Ultraviolet regularity, CPT and the Big Bang quantum vacuum

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In this paper, we further analyze the CPT-invariant vacua in a radiation-dominated spacetime, recently described in [1, 2], by imposing the quantum states to be ultraviolet regular. To this end we provide an alternative description of the CPT-invariant vacuum states by naturally setting invariant “initial” conditions at the big bang. We identify a family of CPT-invariant and ultraviolet regular vacuum states for both scalars and spin-1/2 fields. We give the asymptotic conditions that these states must satisfy and discuss some interesting vacuum choices.

I. INTRODUCTION

The Universe and its very early stages are of upmost interest to fundamental physics. Observations indicate that, soon after the big bang, the Universe is well described by a spatially flat radiation-dominated Friedmann-Lemaître-Robertson-Walker (FLRW) geometry. On top of this homogeneous spacetime, the early Universe requires small scalar perturbations with an almost Gaussian and scale-free power spectrum [3]. Inflationary cosmology has proved to be very successful at predicting the properties of the primordial power spectrum and hence the anisotropies observed in the cosmic microwave background and the inhomogeneities of the large-scale structure of the Universe [4, 5]. Unfortunately, the amount of possibilities driving a very early epoch of accelerated expansion seems to be very large, at least when it is compared to the extraordinary simplicity of the Universe as a whole on the largest scales. A natural way to bypass this tension is to push new model-building strategies for inflation, especially to account for the current absence of signals of tensor perturbations.

In a general spacetime, there is no preferred choice of a vacuum state, as it was already displayed in the pioneering studies of quantum field theory in curved spacetime [6]. In a cosmological scenario, this question translates to asking about how to select the initial quantum state. This issue is of major relevance since physical predictions depend upon the fixing of the initial vacuum. For instance, the main predictions of inflationary cosmology rely on the choice of the initial quantum state at the onset of inflation. This choice is made out by somewhat identifying the initial state of the quasi-exponential expansion assumed by inflation with the natural state in the exact de Sitter space [4, 5]. The preferred vacuum state in de Sitter is naturally justified by invoking that the secret of nature is symmetry. de Sitter isometries play a very important role in selecting a preferred vacuum [6]. Any sensible description of cosmic evolution is also expected to be based on deep underlying symmetries.

An interesting example of the latter is the recent proposal [1, 2] for a CPT-symmetric cosmology in which the gravitational background is assumed to be time-reversal symmetric with respect to the big bang event \( \tau = 0 \) (for a related proposal see also [8]). A radiation-dominated era emerges from this special event, and a universe-antiuniverse pair is created. This is done by assuming a natural analytic continuation of the (odd) expansion factor \( a(\tau) \sim \tau \) to negative values of conformal time \( \tau \). The crucial point to derive one of the main physical implications of the model, namely, the abundance of dark matter (assumed to be formed by heavy right-handed neutrinos created by the expansion of the universe), requires the selection of a vacuum state. This is done by choosing a preferred CPT-invariant vacuum, selected by imposing adiabatic conditions at \( \tau \to \pm \infty \).

This paper aims to carry out a detailed reanalysis of the proposal in [1, 2] by introducing two extra ingredients: i) we parametrize the potential CPT-invariant vacua just at the big bang event \( \tau = 0 \), ii) we restrict the allowed CPT-invariant states by demanding ultraviolet (UV) regularity. A preliminary analysis of the UV adiabatic regularity
condition without interfering with the CPT symmetry has been displayed in [9]. Here we further impose the discrete CPT symmetry for both scalar and spin-1/2 fields. This simplifies the long-standing issue of choosing a preferred vacuum in the quantum theory [10–12]. It also make simple the implementation of the UV regularity condition and renormalization in an expanding universe [13, 14] which is the main novelty of our analysis, in comparison with [1, 2].

The modes characterizing the preferred vacuum \( |0_{\eta=0} \rangle \) in [1] are constructed by a simple linear combination of the modes defining the adiabatic vacua \( |0_\pm \rangle \) (the natural vacua at \( \tau \to \pm \infty \)). \( \text{CPT} |0_{\eta=0} \rangle = |0_{\eta=0} \rangle \), while \( \text{CPT} |0_\pm \rangle = |0_\pm \rangle \). We have checked that the state \( |0_{\eta=0} \rangle \) is UV regular and entirely consistent with renormalization, but not every CPT-invariant state is. Furthermore, as a byproduct of our analysis, it is also possible to conceive alternatives for a preferred CPT-invariant vacuum. We find out that the Bogoliubov \( \beta_k \) coefficients associated to these alternative renormalizable vacua do not behave as a decaying exponential in momenta, as predicted in [1] for CPT symmetry for both scalar and spin-1/2 fields. This simplifies the long-standing issue of choosing a preferred vacuum from the viewpoint of renormalization theory. It is an adiabatic state of infinite adiabatic order, as the Bunch-Davies vacuum in inflationary cosmology.

It is interesting to point out the analogies and differences of the problem of choosing a preferred vacuum in a radiation-dominated universe concerning the same problem in de Sitter space [15]. In planar coordinates \( ds^2 = dt^2 - e^{2Ht}d\vec{x}^2 \), the de Sitter metric possesses manifest invariance under tridimensional translations and rotations. These isometries are not fixed to be a preferred vacuum. The additional symmetry defined by the transformation: \( t \to t + t_0, \vec{x} \to e^{-Ht_0} \vec{x} \) reduces the vacuum ambiguity to a one-complex parameter family of invariant states (i.e., the so-called \( \alpha \) vacua) [13, 16] (see also [17]). However, those \( \alpha \)-vacua are not ultraviolet regular [13], up to the minimal case \( \alpha = 0 \) which turns out to be the Bunch-Davies vacuum [7]. Only for this preferred vacuum \( \alpha = 0 \) the quantum stress-energy tensor \( \langle \alpha | T_{\mu\nu} | \alpha \rangle \) can be renormalized and hence \( \alpha = 0 \) can be admitted as an acceptable physical state [18]. For the radiation-dominated universe, one can also reduce the vacuum ambiguity by imposing the discrete CPT symmetry at \( \tau = 0 \). [Parity and charge conjugation are trivially satisfied for free fields. The non-trivial symmetry in our context is time-reversal]. This way, we get a \( \theta_k \)-parameter family of invariant vacua. Here, however, many of those CPT-invariant vacua are still ultraviolet regular, and some of them can also be regarded as natural candidates for a preferred physical vacuum.

