### Low-energy states and CPT invariance at the big bang

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In this paper, we analyze the quantum vacuum in a radiation-dominated and CPT-invariant universe by further imposing the quantum states to be ultraviolet regular i.e., satisfying the Hadamard/adiabatic condition. For scalar fields, this is enforced by constructing the vacuum via the states of low-energy proposal. For spin- $\frac{1}{2}$  fields, we extend this proposal for a FLRW spacetime and apply it for the radiation-dominated and CPT-invariant universe. We focus on minimizing the smeared energy density around the big bang and give strong evidence that the resulting states satisfy the Hadamard/adiabatic condition. These states are then selfconsistent candidates as effective big bang quantum vacuum from the field theory perspective.

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### I. INTRODUCTION

One of the basic issues in the theory of quantized fields in curved spacetime [1–4] is the fixing of a preferred vacuum state. The canonical quantization approach soon exhibited that the vacuum state is not unique in a timedependent spacetime. Only for stationary spacetimes, or adiabatic regions in expanding universes, one can naturally find a privileged definition of the vacuum. A major consequence of this ambiguity is the particle creation phenomena, as first discovered in cosmology [5-8] and also in the vicinity of black holes [9]. However, a requirement that a physically admissible quantum state should satisfy is the Hadamard condition [10], which specifies the singularity structure of the two-point function. This condition ensures the existence of Wick polynomials of arbitrary order [11–13] and hence, the perturbative series of an interacting theory to be well-defined at any order. The necessity of the Hadamard condition was further motivated in [14]. The Hadamard condition, which is defined for arbitrary spacetimes, can be transformed into the adiabatic condition [2,3,15,16] in homogeneous spacetimes. The adiabatic condition fixes the large momentum structure of admissible states.

On a generic time-varying spacetime one cannot single out a preferred vacuum. This lack of a unique vacuum choice is strongly manifested in Friedmann-Lemaître-RobertsonWalker (FLRW) spacetimes. Several approaches have been considered to select a preferred vacuum state at early times, based on different viewpoints [17–22], from which one can predict late time quantum effects. Furthermore, it is also highly nontrivial to obtain a vacuum state satisfying the Hadamard condition. An especially appealing proposal is the states of low energy (SLE) prescription [23,24]. These states of low energy are obtained by minimizing the expectation value of the energy density after smearing it with a time-dependent test function. This prescription ensures the Hadamard condition or, equivalently, the (all orders) adiabatic condition [3]. The SLE were introduced originally only for scalar fields (and for minimal coupling). It is easy to show that the Minkowski vacuum is the state of low energy, irrespectively of the specific form of the smearing function. For simple asymptotically flat regions, where the expansion factor a(t) approaches constant values at  $t \to \pm \infty$ , the initial and final Minkowski vacua, corresponds to the state of minimal energy when the time averaging has support at early and late times respectively. For de Sitter spacetime, the Bunch-Davies vacuum is the state of low energy, irrespective of the particular form of the smearing function, as long as it has support at the distant past [25,26]. However, the states of low energy depend, in general, on the choice of the smearing function. This method was recently applied to obtain physically motivated vacua in the Schwinger effect [27] and for scalar fields with Yukawa interaction [28].

Of special physical interest is to analyze this issue for a radiation-dominated universe. The study of this particular expansion rate has different motivations. It can be thought of as a natural pre-inflationary phase, as it has been recently

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discussed in [29-31]. The vacuum in this pre-de Sitter space should smoothly evolve to a state that is approximately equivalent to the Bunch-Davies state for large k's, but differs significantly from it at small k's. Furthermore, from a noninflationary perspective, the issue of how to define a preferred vacuum in a radiation-dominated universe is also of special relevance in general, particularly in relation to the interesting and recent proposal of Ref. [32,33]. In this view of cosmic evolution, the CPT symmetry plays a crucial role to single out privileged vacua. The gravitational background is assumed to be timereversal symmetric with respect to the big bang event  $\tau = 0$ . A radiation-dominated era emerges from this special event, for which a natural analytic continuation of the expansion factor  $a(\tau) \sim \tau$  to negative values of conformal time  $\tau$  is assumed. A radiation-dominated universe going back to the big bang is also the simplest way to enforce Penrose's Weyl curvature hypothesis [34].

The goals of this paper are to:

- (i) Extend the prescription of states of low energy for  $spin-\frac{1}{2}$  fields on FLRW spacetimes.
- (ii) Characterize the possible CPT-invariant Hadamard states for scalars and spin- $\frac{1}{2}$  fields just at the big bang event  $\tau=0$ , obtaining a  $\{\theta_k,\Theta_k\}$ -family of CPT-invariant Hadamard states for scalars and fermions respectively.
- (iii) Study the possible CPT-invariant states of low energy in a radiation-dominated universe and analyze whether the smeared energy density can be minimized around the big bang for both scalar and spin-½ fields. We check that the resulting family of CPT-invariant states of low energy, indeed satisfy the Hadamard/adiabatic condition.

