How to define a unique vacuum in cosmology

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Abstract

We propose a distinguished set of positive and negative energy modes of the Klein-Gordon equation as a time independent definition of the vacuum state of a quantized scalar field.

a.- Klein-Gordon equation. Given any space-time with line element:

\[ ds^2 = g_{\alpha\beta}(x^\rho)dx^\alpha dx^\beta, \quad \alpha, \beta, \cdots = 0, 1, 2, 3 \]  

(1)

the Klein-Gordon equation for a classical field \( \psi(x^\rho) \) reads, using a system of units such that \( c = 1 \):

\[ (\Box - \frac{m^2}{\hbar^2})\psi = (g^{\alpha\beta}\partial_{\alpha\beta} - \Gamma^\alpha \partial_\alpha - \frac{m^2}{\hbar^2})\psi = 0 \]  

(2)

where:

\[ \Gamma^\alpha = g^{\lambda\mu}\Gamma_{\lambda\mu}^\alpha \]  

(3)

If \( \psi_1 \) and \( \psi_2 \) are two, in general complex, solutions then the current:

\[ J^\alpha(\psi_1, \psi_2) = -i\hbar g^{\alpha\beta}(\psi_1^* \partial_\beta \psi_2 - \psi_2 \partial_\beta \psi_1^*) \]  

(4)

is conserved:

\[ \nabla_\alpha J^\alpha = \frac{1}{\sqrt{-g}} \partial_\alpha(\sqrt{-g}J^\alpha) = 0, \quad g = \text{det}(g_{\alpha\beta}) \]  

(5)
and this allows to define the invariant scalar product \((\psi_1, \psi_2)\) of two well behaved solutions as the flux of the preceding current across any space-like hypersurface \(\Sigma\):

\[
(\psi_1, \psi_2) = \int_{\Sigma} J^\alpha d\Sigma^\alpha
\] (6)

b.- Quantization of a scalar field. The canonical quantization of a scalar field is a two step process. The first step consists in selecting a distinguished set of modes of the Klein-Gordon equation to define what in the jargon of Quantum field theory is called the Vacuum state. The second step consists in implementing the so-called canonical commutation relations to be satisfied by the field operator and its conjugate momentum. Only the first step raises new problems in general relativity and this paper is entirely dedicated to it.

A common belief\(^1\) is that in general and in particular in cosmology there is no unique way of choosing a unique vacuum state and therefore that there is an inevitable spontaneous creation of particles. We claim in this paper that for Robertson-Walker models with flat space-sections it is possible to distinguish a preferred set of modes, with no time mixing of positive and negative modes, thus defining a unique vacuum state and suppressing the spontaneous particle creation out from the vacuum state.

In Minkowski space-time and in a galilean frame of reference the vacuum state is defined by the set of modes \((\epsilon = \pm)\):

\[
\varphi_\epsilon(x^\alpha, \vec{k}) = [2\omega(\vec{k})(2\pi\hbar)^3]^{-1/2} u_\epsilon(t, \vec{k}) e^{i\vec{k}\vec{x}}; \quad \varphi_{-\epsilon}(x^\alpha, \vec{k}) = \varphi_\epsilon^*(x^\alpha, -\vec{k}) \quad (7)
\]
with:

\[
u_\pm(t, \vec{k}) = (2\omega)^{-1/2} e^{-\vec{k}\omega t} \quad \omega(\vec{k}) = + (\vec{k}^2 + m^2)^{1/2} \quad (8)
\]

where \(\vec{k}\) is a constant index vector. The modes \(\varphi_+\) are by definition the positive energy modes and \(\varphi_-\) the negative energy modes. This set of modes can be characterized by the following conditions:

i) The set of modes, having the general form 7, must be a complete orthonormal set of particular solutions of the Klein-Gordon equation. Orthonormality here means that the scalar product of two modes is:

\[^1\text{See for example [1]}\]
and completeness means that any solution of the Klein-Gordon equation that can be written as a Fourier transform on the flat space-sections \( t = \text{const} \):

\[
\psi(t, \vec{x}) = \frac{1}{(2\pi \hbar)^{3/2}} \int c(t, \vec{k}) e^{i \vec{k} \cdot \vec{x}} d^3\vec{k}
\]