The paper is organized as follows. In Section II we study the CPT-invariant vacuum states for scalar fields. We parametrize the CPT-vacua in terms of an initial hyperbolic phase \( \theta_k \) and study their associated late-times particle production. After this, we investigate the UV regularity of these quantum states and establish the asymptotic conditions that must be satisfied to ensure the renormalizability of the stress-energy tensor. We compare the above-mentioned CPT vacuum \( |0_{\eta=0} \rangle \) with the “minimal” (renormalizable) vacuum \( |0_{\eta_k=0} \rangle \) (whose modes match to the conformal modes at the big bang). In Section III we extend the analysis to spin-1/2 fields. In this case, the CPT-invariant vacuum states are described by the initial (trigonometric) phase \( \theta_k^\prime \). Finally, in Section IV we summarize the main conclusions of our work.

II. CPT-IN Variant VACUUM STATES FOR SCALAR FIELDS AT THE BIG BANG

In this section, we consider a massive scalar field \( \phi \) propagating in a flat FLRW spacetime

\[
ds^2 = a^2(\tau)\left(d\tau^2 - d\vec{x}^2\right).
\]

(1)

We also assume that the expansion factor is of the form given in radiation-dominated era near the big bang

\[
a(\tau) \propto \tau.
\]

(2)

It is convenient to expand the quantized field in Fourier modes adapted to the underlying homogeneity of the 3-space

\[
\phi(\tau, \vec{x}) = \int \frac{d^3k}{\sqrt{2(2\pi)^3}} \left( A_k e^{ik\vec{x}} \phi_k(\tau) + A_k^\dagger e^{-ik\vec{x}} \phi_k^*(\tau) \right),
\]

(3)

where the creation and annihilation operators satisfy the usual commutation relations \( [A_k, A_{k'}^\dagger] = \delta^3(\vec{k} - \vec{k}') \), etc. The normalization of the modes is fixed by the condition

\[
\phi_k \phi_k^* - \phi_k^* \phi_k = \frac{2i}{a^2},
\]

(4)
where the prime denotes derivative with respect to the conformal time. For our purposes it is convenient to work with the rescaled Weyl field \( \varphi \equiv a \phi \) and the rescaled modes \( \varphi_k(\tau) \equiv a(\tau)\phi_k(\tau) \). The field equation implies \( (\mu^2 \equiv a^2m^2 = \gamma^2 \gamma^2) \)

\[
\varphi''_k(\tau) + [k^2 + \mu^2(\tau)] \varphi_k(\tau) = 0 ,
\]

and the normalization condition is given by

\[
\varphi_k \varphi_k' - \varphi_k' \varphi_k' = 2i .
\]

The general solution of (5) can be expressed in terms of parabolic cylindrical functions \( D_k(z) \)

\[
\varphi_k(\tau) = \frac{1}{(2\gamma \tau)^{1/4}} \left[ C_1 D_{\frac{1}{2} - 2i\kappa} (e^{\frac{i4}{4} \sqrt{2\gamma} \tau}) + C_2 D_{\frac{1}{2} + 2i\kappa} (e^{i\frac{3\pi}{4} \sqrt{2\gamma} \tau}) \right] ,
\]

where \( \kappa = \frac{k^2}{2\gamma} \). Any choice of \( k \)-functions \( C_1(k), C_2(k) \) defines a set of modes characterizing a given vacuum state. All these vacua are, by construction, invariant under spatial translations, rotations, parity and charge conjugation (which is here trivial since our scalar field is real). Time translation is not a symmetry for an expanding universe, and time-reversal has not been considered so far. As remarked in the introduction, there is no natural way to select a preferred Fock vacua. In the radiation dominated universe, and due to the very special form of the expansion factor in conformal time, one can further reduce the freedom in choosing a vacuum by exploiting the time-reversal symmetry \( \tau \rightarrow -\tau \) of the background \( ds^2 \propto \tau^2(d\tau^2 - d\vec{x}^2) \).

Generically, the action of charge conjugation \( C \), parity \( P \), and time-reversal \( T \) on a classical scalar field is given by

\[
C : \phi(\tau, \vec{x}) \rightarrow \xi_c^* \phi^*(\tau, -\vec{x}) ; P : \phi(\tau, \vec{x}) \rightarrow \xi_P^* \phi(\tau, -\vec{x}) ; T \phi(\tau, \vec{x}) \rightarrow \xi_T^* \phi(-\tau, \vec{x}) . \]

The \( \xi \)'s are the associated phases of the \( C, P, T \) transformations. In the quantized theory, \( C, P \) are represented as unitary operators, while \( T \) is converted into a antiunitary operator. In our case \( C \) and \( P \) are trivially implemented in the assumed Fourier expansion. Enforcing \( T \) is the key ingredient. However, it seems more useful \([1,2]\) to consider \( CPT \) all at once in the analysis (furthermore, we also choose \( \xi_c \xi_P \xi_T = 1 \) \([21]\) and \( CPT \phi(x)(CPT)^{-1} = \phi(-x)^\dagger \)). The condition for a CPT-invariant vacuum state takes a very simple form on the time-dependent part of scalar field modes

\[
\varphi_k(-\tau) = \varphi_k^*(\tau) .
\]