For pedagogical reasons the organization of the paper is as follows. In Sec. II we parametrize the possible CPT-invariant states in a radiation-dominated universe for scalar fields and give the asymptotic ultraviolet condition that they have to satisfy in order to be Hadamard. In Sec. III we review the SLE characterization, extending it for a general coupling to the scalar curvature and paying special attention to the big bang singularity. We restrict the SLE characterization to the CPT-invariant states. In Sec. IV, we study the possible SLE with smearing functions with support around the big bang for scalar fields. In Sec. V we parametrize the possible CPT-invariant states in a radiation-dominated universe for spin- $\frac{1}{2}$  fields and characterize the asymptotic ultraviolet condition that they have to satisfy in order to be Hadamard. In Sec. VI we provide the SLE characterization for fermions. In Sec. VII, we study the possible SLE with smearing functions with support around the big bang for spin- $\frac{1}{2}$  fields. Finally, in Sec. VIII we summarize our results and discussions. Most of the computations in this paper have been done with the aid of the Mathematica software. Throughout this paper, we use units in which  $\hbar = c = 1$ .

### II. CPT-INVARIANT STATES FOR SCALARS IN A RADIATION-DOMINATED SPACETIME

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

$$ds^{2} = a^{2}(\tau)(d\tau^{2} - d\vec{x}^{2}). \tag{1}$$

We will assume a radiation-dominated universe. The expansion factor is given, in conformal time, by

$$a(\tau) \propto \tau.$$
 (2)

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

$$\phi(\tau, \vec{x}) = \int \frac{\mathrm{d}^3 k}{\sqrt{2(2\pi)^3}} \left( A_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} \phi_k(\tau) + A_{\vec{k}}^{\dagger} e^{-i\vec{k}\cdot\vec{x}} \phi_k^*(\tau) \right), \tag{3}$$

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

$$\phi_k \phi_k^{\prime *} - \phi_k^{\prime} \phi_k^{*} = \frac{2i}{a^2},\tag{4}$$

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

$$\varphi_k''(\tau) + [k^2 + \gamma^2 \tau^2] \varphi_k(\tau) = 0,$$
 (5)

and the normalization condition is given by

$$\varphi_k \varphi_k'^* - \varphi_k' \varphi_k^* = 2i. \tag{6}$$

The general solution of (5) can be expressed in terms of parabolic cylindrical functions  $D_{\nu}(z)$  [35]

$$\varphi_k(\tau) = C_{k,1} S_k(\tau) + C_{k,2} S_k^*(-\tau), \tag{7}$$

where

$$S_k(\tau) = \frac{1}{(2\gamma)^{1/4}} D_{-\frac{1}{2} - 2i\kappa} (e^{i\frac{\pi}{4}} \sqrt{2\gamma}\tau), \tag{8}$$

and

$$\kappa = \frac{k^2}{4\gamma}.\tag{9}$$

Any choice of k-functions  $C_{k,1}$  and  $C_{k,2}$  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  $\tau \to -\tau$  of the background  $\mathrm{d} s^2 \propto \tau^2 (\mathrm{d} \tau^2 - \mathrm{d} \vec{x}^2)$ .

Following [32,33], we directly study the effect of charge conjugation C, parity P, and time-reversal T on the Weyl transformed scalar field  $\varphi$ . The action of these transformations is [36],  $C: \varphi(\tau, \vec{x}) \to \xi_c^* \varphi^*(\tau, \vec{x})$ ;  $P: \varphi(\tau, \vec{x}) \to \xi_p^* \varphi(\tau, -\vec{x}); T: \varphi(\tau, \vec{x}) \to \xi_t^* \varphi^*(-\tau, \vec{x}).$  [The  $\xi$ 's are the associated phases of the C, P, T transformations]. In the quantized theory, C and 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 to consider CPT all at once in the analysis [furthermore, we also choose  $\xi_c \xi_p \xi_t = 1$  [37]; therefore  $CPT \varphi(x) (CPT)^{-1} = \varphi(-x)^{\dagger}$ . The condition for a CPT-invariant vacuum state takes a very simple form on the time-dependent part of scalar field modes,

$$\varphi_k(-\tau) = \varphi_k^*(\tau). \tag{10}$$

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  $C_{k,1} = C_{k,2}^*$ . It seems natural to characterize the *CPT*-invariant state by specifying initial data at  $\tau = 0$ . In the limit of  $\tau \to 0$ , the mode equation becomes

<sup>1</sup>From the Wronskian condition (6) we get the following normalization condition for  $C_{k,1}$  and  $C_{k,2}$ :

$$\begin{split} \frac{e^{\pi\kappa}}{2} \left( |C_{k,1}|^2 + |C_{k,2}|^2 \right) + \frac{\sqrt{2}\cosh\left(2\pi\kappa\right)}{\sqrt{\pi}} \\ \times \operatorname{Re} \left[ e^{-i\frac{\pi}{4}} C_{k,1} C_{k,2}^* \Gamma\left(\frac{1}{2} - 2i\kappa\right) \right] = 1. \end{split}$$