(10)
can also be written as:

\[
\psi(t, \vec{x}) = \int (a_+(\vec{k}) \varphi_+(x^\alpha, \vec{k}) + a_-(\vec{k}) \varphi_-(x^\alpha, \vec{k})) d^3\vec{k}
\]

(11)
i) The functions \( u_\epsilon \) are solutions of the first order differential equation:

\[
i\hbar \dot{u}_\pm = \pm \omega u_\pm, \quad \dot{u} = \frac{du}{dt}
\]

(12)
It is this condition that guarantees that there will not be time mixing of positive and negative modes. Generalizing to Roberson-Walker space-times with flat space-sections this second condition is the main contribution of this paper.

c.-Robertson-Walker models. The line-element of a Robertson-Walker cosmological model with flat space-sections is:

\[
ds^2 = -dt^2 + e^{2\sigma(t)} \delta_{ij} dx^i dx^j, \quad i, j, \cdots = 1, 2, 3
\]

(13)
and the Klein-Gordon equation reads:

\[
(-\partial_t^2 - 3\dot{\sigma} \partial_t + e^{-2\sigma} \Delta - \frac{m^2}{\hbar^2}) \psi = 0
\]

(14)
where:

\[
\dot{\sigma} = \frac{d\sigma}{dt}, \quad \Delta = \delta^{ij} \partial_{ij}
\]

(15)
The scalar product of two solutions can then be written using as hypersurface \( \Sigma \) any space-section \( t = \text{const} \):

\[
(\psi_1, \psi_2) = i\hbar e^{3\sigma} \int_t (\psi_1^* \partial_t \psi_2 - \psi_2 \partial_t \psi_1^*) d^3\vec{x}
\]

(16)
d. Modes. We shall define a mode, as it is usual in this case, as a solution of the following form:

\[ \varphi(x^\alpha, \vec{k}) = \frac{1}{(2\pi \hbar)^{3/2}} u(t, \vec{k}) e^{i\vec{k}\cdot\vec{x}} \]

where \( \vec{k} \), the index of the mode, is a constant vector and where \( u \) must therefore be a solution of the following evolution second order differential equation:

\[ \hbar^2 \dot{u} + 3\hbar^2 \dot{\sigma} \dot{u} + \omega^2 u = 0, \quad \omega^2 = e^{-2\sigma} \vec{k}^2 + m^2 \]

The scalar product of two modes corresponding to any two vector indices is:

\[ (\varphi(x^\alpha, \vec{k}_1), \varphi(x^\alpha, \vec{k}_2)) = i\hbar e^{3\sigma} (u^*(t, \vec{k}_1) \dot{u}(t, \vec{k}_2) - u(t, \vec{k}_2) \dot{u}^*(t, \vec{k}_1)) \delta(\vec{k}_1 - \vec{k}_2) \]

e. Reduction of the evolution equation\(^2\). Let us consider for each index \( \vec{k} \) the following first order differential equation:

\[ i\hbar \dot{u}(t, \vec{k}) = f(t, \vec{k}) u(t, \vec{k}) \]

We say that this equation is a reduction of the corresponding evolution equation 18 if the function \( f \) is such that every solution of 20 is also a solution of 18. Or equivalently, if \( f \) is such that

\[ u(t, \vec{k}) = A(t_0, \vec{k}) e^{-\frac{i}{\hbar} \int_{t_0}^{t} f(s, \vec{k}) ds} \]

where \( A \) is a constant which will depend on a normalization condition and on the lower limit of integration that has been chosen, is a solution of 18.

Deriving both members of eq. 20, multiplying by \( i\hbar \) and taking into account eq. 20 itself we get:

\[ -\hbar^2 \ddot{u} = i\hbar \dot{f} u + f^2 u, \]

and using eq. 18 and dividing by \( u \):

\(^2\)The concept of order reduction has been used widely in many contexts. The use of this concept here is elementary. Another, non elementary, application to cosmology can be seen in [2]
\[ i\hbar \dot{f} + f^2 + 3i\hbar \dot{\sigma} f - \omega^2 = 0 \]  
(23)

This is a Riccati equation that \( f \) has to satisfy if eq. 18 is to be a reduction of eq. 20.