Using standard properties of the parabolic cylindrical functions it can be easily shown that in terms of the general solution (7), the condition above implies \( C_1 = C_2^* \). For our purposes it is convenient to characterize the CPT-invariant condition at \( \tau = 0 \). We easily find

\[
\begin{align*}
\varphi_k(0) &= \varphi_k^*(0) , \\
\varphi_k'(0) &= -\varphi_k'^*(0) .
\end{align*}
\]

The general solution with the above constraints and the normalization condition (6) can be parametrized as

\[
\begin{align*}
\varphi_k(0) &= \frac{1}{\sqrt{k}} e^{\theta_k} , \\
\varphi_k'(0) &= -i\sqrt{k} e^{-\theta_k} ,
\end{align*}
\]

where \( \theta_k \) is an arbitrary real function. A potential sign ambiguity in (10-11) has been removed by matching the sign with the standard initial conditions for a massless (conformal) field \( \varphi_k(0) = \frac{1}{\sqrt{k}}, \varphi_k'(0) = -i\sqrt{k} \). Note that we have used the freedom of phase-rotate the modes to make them real and non-negative at \( \tau = 0 \). In summary, the CPT requirement reduces the space of possible vacuum states to a family of states characterized by the hyperbolic initial \( (\tau = 0) \) phase \( \theta_k \). In terms of this parameter, the functions \( C_1(k) \) and \( C_2(k) \) read

\[
C_1(k) = 2^{2i\kappa} \sqrt{\pi} e^{\frac{\pi}{2} i\kappa} \left( e^{-\frac{\pi}{4} \Gamma(\frac{1}{4} - i\kappa)} + i \frac{iK}{4} e^{-\theta_k} \Gamma(\frac{1}{4} - i\kappa) \right) .
\]
and $C_2(k) = C_1^*(k)$. We note that the minimal initial conditions (i.e., $\theta_k = 0$) can also be imposed even for a massive field. Hence as $\tau \sim 0$,

$$\varphi_k \sim \frac{1}{\sqrt{k}} e^{-i k \tau}.$$  \hfill(13)

This vacuum is a natural choice because the field modes behave at the big bang as the modes of a massless conformally coupled field. This is consistent since $R = 0$ and the mass is negligible at $\tau \rightarrow 0$, as explained in [9].

### A. Particle production

For each choice of the initial $m$-vacuum $|0_{in}\rangle$ we have a different prediction for the particle creation spectrum at late times. Particles are defined at $\tau \rightarrow +\infty$ as excitations of the $out$-vacuum $|0_{+}\rangle$. The particle production rate can be obtained by the frequency-mixing approach [6]. It has been reviewed in [13, 14, 22, 23] and used extensively in the literature for decades (see, for instance, [24–33]). In our case we find the following expression for the average density number of created particles in the mode $\vec{k}$

$$n_k \equiv |\beta_k|^2 = \frac{1}{2} + \frac{e^{-\pi \kappa} \cosh(2\pi \kappa)}{4\pi} \left( e^{-2\theta_k \kappa} \frac{1}{2} |\Gamma(\frac{1}{4} + i\kappa)|^2 + e^{2\theta_k \kappa} \frac{1}{2} |\Gamma(\frac{1}{2} + i\kappa)|^2 \right).$$  \hfill(14)

It is interesting to remark that the above general expression can be reexpressed, after some manipulations, as

$$|\beta_k|^2 = \frac{1}{2} \left( \cosh(2\eta_k) \cosh(\Lambda_k) - 1 \right),$$  \hfill(15)

where we have defined $\cosh(\Lambda_k) = \sqrt{1 + e^{-4\pi \kappa}}$, and where

$$2\eta_k = -2\theta_k + \frac{1}{2} \ln \left( \frac{\kappa \cosh(2\pi \kappa)}{2\pi^2} |\Gamma(\frac{1}{4} + i\kappa)|^4 \right).$$  \hfill(16)

Following [2] we observe that the number of created particles is minimized when $\eta_k = 0$. This condition can be used to choose a preferred CPT-invariant vacuum and it is characterized by

$$\theta_k^{ad} = \frac{1}{4} \ln \left( \frac{\kappa \cosh(2\pi \kappa)}{2\pi^2} |\Gamma(\frac{1}{4} + i\kappa)|^4 \right).$$  \hfill(17)

[As we will explain shortly, the super-index $ad$ refers to the fact that this vacuum state is an adiabatic vacuum to all orders]. Therefore, we can regard (17) as an equivalent characterization of the preferred CPT-invariant vacuum proposed in [1, 2].

### B. Ultraviolet regularity of the CPT-invariant vacuum states

For a quantum state $|0_{in}\rangle$ to be admitted as physically acceptable we should demand it to be ultraviolet regular. This means that the high-energy behaviour of the state must approach the behaviour of Minkowski space at a rate such that basic composite operators, as the stress-energy tensor, can be renormalized. Therefore, it is natural to require that the renormalized form of $\langle 0_{in}|T_{\mu\nu}|0_{in}\rangle_{ren}$ be well-defined. Since the renormalization subtractions in evaluating $\langle 0_{in}|T_{\mu\nu}|0_{in}\rangle_{ren}$ are essentially unique (up to finite counterterms), the ultraviolet behaviour of the modes must be compatible with the subtractions.