<sup>2</sup>We note that if the T transformation is directly applied on the original scalar field  $\phi(x)$  there will be a difference of sign with respect to the transformation defined here. This sign can be always absorbed in the phase  $\xi_t^*$  or by making a redefinition of the (Weyl transformed) modes  $\varphi_k \to i\varphi_k$  to keep our choices (e.g.,  $\xi_c \xi_p \xi_t = 1$ ), and hence, the final form of the CPT transformation unaltered. For convenience we have adopted the conventions used in [32,33].

$$\varphi_k''(\tau) + k^2 \varphi_k(\tau) \sim 0. \tag{11}$$

Then,

$$\varphi_k(\tau) \sim c_k e^{-ik\tau} + d_k e^{ik\tau}. \tag{12}$$

The normalization condition implies  $|c_k|^2 - |d_k|^2 = k^{-1}$ . This condition, together with the required *CPT* invariance  $[c_k = c_k^* \text{ and } d_k = d_k^*, \text{ i.e., } c_k \text{ and } d_k \text{ must be real] allows us to reparametrize the constants <math>c_k$  and  $d_k$  in terms of an hyperbolic angle  $\theta_k$  as

$$c_k = \frac{\cosh(\theta_k)}{\sqrt{k}}, \qquad d_k = \frac{\sinh(\theta_k)}{\sqrt{k}}.$$
 (13)

Therefore, the *CPT*-invariant solution for  $\tau \to 0$  should go as

$$\varphi_k(\tau) \sim \frac{1}{\sqrt{k}} e^{-ik\tau} \cosh \theta_k + \frac{1}{\sqrt{k}} e^{ik\tau} \sinh \theta_k.$$
 (14)

At  $\tau = 0$  this results into

$$\varphi_k(0) = \frac{e^{\theta_k}}{\sqrt{k}}, \qquad \varphi'_k(0) = -i\sqrt{k}e^{-\theta_k}. \tag{15}$$

where  $\theta_k$  is an arbitrary real function. 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  $C_{k,1}$  and  $C_{k,2}$  read<sup>3</sup>

$$C_{k,1} = 2^{i\kappa} \sqrt{\pi} e^{\pi\kappa} \left( \frac{e^{-\frac{i\pi}{4}} e^{\theta_k}}{\kappa^{\frac{1}{4}} \Gamma\left(\frac{1}{4} - i\kappa\right)} + \frac{i\kappa^{\frac{1}{4}} e^{-\theta_k}}{\Gamma\left(\frac{3}{4} - i\kappa\right)} \right), \quad (16)$$

with  $\kappa$  defined in (9) and  $C_{k,2} = C_{k,1}^*$ . In other words, any *CPT*-invariant solution can be written in terms of the  $\theta_k$  angle as

$$\varphi_k^{CPT}(\tau) = C_{k,1} S_k(\tau) + C_{k,1}^* S_k^*(-\tau), \tag{17}$$

with  $C_{k,1}$  given above. We can regard this result as an equivalent characterization of the *CPT*-invariant vacua proposed in [32,33]. The main advantage of this reparametrization is that it allows us to characterize the nontrivial ultraviolet behavior of the modes at large k. Also, in the Heisenberg picture we understand now the time reversal

<sup>&</sup>lt;sup>3</sup>The final expression for  $C_{k,1}$  can be written in several ways by using some properties of the gamma functions. In particular we have used  $\Gamma(z)\Gamma(z+\frac{1}{2})=2^{1-2z}\sqrt{\pi}\Gamma(2z)$  and  $\Gamma(z)\Gamma(1-z)=\frac{\pi}{\sin(\pi z)}$ .

vacuum state  $|0\rangle$  as defined by giving initial data  $\varphi_k^{CPT}(\tau_0)$  at  $\tau_0=0$ .

To clarify the discussion above, it is interesting to present states that are not CPT invariant. As time evolves the expansion of the universe slows down and one can naturally define a late-times (infinite order) adiabatic vacuum  $|0_{+}\rangle$  [38]. In this asymptotic region  $(\tau \to \infty)$ , the general solution (7) behaves as a linear combination of positive and negative-frequency solutions, and the preferred (positive-frequency) solution for the late-times modes at  $\tau \to \infty$  reads

$$\varphi_k^{(+)}(\tau) \sim \frac{e^{-i\int_{\tau}\omega(u)du}}{\sqrt{\omega(\tau)}} \sim \frac{e^{-i(\frac{\gamma}{2}\tau^2 + \kappa \ln(2\gamma\tau^2))}}{\sqrt{\gamma\tau}}, \qquad (18)$$

where  $\omega = \sqrt{k^2 + m^2 a^2}$ . The constants  $C_{k,1}$  and  $C_{k,2}$  can be fixed imposing this late-times behavior. We directly find

$$C_{k1} = \sqrt{2}e^{-\frac{\pi\kappa}{2}}e^{i\frac{\pi}{8}}, \qquad C_{k2} = 0.$$
 (19)