Let us require that \( f \) could be expanded as a Laurent series:

\[
f = \sum_{n=-s}^{\infty} (i\hbar)^n f_n, \quad s < \infty
\]  
(24)

Substituting this expression into 23 we obtain to begin with:

\[
f_n = 0 \quad \text{for} \quad -s \leq n < 0
\]  
(25)

and:

\[
f_0^2 = \omega^2
\]  
(26)

The following terms are all given by an equation of the following type:

\[
f_n = \frac{1}{2f_0} A(f_1, f_2, \cdots, f_{n-1}, \dot{f}_1, \dot{f}_2, \cdots, \dot{f}_{n-1}, t)
\]  
(27)

and can be calculated successively starting with either one of the solutions of eq. 26. In particular we have

\[
f_1 = -\frac{1}{2}(3\dot{\sigma} + f_0^{-1}\dot{f}_0)
\]  
(28)

and therefore the behavior of 21 when \( \hbar \to 0 \) is:

\[
u(t, \vec{k}) \to Ae^{3/2(\sigma(t_0) - \sigma(t))} (f_0(t_0)/f_0(t))^{1/2} e^{-\frac{i}{\hbar} \int_{t_0}^{f}(f(s, \vec{k})\,ds}
\]  
(29)

We shall write:

\[
f_0^+ = +\omega, \quad f_0^- = -\omega, \quad \omega > 0
\]  
(30)

and note \( f_+ \) and \( f_- \) the two particular solutions of the Riccati equation 23 that they generate.

The complex conjugate of eq. 23 can be written as:

\[ i\hbar \frac{d}{dt} (-f^*) + (-f^*)^2 + 3i\hbar \dot{\sigma}(-f^*) - \omega^2 = 0 \]  
(31)
which proves that if \( f \) is a solution of (23) then \( -f^* \) is also a solution. Since \( f_0^* = -(f_0^+)^* \) because \( \omega \) is real, and since each of these initial terms characterizes the corresponding solution \( f_- \) and \( f_+ \) it follows that:

\[
f_- = -f_+^*
\] (32)

Notice that since \( \omega \) in (18) is a function of \( \vec{k}^2 \) both functions \( f_\pm \) are even functions of \( \vec{k} \):

\[
f(t, \vec{k}) = f(t, -\vec{k})
\] (33)

**f.- Positive and negative energy modes.** We shall define the positive (respectively negative) energy modes \( u_+ \) (resp. \( u_- \)) as those modes for which \( u \) is a solution of (20), \( f \) being \( f_+ \) (respectively \( f_- \)):

\[
i\hbar \dot{u}_\pm(t, \vec{k}) = f_\pm(t, \vec{k})u_\pm(t, \vec{k})
\] (34)

or:

\[
u_\pm(t, \vec{k}) = A_\pm(t_0, \vec{k})e^{-\frac{\sqrt{\hbar}}{\vec{k}} \int_{t_0}^{t} f_\pm(s, \vec{k}) ds}
\] (35)

Let \( c(t, \vec{k}) \) be a solution of the second order equation (18) corresponding to initial conditions \( c(t_0, \vec{k}) \) and \( \dot{c}(t_0, \vec{k}) \) on some space-section \( t = t_0 \). If \( u_+ \) and \( u_- \) are two particular energy modes, one positive and the other negative there will exist two constants \( a_\pm(\vec{k}) \) such that:

\[
c(t_0, \vec{k}) = a_+(\vec{k})u_+(t_0, \vec{k}) + a_-(\vec{k})u_-(t_0, \vec{k})
\] (36)

and from (20) we shall have also:

\[
i\hbar \dot{c}(t_0, \vec{k}) = a_+(\vec{k})f_+(t_0, \vec{k})u_+(t_0, \vec{k}) + a_-(\vec{k})f_-(t_0, \vec{k})u_-(t_0, \vec{k})
\] (37)

Solving for \( a_\pm \) we obtain:

\[
a_\pm(\vec{k}) = \frac{i\hbar \dot{c}(t_0, \vec{k}) - f_\pm(t_0, \vec{k})c(t_0, \vec{k})}{u_\pm(t_0, \vec{k})(f_\pm(t_0, \vec{k}) - f_\mp(t_0, \vec{k}))}
\] (38)

If \( c \) is itself a positive (resp. negative) energy mode then \( a_+ = 0 \) (resp. \( a_- = 0 \)) demonstrating explicitly that an energy mode is positive (resp. negative)
independently of the choice of the space-section and initial condition on it, as far as it satisfies the appropriate first order equation 34.