The mode decomposition [3] allow us to write the formal vacuum expectation values of the stress-energy tensor as a sum over modes

$$\langle T_{\mu\nu} \rangle = \int d^3k T_{\mu\nu}(\vec{k}, \tau).$$  \hfill(18)

A very useful renormalization scheme, which works in momentum space and does not depend on an explicit regulator, was introduced by Parker and Fulling [34, 35]. It involves a subtraction algorithm directly for the integrand in (18). The method is based on the adiabatic WKB expansion of the field modes

$$\varphi_k(\tau) \sim \frac{1}{\sqrt{W_k(\tau)}} e^{-i \int^\tau W_k(\tau') d\tau'}.$$  \hfill(19)
where
\[ W_k = \omega_k + \omega_k^{(2)} + \omega_k^{(4)} + \cdots , \]  
(20)
with \( \omega_k = \sqrt{k^2 + m^2 a^2} \), and \( \omega_k^{(n)} \) is the \( n \)-order term in a systematic adiabatic expansion. The adiabatic order is fixed by the number of \( \tau \)-derivatives of the scale factor \( a(\tau) \). The above expansion of the modes is translated to an adiabatic expansion of \( T_{\mu\nu}(\vec{k}, \tau) \). This operation allows to extract from the integrand \( T_{\mu\nu}(\vec{k}, \tau) \) the divergent part of the overall integral \( \langle T_{\mu\nu} \rangle_{\text{ren}} \). Therefore, one can write
\[ \langle T_{\mu\nu} \rangle_{\text{ren}} = \int d^3k \left[ T_{\mu\nu}(\vec{k}, \tau) - T_{\mu\nu}^{\text{N-ad}}(\vec{k}, \tau) \right], \]  
(21)
where \( N \) is the adiabatic order required to cancel the UV divergences of the integral \( \langle T_{\mu\nu} \rangle_{\text{ren}} \). \( T_{\mu\nu}^{\text{N-ad}}(\vec{k}, \tau) \) is the associate adiabatic expansion of \( T_{\mu\nu}(\vec{k}, \tau) \) at order \( N \). We note that \( N \) can be regarded as the degree of divergence of \( \langle T_{\mu\nu} \rangle_{\text{ren}} \).

For the stress-energy tensor \( N = 4 \) (in four spacetime dimensions). Since \( \nabla_{\mu} T_{\mu\nu}^{\text{N-ad}}(\vec{k}, \tau) = 0 \), the subtractions constructed this way preserve general covariance and also locality. The above expression for \( \langle T_{\mu\nu} \rangle_{\text{ren}} \) can be shown [34] to agree with the result of the method introduced by Zeldovich and Starobinsky [36]. A similar discussion can be performed for other composite operators, like the basic two-point function at coincidence \( \langle \phi^2 \rangle \). In this case we have
\[ \langle \phi^2 \rangle_{\text{ren}} = \frac{1}{2(2\pi)^3a^2} \int d^3k \left[ |\varphi_k(\tau)|^2 - (|\varphi_k(\tau)|^2)^{N-\text{ad}} \right]. \]  
(22)
Here we need \( N = 2 \). The adiabatic subtraction method can also be regarded as an upgraded version of the general DeWitt-Schwinger renormalization method when the spatial translations symmetry of the background is assumed [37]. More details can be found in [13, 14] and a brief sketch in the associated reference [3].

Since the subtractions \( T_{\mu\nu}^{\text{N-ad}}(\vec{k}, \tau) \) are essentially fixed, the major point now is to restrict the field modes involved in \( T_{\mu\nu}(\vec{k}, \tau) \), defining \( |0_{\text{in}}\rangle \), such that \( \langle 0_{\text{in}}|T_{\mu\nu}|0_{\text{in}}\rangle_{\text{ren}} \) be convergent. To this end, and in the context of our analysis, it is useful to evaluate the complete adiabatic expansion of the modes at \( \tau = 0 \). We get
\[ \varphi_k(0) \sim \frac{1}{\sqrt{k}} + \frac{\gamma^2}{8 k^{9/2}} + \frac{41\gamma^4}{128 k^{17/2}} + \cdots. \]  
(23)
From this we infer the asymptotic expansion of \( \theta_k \)
\[ \theta_k \sim \frac{\gamma^2}{8k^4} + \frac{5\gamma^4}{16k^6} + \frac{61\gamma^6}{24k^{12}} + \cdots. \]  
(24)
The set of vacuum states that fit the above large \( k \) expansion can be generically referred to as adiabatic (CPT-invariant) vacua. It is not difficult to check that [17] defines a vacuum of infinite adiabatic order. This is so because the large \( k \) asymptotic expansion of \( |\text{CPT-invariant} \rangle \) exactly match the adiabatic expansion \( \langle \phi^2 \rangle \) at any order.

A consequence of having an in-vacuum of infinite adiabatic order is that the number density of created particles in the mode \( \vec{k} \) (i.e., \( n_k \)) with respect to the out-vacuum (which is also of infinite adiabatic order) decays for large \( k \) faster than any power \( k^{-N} \). Typically, an exponential decay. This very smooth behavior of the field modes characterizing \( |0_{\text{in}}\rangle \) also ensures the ultraviolet convergence of \( \langle 0_{\text{in}}|T_{\mu\nu}|0_{\text{in}}\rangle_{\text{ren}} \). In contrast, for an in-vacuum of a finite adiabatic order the decay is a power-law. If we choose \( \theta_k \) different from [24] we get these kind of vacua. For instance, choosing \( \theta_k = 0 \) (zero adiabatic order) we find [3] \( n_k \sim k^{-8} \). Furthermore, for \( \theta_k \sim 1/k^4 \) we also get \( n_k \sim k^{-8} \), except for the case \( \theta_k = \gamma^2/(8k^4) \), for which \( n_k \sim k^{-16} \). This behavior ensures the UV convergence of the total number density of created particles
\[ \int \frac{d^3k}{(2\pi a)^3} n_k < +\infty. \]  
(25)
In contrast, for \( \theta_k \sim 1/k \) we get \( n_k \sim k^{-2} \) and the integral evaluating the total number density is divergent.