We note that the late-times adiabatic vacuum is not *CPT* invariant, since  $C_{k,1} \neq C_{k,2}^*$ . Analogously, the early-times adiabatic vacuum  $|0_-\rangle$  is determined by the asymptotic condition  $(\tau \to -\infty)$ 

$$\varphi_k^{(-)}(\tau) \sim \frac{e^{-i\int_{\tau} \omega(u)du}}{\sqrt{\omega(\tau)}} \sim \frac{e^{i(\frac{\gamma}{2}\tau^2 + \kappa \log(2\gamma(-\tau)^2))}}{\sqrt{-\gamma\tau}}, \qquad (20)$$

and  $C_{k,1}=0$ ,  $C_{k,2}=\sqrt{2}e^{-\frac{\pi x}{2}}e^{-i\frac{\pi}{8}}$ , which is also not CPT invariant. Given the constants  $C_{k,1}$  and  $C_{k,2}$  for each solution, it is direct to see that  $CPT|0_{\pm}\rangle=|0_{\pm}\rangle$ .

# A. Ultraviolet regularity of the *CPT*-invariant vacuum states

For a quantum state  $|0\rangle$ , to be admitted as physically acceptable we should demand it to be ultraviolet regular. This means that the high-energy behavior of the state must approach the behavior of Minkowski space at a rate such that basic composite operators can be renormalized. In cosmological backgrounds this translates into the adiabatic condition: for large k, the behavior of the field modes  $\varphi_k$  should follow the Wentzel-Kramers-Brillouin (WKB) type asymptotic condition at all orders [39–42]

$$\varphi_k(\tau) \sim \frac{1}{\sqrt{\Omega_k(\tau)}} e^{-i\int^{\tau} \Omega_k(\tau')d\tau'},$$
(21)

where the function  $\Omega_k(\tau)$  admits an asymptotic expansion in terms of the derivatives of  $a(\tau)$ 

$$\Omega_k = \omega + \omega_k^{(1)} + \omega_k^{(2)} + \omega_k^{(3)} + \omega_k^{(4)} + \cdots$$
 (22)

The coefficients of the expansion  $\omega_k^{(n)}$  are obtained by systematic iteration from the mode equation, and depend on derivatives of a up to and including order n. The expansion above dictates the ultraviolet behavior that the fields modes must obey in order to define an admissible quantum state. Note that (21) and (22) should be satisfied at all orders to be equivalent to the Hadamard condition. This expansion is in general asymptotic, and therefore cannot define a unique vacuum state, but rather a family of acceptable states. Furthermore, the two-point function inherits from (21) and (22) an adiabatic expansion which produces the same renormalized stress-energy tensor as the DeWitt-Schwinger expansion when it is restricted to FLRW spacetimes in four spacetime dimensions [43–45]. In Appendix A we give more detail about the adiabatic method for scalars.

For the CPT-invariant vacua, parametrized by the real and time-independent function  $\theta_k$ , this condition should be reexpressed in terms of the hyperbolic initial phase. It is important to note that the adiabatic modes  $\varphi_k^{(N)}$  of order N satisfy the equation of motion at order N. Therefore, adiabaticity is preserved in time and it is enough to study the large momentum behavior of the modes  $\varphi_k$  at a given instant of time  $\tau_0$  to study its ultraviolet behavior.

In the context of our analysis, it is natural to evaluate the complete adiabatic expansion of the modes (21) at  $\tau = 0$ . We get

$$\varphi_k(0) \sim \frac{1}{\sqrt{k}} + \frac{\gamma^2}{8k^{9/2}} + \frac{41\gamma^4}{128k^{17/2}} + \cdots$$
 (23)

From this, we infer an asymptotic expansion for  $\theta_k$ 

$$\theta_k \sim \frac{\gamma^2}{8k^4} + \frac{5\gamma^4}{16k^8} + \frac{61\gamma^6}{24k^{12}} + \cdots$$
 (24)

The set of vacuum states that fit the above large k expansion can be generically referred to as adiabatic (CPT-invariant) vacua. In Appendix B we show that only if  $\theta_k$  behaves as in (24), the high-energy behavior of the field modes is compatible with the adiabatic condition after time evolution (i.e., for  $\tau > 0$ ).

### III. STATES OF LOW ENERGY FOR SCALARS

Let us briefly summarize the method for constructing states of low energy. We follow the prescription described in [23,24]. The main idea of this construction is to fix the free parameters of the problem (e.g.,  $\theta_k$  in our *CPT*-invariant model) by requiring that the vacuum expectation value of the smeared energy density over a temporal window should be minimal. A special and very important virtue of this construction is that it guarantees that the resulting states are Hadamard for smooth regions of the

spacetime. We first review the general method for arbitrary  $a(\tau)$  emphasizing the aspects that will be relevant for our analysis and then we particularize it for the CPT-invariant model under consideration. We further generalize the standard result by including an arbitrary coupling to the scalar curvature  $\xi$ . The starting point is to fix a fiducial set of normalized modes  $\phi_k(\tau)$ . They are related to the Weyl modes of the previous section by  $\varphi_k = a\phi_k$ . One can parametrize a general set of modes  $T_k(\tau)$  in the form

$$T_k(\tau) = \lambda_k \phi_k(\tau) + \mu_k \phi_k^*(\tau), \tag{25}$$

where  $\lambda_k$  and  $\mu_k$  are complex numbers that must obey  $|\lambda_k|^2 - |\mu_k|^2 = 1$ . The goal now is to find for which values of  $\lambda_k$  and  $\mu_k$  the smeared energy density is minimal.

