \le e^{F/k}-1 \ ,$$
$$F=\int_{z_m}^{z} |\psi(v)|\,dv \ .$$

In addition one has

$$h_k(z)=-\frac{1}{2ik}\int_{zm}^{z} dv\,\psi(v)(1-e^{-2ik(v-z)})[1+h_k(z)] \quad (A2)$$

(see p. 196 of Ref. 47). With the required conditions it is easy to see that

$$h_k(z)=\frac{\alpha}{k}+\frac{g_0 z}{2ikp_0}+O(k^{-2}),\ \ z_0<z<z_1 \quad (A3)$$

where α=constant, $g_0=g(\eta_0)$, and $p_0=p(\eta_0)$. On the other hand, the out basis is

$$\varphi_{\vec k}^{\rm out}(z)=\frac{e^{-i(k^2p_0+g_0)^{1/2}}}{[2(k^2p_0+g_0)^{1/2}]^{1/2}}$$
$$=\frac{e^{-ikz}}{(2kp_0{}^{1/2})^{1/2}}\left[1+\frac{g_0 z}{2ikp_0}+O(k^{-2})\right]$$
$$(z>z_0) \ . \quad (A4)$$

If we write

$$\varphi_{\vec k}^{\rm in}=(1+A_{\vec k})\varphi_{\vec k}^{\rm out}+\beta_{\vec k}\varphi_{\vec k}^{\rm out*} \ , \quad (A5)$$

then

$$A_{\vec k}=\frac{\alpha}{k}+O(k^{-2}) \ ,$$
$$\beta_{\vec k}=O(k^{-2}) \ , \quad (A6)$$

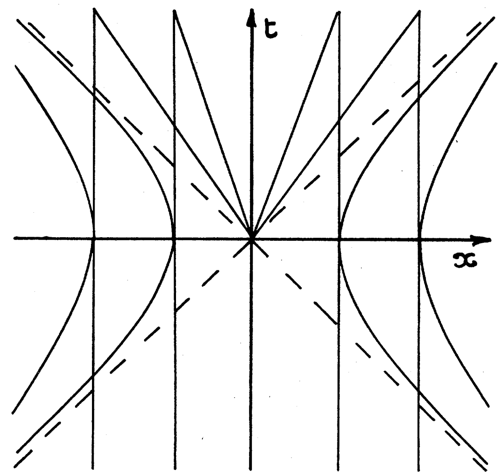

FIG. 1. World lines of Minkowski observers (vertical lines), Rindler observers (hyperbolas), and Kasner observers (radial lines).

that is,

$$\int |\beta_{\vec k}|^2 d^3k < \infty \ . \quad (A7)$$

APPENDIX B

The particle notion and the corresponding vacuum definition is always tied to a reference system, e.g., in Minkowski flat space-time the inertial systems. In all the work we have used the comoving system, i.e., the "local" inertial systems in Bianchi type-I universes, leaving for a forthcoming paper an eventual generalization.

In any event, let us settle the point through an example. Let t,x,y,z be an inertial system of Minkowski space. And let us change the coordinates with the transformation

$$t=\xi\sinh\tau,\ \ x=\xi\cosh\tau \ ,$$
$$y=y,\ \ z=z \ . \quad (B1)$$

The Minkowski metric

$$ds^2=-dt^2+dx^2+dy^2+dz^2 \quad (B2)$$

becomes in the new coordinates

$$ds^2=-\xi^2 d\tau^2+d\xi^2+dy^2+dz^2 \ . \quad (B2')$$

It is the Rindler static metric.

As it is static it has a well-defined vacuum, the Rindler vacuum, which is different from the Minkowski vacuum. In fact, while Minkowski observers follow x=const lines (the vertical lines of Fig. 1), Rindler observers follow τ=const lines (the hyperbolas), and have a constant acceleration. Thus, it can be shown (cf. Refs. 20 and 39) that Rindler observers see a thermal radiation in the Minkowski vacuum and vice versa.

On the contrary, if we perform the change of coordinates

$$t=\tau\sinh\xi,\ \ x=\tau\cosh\xi \ ,$$
$$y=y,\ \ z=z \ , \quad (B3)$$

we obtain

$$ds^2 = -d\tau^2 + \tau^2 d\xi^2 + dy^2 + dz^2 \ ,$$

a nonstatic metric that corresponds to the Bianchi type-I Kasner (1,0,0) metric. In this case, the observer follows the radial lines, with constant velocity and no acceleration, and we are in a completely different physical situation where, according to a naive interpretation of our theory, we shall only have strong vacuum in $\tau \to \infty$. This interpretation is naive because in this case we do not use a "comoving" system. (Flat space-time is empty, but we usually consider the inertial system as the comoving ones because, in fact, empty flat space-time is only a limit case of a nonempty universe where the notion of comoving system is meaningful.) Thus, this case deserves a deeper study. In any event it is clear that different systems have different vacua, even if the geometry is the same.

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*Present address: Comisión Nacional de Energía Atomica-Centroatomico Bariloche, 8400 Bariloche, Argentina.

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