It is less clear whether the convergence of [15] is enough to ensure the UV convergence of the most relevant quantities such as the energy density and pressure \( \langle 0_{\text{in}}|T_{\mu\nu}|0_{\text{in}}\rangle_{\text{ren}} \). In Ref. [3] we have analyzed with many details this issue for the minimal solution \( \theta_k = 0 \). The finiteness of the adiabatic order of the in-state originates the emergence of
oscillatory terms, or even extra negative powers in \( k \), in \( T_{\mu\nu}(\vec{k}, \tau) \). UV regularity of the \( in \) state is achieved if those terms do not nullify the UV convergence of the overall \( k \)-integral. In Appendix A we have analyzed the general case. To ensure renormalizability of the stress-energy tensor, the asymptotic behaviour of \( \theta_k \) should be

\[
\theta_k \sim 0 + \mathcal{O}\left(\frac{1}{k^n}\right), \quad n > 3. \tag{26}
\]

If we choose \( \theta_k \) matching with the adiabatic expansion \( \langle 21 \rangle \) up to a given order \( k^{-N} \), and assume this expression as valid for arbitrary momenta, we will obtain a vacuum of finite adiabatic order. The larger is \( N \), the faster is the decay rate of the oscillatory terms and the faster is the decay of the particle number at large \( k \). In the limit \( N \rightarrow \infty \) we have vacua of infinite adiabatic order (one example is \( (17) \), for which the decay of the particle number is exponential and no oscillatory terms are present in \( T_{\mu\nu}(\vec{k}, \tau) \).

III. CPT-IN Variant Quantum States for a Spinor Field

Let us consider now a spin-1/2 field Dirac equation propagating in the same background metric \( ds^2 = a^2(\tau)(d\tau^2 - dx^2) \). The field equation \( (i\gamma^\mu \nabla_\mu - m)\Psi = 0 \), where \( \gamma^\mu = \frac{1}{2} \gamma^\mu \) and \( \gamma^\mu \) are the flat spacetime Dirac matrices become (we use the conventions of \( [13, 14] \))

\[
\left( \gamma^0 \partial_\tau + \vec{\gamma} \cdot \vec{\nabla} + \frac{3\alpha'}{2a} \gamma^0 + ima \right)\Psi = 0. \tag{27}
\]

It is also convenient to perform a Weyl transformation for the spinor field of the form \( \psi = a^{3/2} \Psi \). The mode expansion for the quantized \( \psi \) field is given by \( (D_{\vec{k}\lambda} = B_{\vec{k}\lambda} \) for Majorana spinors)

\[
\psi(x) = \int d^3k \sum_\lambda \left[ B_{\lambda k}^\dagger u_{\lambda k}(x) + D_{k\lambda}^\dagger v_{\lambda k}(x) \right], \tag{28}
\]

where the \( u \)-modes in the Dirac representation

\[
\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix} \tag{29}
\]

can be written as (we have re-expressed the results in \( [38] \) in terms of the conformal time, up to the above \( a^{-3/2}(\tau) \) Weyl rescaling factor)

\[
u_{\lambda k}(x) = \frac{e^{i\vec{k} \cdot \vec{x}}}{\sqrt{(2\pi)^3}} \begin{pmatrix} h^I_{k\lambda}(\tau)\xi_{\lambda}(\vec{k}) \\ h^{II}_{k\lambda}(\tau)\xi_{\lambda}(\vec{k}) \end{pmatrix}, \tag{30}
\]

and where \( \xi_{\lambda} \) is a constant and normalized two-component spinor \( \xi^\dagger_{\lambda} \xi_{\lambda'} = \delta_{\lambda\lambda'} \) that represent the helicity eigenstates. \( \nu_{\lambda k}(x) \) is obtained by the charge conjugation operation. The Dirac equation for the functions \( h^I_{k\lambda}(\tau) \) and \( h^{II}_{k\lambda}(\tau) \) is transformed into \( [ \text{we define } ma(\tau) = \gamma^\tau = \mu(\tau) ] \)

\[
h^I_{k\lambda} + ik h^I_{k\lambda} + i\mu h^I_{k\lambda} = 0, \tag{31}
\]

\[
h^{II}_{k\lambda} + ik h^{II}_{k\lambda} - i\mu h^{II}_{k\lambda} = 0, \tag{32}
\]

together with the normalization condition

\[
|h^I_{k\lambda}|^2 + |h^{II}_{k\lambda}|^2 = 1. \tag{33}
\]

As in the scalar case, the general solution can be given in terms of parabolic cylindrical functions \( D_\nu(z) \) as

\[
h^I_{k\lambda} = \frac{C_1}{\sqrt{2}} D_{-2ik\lambda}(e^{i\frac{\tau}{4}} \sqrt{2\gamma \tau}) + e^{-i\frac{\tau}{4}} \sqrt{\kappa} C_2 D_{-1+2ik\lambda}(e^{i\frac{3\tau}{4}} \sqrt{2\gamma \tau}), \tag{34}
\]

\[
h^{II}_{k\lambda} = \frac{C_3}{\sqrt{2}} D_{2ik\lambda}(e^{i\frac{\tau}{4}} \sqrt{2\gamma \tau}) + e^{i\frac{\tau}{4}} \sqrt{\kappa} C_4 D_{-1-2ik\lambda}(e^{i\frac{3\tau}{4}} \sqrt{2\gamma \tau}), \tag{35}
\]
where again \( \kappa = \frac{1}{4\tau} \). The complex functions \( C_{1,2}(k) \) defining the vacuum state are constrained by the normalization condition \( \text{(53)} \).\

It is very important to note that the equations \( \text{(51), (52)} \) for the time-dependent part of the field modes \( h_k^I(\tau) \) and \( h_k^{II}(\tau) \) remain unchanged under the transformation \( \tau \to -\tau \) and, simultaneously, \( h_k^I \to h_k^{II*} \) and \( h_k^{II} \to h_k^I* \). This is indeed the form of the CPT transformation given in \( \text{(2)} \) on the above characterization of the field modes. Therefore the vacuum will be CPT invariant if the chosen modes verify the relation

\[
h_k^I(\tau) = h_k^{II*}(-\tau).
\]

In terms of the functions \( C_{1,2}(k) \) a CPT-invariant vacuum is characterized by the restriction \( C_1 = C_2^* \). As for the scalar field, we can easily constraint the CPT-invariant initial conditions at \( \tau = 0 \) as

\[
h_k^I(0) = h_k^{II*}(0).
\]