The smeared energy density can be defined as follows. The vacuum expectation value of the Hamiltonian  $H(\tau)$  for a scalar field  $\phi$ , associated to a foliation of a spacelike Cauchy surface  $\Sigma_{\tau}$  and a temporal vector characterizing an observer  $u^b$  is given by

$$H(\tau) = \int_{\Sigma_{-}} d^{3}x \sqrt{|h|} \langle T_{ab} \rangle n^{a} u^{b}.$$
 (26)

 $\sqrt{|h|}$  is the determinant of the induced Riemann metric in  $\Sigma_{\tau}$ ,  $\langle T_{ab} \rangle$  is the vacuum expectation value of the stress-energy tensor,  $n^a$  is the unit normal vector to the foliation. We should take as  $\langle T_{ab} \rangle$  the renormalized values. However, we are interested in the problem of minimizing the energy density, and since the subtraction terms in the renormalization are independent of the vacuum state we can ignore them. We will only consider the contributions of the modes, as in (28). Following [23], we choose the privileged isotropic observer,  $u^a = n^a = (a^{-1}, 0, 0, 0)$  in conformal time coordinates, and the above expression reduces to

$$H(\tau) = \int_{\Sigma_{\tau}} d^3x \sqrt{|h|} \langle T_{ab} \rangle u^a u^b$$

$$= \int_{\Sigma_{\tau}} d^3x \sqrt{|h|} \langle \rho(\tau) \rangle$$

$$= \int_{\Sigma} d^3x \int \frac{d^3k}{(2\pi)^{3/2}} \sqrt{|h|} \rho_k(\tau), \qquad (27)$$

where  $\rho_k(\tau)$  is the formal energy density of a given mode  $T_k$ . In conformal coordinates  $\rho_k(\tau)$  is given by

$$\rho_k(\tau) = \frac{1}{4a^2} \left( |T_k'|^2 + \omega^2 |T_k|^2 + 6\xi \left( \frac{a'^2}{a^2} |T_k|^2 + \frac{a'}{a} (T_k T_k'^* + T_k^* T_k') \right) \right), \quad (28)$$

(remember  $\omega^2 = k^2 + m^2 a^2$ ). It is interesting to stress that, for a radiation-dominated universe,  $T_k \sim a^{-1}$  and therefore

the behavior of  $\rho_k$  near the big bang is  $\rho_k \sim a^{-6}$ . This will be important in the following section.

The smeared Hamiltonian is defined then as

$$H[f] := \int d\tau \sqrt{a^2} f^2(\tau) H(\tau)$$

$$= \int \frac{d^3k}{(2\pi)^{3/2}} \int_{\Sigma} d^3x \int d\tau \sqrt{|g|} f^2(\tau) \rho_k(\tau), \quad (29)$$

where we have used (27), and where the smearing has been done with a positive definite window function  $f^2$ , along the curve of an isotropic observer. One can see that the temporal dependence term to be minimized is indeed the smeared energy density for each mode k with the appropriate factor  $\sqrt{|g|}$  coming from the four-dimensional volume element. Therefore, from now on we will work directly with the smeared energy density

$$\mathcal{E}_{k}[f] := \int d\tau \sqrt{|g|} f^{2} \rho_{k}. \tag{30}$$

As stated above, the SLE prescription is based on choosing the (Hadamard) state that minimizes the energy density over a temporal window function (30). It is important to stress the appearance of  $\sqrt{|g|}$  which in our case reduces to  $\sqrt{|g|} = a^4$ . We note that this type of factors also appear in the analysis of Ref. [46] to smooth the big bang singularity via quantized fields. In Sec. IV we will apply this prescription to build a Hadamard state around  $\tau=0$  in a radiation-dominated spacetime by taking advantage of this volume element.

In order to minimize  $\mathcal{E}_k$ , it is very convenient to express it explicitly in terms of the free parameters  $\mu_k$  and  $\lambda_k$ , namely

$$\mathcal{E}_k = (2\mu_k^2 + 1)c_{k,1} + 2\mu_k \text{Re}(\lambda_k c_{k,2}), \tag{31}$$

where we have defined

$$c_{1} \equiv c_{k,1} = \frac{1}{4} \int d\tau \sqrt{|g|} \frac{f^{2}}{a^{2}} \left( |\phi'_{k}|^{2} + \omega^{2} |\phi_{k}|^{2} + 6\xi \left( \frac{a'^{2}}{a^{2}} |\phi_{k}|^{2} + \frac{a'}{a} (\phi_{k} \phi'^{*}_{k} + \phi^{*}_{k} \phi'_{k}) \right) \right), \quad (32)$$

$$c_{2} \equiv c_{k,2} = \frac{1}{4} \int d\tau \sqrt{|g|} \frac{f^{2}}{a^{2}} \left( \phi_{k}^{\prime 2} + \omega^{2} \phi_{k}^{2} + 6\xi \left( \frac{a^{\prime 2}}{a^{2}} \phi_{k}^{2} + 2 \frac{a^{\prime}}{a} \phi_{k} \phi_{k}^{\prime} \right) \right).$$
(33)