From 20 and 32 we have:

\[ i\hbar \frac{d}{dt}(u_+ - u_-^*) = f_+(u_+ - u_-^*) \]  \hspace{1cm} (39)

and therefore we shall have:

\[ u_-(t, \vec{k}) = u_+^*(t, \vec{k}) \]  \hspace{1cm} (40)

provided that we choose initial conditions which satisfy this condition on some arbitrary space-section. From 33 we shall have:

\[ u_\pm(t, \vec{k}) = u_\pm(t, -\vec{k}) \]  \hspace{1cm} (41)

Let us consider two modes with energy condition \( \epsilon_1 = \pm \) and \( \epsilon_2 = \pm \).

From 19, and 20 and its complex conjugate, we have:

\[
(\varphi_{\epsilon_1}(x^\alpha, \vec{k}_1), \varphi_{\epsilon_2}(x^\alpha, \vec{k}_2)) = e^{3\sigma}(u_{\epsilon_1}^*(t, \vec{k}_1)u_{\epsilon_2}(t, \vec{k}_2)(f_{\epsilon_1}(t, \vec{k}_2) + f_{\epsilon_2}^*(t, \vec{k}_1))\delta(\vec{k}_1 - \vec{k}_2)
\]  \hspace{1cm} (42)

From this result we can see that the scalar product of two different modes is zero. If \( \vec{k}_1 \neq \vec{k}_2 \) then this follows from the properties of the Dirac \( \delta \) function. If \( \vec{k}_1 = \vec{k}_2 \) and \( \epsilon_1 = -\epsilon_2 \) then this is a consequence of 32. To normalize the modes we shall require the generalized modes to satisfy again conditions 9. This is equivalent to requiring the constant \( A_{\pm}(t_0, \vec{k}) \) in 21 to satisfy:

\[
A_{\pm}A_{\pm}^* = e^{-3\sigma} | f_{\pm}(t_0, \vec{k}) + f_{\pm}^* (t_0, \vec{k}) |^{-1}
\]  \hspace{1cm} (43)

This fixes the norm of \( A_{\pm} \) but not its phase. Since we want to have everywhere the relation 40 we may require that \( A_{\pm} \) satisfy the relation:

\[ A_-(t_0, \vec{k}) = A_+^*(t_0, \vec{k}) \]  \hspace{1cm} (44)

Let \( \psi \) be any solution of the Klein-Gordon equation 14 which can be expressed as a Fourier integral on each space-section \( t = \text{constant} \):

\[
\psi(t, \vec{x}) = \frac{1}{(2\pi \hbar)^{3/2}} \int c(t, \vec{k}) e^{i\hbar \vec{k} \vec{x}} d^3\vec{k}
\]  \hspace{1cm} (45)
Since the $c$’s must be, for each $\vec{k}$, a solution of 18 they will be a linear combination of $u_+$ and $u_-$ as in 36. Substituting in 45, using 41, and after some re-writing we get:

$$
\psi(t, \vec{x}) = \int a_+(\vec{k})\varphi_+(t, \vec{k}) + a_-(\vec{k})\varphi_-(t, \vec{k}) d^3\vec{k}
$$

(46)

where:

$$
\varphi_-(t, \vec{k}) = \varphi_+^*(t, -\vec{k})
$$

(47)

We have thus proved that the set of modes defined above provide a straightforward generalization of the modes 7 associated with the galilean frames of reference of Minkowski space-time. The vacuum state that they define does not depend on time.

**g. Concluding remarks.** We have assumed that the space-sections $t = \text{constant}$ were flat. This is not an essential restriction. Models with non flat space-sections can be dealt with using the eigen-states of the Laplacian of a constant curvature 3-dimensional riemannian metric.

Also, the main idea of this paper which consisted in reducing the Klein-Gordon equation to two complex conjugate first order equations with respect to time can be generalized to more general space-times and frames of reference. This work will be published elsewhere.

**References**


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$^3$See for instance [3]