Furthermore, we have also the normalization condition \( \text{(53)} \) at \( \tau = 0 \) implying

\[
|h_k^I(0)| = |h_k^{II}(0)| = \frac{1}{\sqrt{2}}.
\]

Therefore, the general \((\tau = 0)\) solution to the conditions \( \text{(57, 58)} \) can be written as

\[
\begin{align*}
h_k^I(0) &= \frac{e^{+i\theta_k^I}}{\sqrt{2}}, \\
h_k^{II}(0) &= \frac{e^{-i\theta_k^I}}{\sqrt{2}},
\end{align*}
\]

where \( \theta_k^I \) is an arbitrary trigonometric angle. [The superscript \( f \) refers to the fermionic field, in contrast with the plain notation \( \theta_k \) used previously for the scalar field.] In terms of \( \theta_k^f \), the constants \( C_1 \) and \( C_2 \) read

\[
C_1(k) = 2^{i\kappa} \sqrt{\pi} e^{\pi\kappa} \left( \frac{e^{i\theta_k^f} \Gamma(\frac{1}{2} + i\kappa)}{\Gamma(\frac{3}{2} - i\kappa)} + \frac{\kappa e^{\frac{i3\pi}{2}} e^{-i\theta_k^f}}{\Gamma(1 - i\kappa)} \right),
\]

and \( C_2 = C_1^* \). We note that a tentative minimal solution for the initial CPT-invariant condition is \( \theta_k^f = 0 \), as for the scalar field. However, as we will show later this defines a quantum state that is not ultraviolet regular. A minimal and self-consistent solution requires a more involved analysis. We reconsider this issue in subsection III B.

### A. Particle production

We can also compute the particle creation for an initial vacuum state characterized by \( \theta_k^f \). The vacuum \( |0_{in}\rangle \) is perceived at late times as a collection of particles, defined as quantum excitations of the adiabatic \( out\)-vacuum \( |0_+\rangle \). We find

\[
n_{k,\lambda} = |\beta_{k,\lambda}|^2 = \frac{1}{2} - \frac{e^{-\pi\kappa} \sinh(2\pi\kappa)}{4\pi} \left( e^{-2i\theta_k^f} e^{\frac{3\pi}{2}\Gamma(i\kappa)\Gamma(\frac{1}{2} - i\kappa)} + e^{2i\theta_k^f} e^{-\frac{3\pi}{2}\Gamma(-i\kappa)\Gamma(\frac{1}{2} + i\kappa)} \right),
\]

where the subindex \( \lambda \) refers to the helicity of the created fermionic particles.\(^3\) As for the case of scalar fields, and in agreement with the results of \( \text{[1, 2]} \), the above expression can be rewritten as

\[
|\beta_{k,\lambda}|^2 = \frac{1}{2} (1 - \cos(2n_k) \cos(\Lambda_k)),
\]

\(^3\) In terms of \( C_{1,2} \) the normalization condition reads

\[
\frac{e^{\pi\kappa}}{2} (|C_1|^2 + |C_2|^2) + \frac{2\sqrt{\pi} \sinh(2\pi\kappa)}{\sqrt{\pi}} \text{Re}[e^{-i\frac{3\pi}{2}\Gamma} C_1 C_2^* (2i\kappa)] = 1.
\]

\(^4\) Note that the spectrum is indeed independent of \( \lambda \).
where \(\cos(\Lambda_k) = \sqrt{1 - e^{-4\pi \kappa}}\) and

\[
2\eta_k = -2\theta_k^f + \frac{\pi}{4} + \text{Arg}[\Gamma(\frac{1}{2} - i\kappa)\Gamma(i\kappa)] .
\] (43)

Arg\((z)\) refers to the argument of \(z\). The number of created particles gets its minimal value for \(\eta_k = 0\). For this situation we get

\[
\theta_k^{ad-f} = \frac{\pi}{8} + \frac{1}{2} \text{Arg}[\Gamma(\frac{1}{2} - i\kappa)\Gamma(i\kappa)] .
\] (44)

This offers an alternative characterization of the preferred CPT-invariant vacuum proposed in [1 2].

B. UV regularity of the CPT-invariant vacua

The analysis of the adiabatic expansion for spinors is more involved than for scalars. It does not fit the conventional WKB-type template, as happens for scalar fields. It is given, assuming the definitions [30] for the modes, by [38–40]

\[
h_k^I(\tau) \sim \sqrt{\frac{\omega + ma}{2\omega}} (1 + F^{(1)} + F^{(2)} + \cdots) e^{-i f^+ \Omega_k(\tau) d\tau} ,
\]

\[
h_k^{II}(\tau) \sim \sqrt{\frac{\omega - ma}{2\omega}} (1 + G^{(1)} + G^{(2)} + \cdots) e^{-i f^- \Omega(\tau) d\tau} ,
\]

where \(\omega^2 = k^2 + m^2 a^2\), and \(\Omega(\tau) = \omega + \omega^{(1)} + \omega^{(2)} + \cdots\). The recursive algorithm is displayed in [38–40]. At \(\tau = 0\) we obtain a well-defined large \(k\) asymptotic expansion

\[
h_k^I(0) \sim \frac{1}{\sqrt{2}} \left(1 - i \frac{\gamma}{4k^2} - \frac{\gamma^2}{32k^4} - i \frac{21\gamma^3}{128k^6} - \frac{85\gamma^4}{2048k^8} + \cdots \right)
\]

(47)

and \(h_k^{II}(0) \sim h_k^{I*}(0)\), which requires the following large \(k\) expansion for \(\theta_k^I\):

\[
\theta_k^I \sim - \left(\frac{\gamma}{4k^2} + \frac{\gamma^3}{6k^6} + \frac{4\gamma^5}{5k^{10}} + \cdots \right) .
\] (48)

This determines the appropriated rate for the decaying of \(\theta_k^I\) when \(k \to \infty\) to have a CPT-invariant vacuum of infinite adiabatic order. A good example is the preferred vacuum proposed in [1 2] for the spinor field. The large \(k\) expansion of [14] coincides with [18].