In the above formulas it is assumed that  $c_1$  is a positive quantity, as it is trivially satisfied for  $\xi=0$ . It can be showed that if we take  $\mu_k$  to be real and positive, the minimization problem over the parameters  $\lambda_k$  and  $\mu_k$  determines a unique solution, namely

$$\mu_{k} = \sqrt{\frac{c_{1}}{2\sqrt{c_{1}^{2} - |c_{2}|^{2}}} - \frac{1}{2}};$$

$$\lambda_{k} = -e^{-i\operatorname{Arg}c_{2}}\sqrt{\frac{c_{1}}{2\sqrt{c_{1}^{2} - |c_{2}|^{2}}} + \frac{1}{2}}.$$
(34)

Notice that the minimization problem holds whenever  $\frac{|c_2|}{c_1} < 1$  is satisfied. This is usually the case if  $\phi_k$  do not contain singularities in the support of  $f^2$  [23,24]. This issue will be relevant around the big bang singularity, as we will see in the following sections.

### A. CPT-invariant states of low energy

Let us now extend the method above for the CPT-invariant states in a radiation-dominated universe. If the minimizing problem is restricted to the set of CPT-invariant states, we can parametrize the state of low energy using  $\theta_k$ . For this we choose as a fiducial solution

$$\phi_k(\tau) = \frac{1}{a} \varphi_k^{CPT}(\tau, \theta_k = 0), \tag{35}$$

with  $\varphi_k^{CPT}$  given in (17) and choosing  $\theta_k=0$ . If we impose CPT to our general solution (25), using the CPT conditions at  $\tau=0$ , [i.e.,  $\varphi_k(0)=\varphi_k^*(0)$  and  $\varphi_k'(0)=-\varphi_k'^*(0)$ ] we arrive to

$$\lambda_k = \cosh(\theta_k), \qquad \mu_k = \sinh(\theta_k).$$
 (36)

That is,  $\lambda_k$  and  $\mu_k$  are real functions. Now we proceed to minimize  $\mathcal{E}_k$  with the  $\theta_k$  parametrization

$$\mathcal{E}_k = (2\mu_k^2 + 1)c_1 + 2\mu_k \operatorname{Re}(\lambda_k c_2)$$
  
=  $c_1 \cosh(2\theta_k) + \sinh(2\theta_k) \operatorname{Re}(c_2)$ . (37)

Taking  $\partial_{\theta_{\iota}} W = 0$  we end up with

$$\tanh(2\theta_k) = -\frac{\operatorname{Re}(c_2)}{c_1}.\tag{38}$$

So the state given by

$$T_k = \cosh(\theta_k)\phi_k + \sinh(\theta_k)\phi_k^*, \tag{39}$$

with  $\phi_k$  given in (35) and

$$\theta_k = \frac{1}{2} \operatorname{arctanh} \left( -\frac{\operatorname{Re}(c_2)}{c_1} \right) \tag{40}$$

corresponds to the *CPT*-invariant state of low energy. Note again that, although a particular fiducial solution has been chosen in the minimization process, the final result (39) is

independent of this basis. However it depends, in general, on the choice of  $f^2$ .

### 1. An example: CPT-invariant vacuum of low energy at late times

Let us see how to obtain an example of an adiabatic (Hadamard) vacuum which is also CPT invariant using the prescription above. For each choice of the initial vacuum  $|0\rangle$  we have a different prediction for the particle creation spectrum at late times. Particles are defined at  $\tau \to +\infty$  as excitations of the out-vacuum  $|0_+\rangle$ . The particle production rate can be obtained by the frequency-mixing approach [5–8]. It has been reviewed in [1,3,47,48] and used extensively in the literature for decades (see, for instance, [18,49–57]). In our case, we find the following expression for the average density number of created particles in the mode  $\vec{k}$  as a function of the initial state characterized by  $\theta_k$ ,

$$\begin{split} n_k &\equiv |\beta_k|^2 = -\frac{1}{2} + \frac{e^{-\pi\kappa} \, \cosh{(2\pi\kappa)}}{4\pi} \left( e^{-2\theta_k} \kappa^{\frac{1}{2}} \bigg| \Gamma\bigg(\frac{1}{4} + i\kappa\bigg) \bigg|^2 \right. \\ &+ \left. e^{2\theta_k} \kappa^{-\frac{1}{2}} \bigg| \Gamma\bigg(\frac{3}{4} + i\kappa\bigg) \bigg|^2 \bigg), \end{split} \tag{41}$$

with  $\kappa$  given in Eq. (9). We remark that the above general expression can be reexpressed, after some manipulations, as

$$|\beta_k|^2 = \frac{1}{2}(\cosh(2\eta_k)\cosh(\Lambda_k) - 1),\tag{42}$$

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

$$2\eta_k = 2(\theta_k^{\text{late}} - \theta_k),\tag{43}$$

with

$$\theta_k^{\text{late}} = \frac{1}{4} \ln \left( \frac{\kappa \cosh(2\pi\kappa)}{2\pi^2} \middle| \Gamma\left(\frac{1}{4} + i\kappa\right) \middle|^4 \right). \tag{44}$$