Mimicking the analysis for the scalar field one can probe the elementary solution \(\theta_k^f = 0\). We find that the corresponding Bogoliubov coefficients do not behave as a decaying exponential, as for the choice \(\theta_k^{ad-f}\), but rather as a power law of the form \(|\beta_{k,\lambda}|^2 \sim k^{-4}\). However, the quantum stress-energy tensor \(\langle T_{\mu\nu}\rangle_{ren}\) diverges for this choice of vacuum, hence the vacuum characterized by \(\theta_k^f = 0\) is not UV regular. This can be proved using the cumbersome techniques displayed in the accompanying paper [3]. To ensure an UV regular vacuum we have to demand the trigonometric angle \(\theta_k\) to be different from zero. Furthermore, it should decay to zero for large \(k\) exactly as

\[
\theta_k^I \sim - \frac{\gamma}{4k^2} + \mathcal{O}\left(\frac{1}{k^n}\right) , \quad n > 2 .
\] (49)

In Appendix [15] we give some details about these results. The result [29], together with [26] for scalar fields are the main results of this work. Those formulas provide the large \(k\) characterization of the UV regular and CPT-invariant vacua. We still have freedom to specify the infrared behaviour of \(\theta_k^I\) (as well as for \(\theta_k\) for scalar fields). This can be fixed by introducing extra assumptions, not so fundamental as UV regularity or symmetries. The choice [14] [17] for scalars], although perfectly consistent and elegant, introduces an additional argument by demanding that the number of created particles at \(\tau \sim +\infty\) is minimized. From a more general viewpoint we can consider as consistent CPT-invariant vacua all those that verify the condition [19].
In this context, it is interesting to compare the predictions for particle production for two different examples of CPT-invariant vacua. For instance, let us consider the elementary and illustrative example $\theta_k^{\text{min} - f} = -\frac{i k}{\sqrt{2}}$. The vacuum defined in this way can be proved to have convergent $(T_{\mu\nu})_{\text{ren}}$ and the density of created particles decays as $n_k \sim k^{-12}$. At late times the renormalized comoving energy density of (Majorana) dark matter neutrinos is found to be $\rho_{dm} = m(\gamma/\pi)^{3/2} I_k^\text{min} - f$, where the new numerical constant $I_k^\text{min} - f = 0.02699$. This differs from the constant obtained for the preferred vacuum in $[1] I_k^{\text{eff} - f} = 0.01276$. Therefore, the predicted mass of the assumed sterile dark matter neutrinos (to accommodate the present-day dark matter density) differs by a factor 0.61. One gets now $m_{dm} = 2.9 \times 10^8 \text{GeV}$, instead of $4.8 \times 10^8 \text{GeV}$.

**IV. CONCLUSIONS AND FINAL COMMENTS**

In this paper we have given a simple characterization of the CPT-invariant vacuum states at the big bang through the phase functions $\theta_k$ (for scalar fields) and $\theta_k^f$ (for fermionic fields). We have analyzed intertwining aspects of quantum field theory in the assumed radiation dominated background for those CPT-invariant vacua. We have characterized the asymptotic large $k$ behavior of $\theta_k$ ($\theta_k^f$) to ensure UV regularity. The existence of many CPT-invariant vacua is somewhat analogous to the invariant $\alpha$-vacua in de Sitter space. However, while the $\alpha$-vacua are not ultraviolet regular, up to the Bunch-Davies vacuum, we identify here several examples of CPT-invariant and ultraviolet regular vacuum states.

For instance, in the case of a massive scalar field, it is possible to choose a CPT-invariant vacuum state characterized by elementary initial conditions, namely $\varphi_k \sim \frac{1}{\sqrt{2k}} e^{-ik\tau}$, corresponding to $\theta_k = 0$. In doing so, one is taking advantage of the very special nature of the big bang event $[11]$. As $\tau \to 0$, one can demand that the massive field modes behave as the modes of a conformal theory, as the effective mass of the field is negligible. Furthermore, this choice is fully consistent with renormalizability $[3]$ in the sense that the vacuum expectation value of the stress-energy tensor can be renormalized by the standard subtractions. Apart from this special case, we have seen that the condition for a CPT-invariant vacuum to be UV regular is that the associated $\theta_k$ behaves as $\theta_k \sim O(k^{-n}), n > 3$. For a massive spinor field one can try a similar strategy to construct a CPT-invariant vacuum. The most elementary initial conditions at the big bang are $h_k^{\text{eff} - f} \sim \frac{1}{\sqrt{2k}} e^{-ik\tau}$. This vacuum state, defined at $\tau \sim 0$, is also CPT-invariant. Unfortunately, this apparent legitimate choice is not physically consistent because now the renormalized $(T_{\mu\nu})_{\text{ren}}$ turns out to be divergent. Nevertheless, we have found a family of CPT-invariant vacua that are UV regular, which is characterized by the condition that $\theta_k^f$ must behave at large $k$ as exactly $\theta_k^f \sim -\frac{i k}{\sqrt{2}} + O(k^{-n}), n > 2$. Other well-motivated examples are those characterized by $\theta_k^{\alpha d}$ ($\theta_k^{\text{eff} - f}$), already identified in $[1, 2]$. A by-product of our analysis is to point out that those states are of infinite adiabatic order, and hence ultraviolet regular vacuum states.

Finally, we want to remark that a more sophisticated choice for a preferred vacuum can also be suggested. One of the main ingredients of the approach used here is the possibility of performing Weyl local rescalings in the description of the quantized matter fields. It seems natural to demand an exact cancellation of the geometrical Weyl anomaly among matter fields in the massless limit. This has been explored in $[42]$. The non-geometrical part of the trace of the quantized stress-energy tensor for massive fields strongly depends on the vacuum state (see, for instance, $[39]$). Hence, requiring that it also vanishes at $\tau = 0$ imposes a strong condition on the quantum vacuum. Whether this is enough to univocally fix the vacuum requires further analysis.

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Appendix A: Details on the large momentum expansion of the scalar field modes

This short appendix gives supplementary material to the analysis given in [3] for more general hyperbolic phases \( \theta_k \). For an arbitrary value of \( \theta_k \) we cannot ensure that the stress-energy tensor is renormalizable with the standard subtractions. We have to analyze the problem with the technique displayed in [9]. In short, we have to look at the large \( k \) expansion of the modes \( \varphi_k \)

\[
|\varphi_k(t)|^2 \sim \cosh(2\theta_k) \left( \frac{1}{k} - \frac{\gamma^2 \tau^2}{2k^3} + \frac{3\gamma^4 \tau^4}{8k^5} + \frac{\gamma^2}{4k^5} - \frac{\gamma^2 \cos(2k\tau)}{4k^5} + \mathcal{O}\left(\frac{1}{k^6}\right)\right) \\
+ \sinh(2\theta_k) \left( -\frac{\gamma^2}{4k^5} + \frac{\cos(2k\tau)}{k} - \frac{\gamma^2 \tau^3 \sin(2k\tau)}{3k^2} - \frac{\gamma^4 \tau^6 \cos(2k\tau)}{18k^3} - \frac{\gamma^2 \tau^2 \cos(2k\tau)}{2k^3} + \mathcal{O}\left(\frac{\sin(2k\tau)}{k^4}\right)\right)
\]

To get a finite \( \langle 0|\langle T_{\mu\nu}\rangle|0 \rangle_{\text{ren}} \), the non-oscillatory terms must coincide with the adiabatic expansion obtained from \([19]\) up to and including the order \( k^{-5} \). These are exactly the non-oscillatory terms inside the parenthesis multiplying to \( \cosh(2\theta_k) \). Therefore, the factor \( \cosh(2\theta_k) \) can only add corrections of order \( \sim k^{-5} \). Taking into account the Taylor expansion of the hyperbolic cosine, we can easily conclude that the leading order in the ultraviolet expansion of \( \theta_k \) must be at least of order \( k^{-5/2} \). On the other hand, the leading oscillatory term must also decay, at least, as \( k^{-n}, n > 4 \). This ensures a well behaved integral for the energy density and pressure in the ultraviolet regime, (see [3]). Therefore the factor \( \sin(2\theta_k) \) can only add corrections of order \( k^{-n}, n > 3 \). Using the expansion of the hyperbolic sine, we see that the leading order in the ultraviolet expansion of \( \theta_k \) must be at least of order \( k^{-n}, n > 3 \). Therefore the asymptotic form of \( \theta_k \) should be \( \theta_k \sim \mathcal{O}(k^{-n}), n > 3 \).

Appendix B: Details on the large momentum expansion of the spin-1/2 field modes

In this brief appendix, we give the large \( k \) expansion of the integrand of the formal vacuum expectation value of the energy density \( \rho(k, \tau) \), defined as

\[
\langle T_{tt} \rangle = \frac{1}{(2\pi)^2 a^3} \int_0^\infty k^2 dk \rho(k, \tau),
\]

for the CPT-invariant vacuum states defined in Section [3](see Ref. [39] for details regarding \( \langle T_{\mu\nu}\rangle_{\text{ren}} \) for Dirac fields in spatially flat FLRW backgrounds). Using the techniques displayed in [4], we find

\[
m^{-1} \rho(k, \tau) \sim \cos(2\theta_k) \left( -\frac{2k}{\gamma \tau} - \gamma \frac{\tau}{k} + \frac{\gamma^3 \tau^3}{2k^3} - \frac{\gamma \cos(2k\tau)}{2k^3} + \mathcal{O}\left(\frac{\sin(2k\tau)}{k^4}\right)\right) \\
+ \sin(2\theta_k) \left( +\frac{1}{k \tau} + \frac{\gamma^2}{2k^3} - \frac{\cos(2k\tau)}{k \tau} + \frac{\gamma^2 \tau^2 \sin(2k\tau)}{3k^2} + \mathcal{O}\left(\frac{\cos(2k\tau)}{k^3}\right)\right).
\]

This expression has to be compared with the large \( k \) expansion of the adiabatic expansion of the energy density, namely

\[
m^{-1} \rho(k, \tau)^{\text{adi}} \sim -\frac{2k}{\gamma \tau} - \gamma \frac{\tau}{k} + \frac{\gamma^3 \tau^3}{4k^3} + \mathcal{O}\left(\frac{1}{k^5}\right).
\]

In this case, and since we are directly looking at the energy density, we need to find coincidence with the adiabatic expansion up to and including order \( \mathcal{O}(k^{-3}) \). We directly see that, for \( \theta_k = 0 \), there is one term in \([12] \), \( \gamma/(2k^3 \tau) \), that does not coincide with the adiabatic expansion, generating a logarithmic divergence after renormalization. On the contrary, for \( \theta_k \sim -\frac{\gamma}{4k^2} \), and using the large \( k \) expansion of the trigonometric functions, we see that the part

\[5\] Note that, \( \langle \rho \rangle \propto \int dk k^2 \rho(k, \tau) \), and therefore, a term going as \( \sim k^{-3} \) generates a logarithmic divergence.
proportional to $\sin(2\theta_k)$ contributes to the large $k$ expansion in such a way that we recover the adiabatic expansion making the state UV regular. Furthermore, in this case we find also cancellations for the oscillatory terms. We have also performed a similar analysis with the two-point function and the pressure, finding analogous results. We have found that, to ensure the convergence of these three quantities, the trigonometric phase should behave, at large $k$, as $\theta_k \sim -\frac{\gamma}{4k^2} + O(k^{-n}), \ n > 2$.

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