The state producing the minimal amount of particles at late time is therefore given by

$$\theta_k = \theta_k^{\text{late}}.\tag{45}$$

This state can be seen as a CPT-invariant low-energy state associated to a smearing function with support at  $|\tau| \sim \infty$  since at late times (here we include the conventional renormalization subtractions),

$$\mathcal{E}_k[f] \propto \frac{1}{2} \int d\tau f^2 \omega |\beta_k|^2.$$
 (46)

It is important to remark that, in this case, this state minimizes the smeared energy density at late times independently of the choice of smearing function  $f^2$ . One can check that this state is Hadamard by evaluating the asymptotic large k expansion of  $\theta_k^{\text{late}}$ 

$$\theta_k^{\text{late}} = \frac{1}{4} \ln \left( \frac{\kappa \cosh(2\pi\kappa)}{2\pi^2} \middle| \Gamma\left(\frac{1}{4} + i\kappa\right) \middle|^4 \right) \\ \sim \frac{\gamma^2}{8k^4} + \frac{5\gamma^4}{16k^8} + \frac{61\gamma^6}{24k^{12}} + \cdots$$
 (47)

and comparing with the adiabatic expansion (24). As expected, they agree at all orders. This Hadamard and *CPT*-invariant state is equivalent to the one proposed in [32,33]. We note that, if we do not impose *CPT* invariance, the states of low energy at early and late times are just  $|0_{\pm}\rangle$ , which have zero energy [see Eqs. (18) and (20)]. Finally, we also point out that this identification of the low-energy state at late times is somewhat similar to the characterization of the Bunch-Davies vacuum as the low-energy state in de Sitter when the smearing function has support at very early times. This is also independent of the particular smearing function [25,26].

In the following section we will study states of low energy in a *CPT*-symmetric radiation-dominated universe but with  $f^2$  supported around the big bang ( $\tau = 0$ ). As we will see, in this case we find that the result strongly depends on the choice of  $f^2$ , and also on  $\xi$ . For  $\xi \neq \frac{1}{6}$  the issue is more subtle, and an extra condition has to be imposed on  $f^2$ . For  $\xi = \frac{1}{6}$  this constraint is alleviated.

## IV. CPT-INVARIANT STATES OF LOW ENERGY AT $\tau$ =0 FOR SCALARS

In the last subsection, we have obtained a CPT-invariant state by minimizing the smeared energy density at  $|\tau| \to \infty$ . However, this may seem an unnatural vacuum state since we are imposing an initial condition  $\theta_k = \theta_k^{\text{late}}$  which is determined by the late time behavior of the Universe. Therefore, a simple question arises; can we obtain a Hadamard state by minimizing the smeared energy density supported around the big bang,  $\tau = 0$ ? We will study the above question using a Gaussian smearing function

$$f_g^2(\tau) = \frac{1}{\sqrt{\pi}\epsilon} e^{-\frac{\tau^2}{\epsilon^2}}.$$
 (48)

In this section we will work with minimally coupled scalars  $\xi=0$  for simplicity. The results can be generalized to other couplings except for the very special conformal coupling  $\xi=1/6$ . We detail this last for completeness in Appendix C.

#### A. Massless case

Let us first analyze the massless case, where we can find analytic solutions. We take the fiducial solution given in (35), that in this case corresponds to the conformal solution

 $\phi_k = \frac{e^{-ik\tau}}{a\sqrt{k}}$ . We proceed to obtain the *CPT*-invariant state of low energy with the Gaussian function centered at  $\tau = 0$ , i.e.,  $f^2 = f_q^2$ . We first evaluate  $c_1$  and  $c_2$ 

$$c_1 = \frac{1}{4} \int d\tau \, f_g^2 \left( \frac{1}{2k\tau^2} + k \right) = \frac{k}{4} - \frac{1}{4k\epsilon^2}, \tag{49}$$

$$c_2 = \frac{1}{4} \int d\tau f_g^2 e^{-2ik\tau} \left( \frac{1}{2k\tau^2} + \frac{i}{\tau} \right) = -\frac{e^{-k^2 \epsilon^2}}{4k\epsilon^2}.$$
 (50)

We note that, in evaluating them, we made use of the distributional character of the integrand (see, for example, [46]). However, although this quantities give finite results,  $c_1$  changes sign depending on the value of k, and therefore the quotient  $\frac{|c_2|}{c_1}$  is not necessarily smaller than 1 for all k, thus the minimization prescription cannot be applied around  $\tau = 0$  whenever we have a divergence in the above integrals. To bypass this problem and to be able to minimize the smeared energy density for all k we require the condition

$$\lim_{\tau \to 0} \frac{f^2(\tau)}{\tau^2} < \infty. \tag{51}$$

For example, using  $f^2 = a^2 f_g^2$  one obtains the following state of low energy for all k centered at  $\tau = 0$ 

$$\theta_k^{m=0} = -\frac{1}{2} \coth^{-1} \left( e^{(\epsilon k)^2} \frac{1 + (\epsilon k)^2}{1 + 2(\epsilon k)^2} \right).$$
 (52)

The resulting state is Hadamard because the large momentum expansion of  $\theta_k$  decays faster than any power of  $k^{-n}$  [see Eq. (24) for  $\gamma=0$ ]. The divergent terms  $\tau^{-2}$  in the integrands of Eqs. (49) and (50) disappear for a conformally coupled field (see Appendix C) and the  $\sqrt{|g|}=a^4$  factor from the volume element is enough to render both integrals finite. However, because we are minimizing the state around the big bang, the resulting state depends on the test function  $f^2$ .

#### B. Massive case

Let us now study the massive case. In this context we cannot obtain an analytic expression for the state of low energy centered at  $\tau=0$ . However, we can obtain an approximated state given by the expansion of the modes  $\phi_k$  around  $\tau\sim0$ , and study its large-k behavior. We have explicitly checked that this approximated solution for  $\theta_k$  follows the adiabatic condition (24) up to a given order, that increases as we increase the order of the expansions in powers of  $\tau$ .

This analysis can be done as follows. We start from the definition of  $c_1$  and  $c_2$  given in Eqs. (32) and (33) with the fiducial modes  $\phi_k$  proposed in Eq. (35), and using

 $f^2 = a^2 f_g^2$  as the smearing function to ensure a well posed minimization problem. We then expand the modes in powers of  $\tau$  around  $\tau = 0$  (where the center of the temporal window is located), and find

$$c_1 = \frac{1}{4} \int d\tau \, a^2 f_g^2 \left( \frac{1}{k\tau^2} + 2k + \frac{3\gamma^2 \tau^2}{2k} - \frac{1}{9} \gamma^2 k \tau^4 \cdots \right), \quad (53)$$

$$c_2 = \frac{1}{4} \int d\tau \, a^2 f_g^2 \left( \frac{1}{k\tau^2} + 2k - \frac{8}{3} i k^2 \tau - 2k^3 \tau^2 + \frac{3\gamma^2 \tau^2}{2k} \cdots \right).$$
(54)

We remark that we have chosen  $f^2 = a^2 f_g^2$  for the smearing function so that the minimization problem is well posed for all k.

Finally, using Eq. (40), we take the expansions above and use them to obtain an approximated (and very involved) expression for the initial phase  $\theta_k$ . As a byproduct, we can use this result to check that the state obeys the Hadamard condition. Namely, if we expand our result for large k we recover order-by-order the expected asymptotic behavior (24). As we include more terms of the  $\tau$  expansion, more terms in the large k expansion are recovered. We have explicitly proved that for  $\mathcal{O}(\tau^{14})$  in (53) and (54) we obtain the expected large momentum expansion up to  $\mathcal{O}(k^{-16})$ .

$$\theta_k \sim \frac{\gamma^2}{8k^4} + \frac{5\gamma^4}{16k^8} + \frac{61\gamma^6}{24k^{12}} + \mathcal{O}(k^{-16}).$$
 (55)

These computations involves very long analytical expressions and have required the intensive use of the *Mathematica* software.

In summary, with the prescription of states of low energy we can obtain a CPT-invariant Hadamard state which minimizes the smeared energy density around the big bang for a smearing function  $f^2$  such as  $f^2 = a^2 f_g^2$ . We note that the asymptotic expansion (55) is not sensitive to the particular smearing function  $f^2$  that we are using; the particular choice of  $f^2$  only matters in the infrared regime. We also note that the result above (55) is independent of the scalar coupling  $\xi$ . We have explicitly checked that the large k expansion of the hyperbolic angle  $\theta_k$  obtained via the SLE prescription does not depend on  $\xi$ .

# V. CPT-INVARIANT STATES FOR FERMIONS IN A RADIATION-DOMINATED SPACETIME

Let us consider now a spin one-half field  $\Psi$  propagating in the same background metric  $\mathrm{d}s^2=a^2(\tau)(\mathrm{d}\tau^2-\mathrm{d}\vec{x}^2)$ . The field equation  $(i\underline{\gamma}^\mu\nabla_\mu-m)\Psi=0$ , where  $\underline{\gamma}^\mu=\frac{1}{a}\gamma^\mu$  and  $\gamma^\mu$  are the flat spacetime Dirac matrices, become  $^4$ 

$$\left(\gamma^0 \partial_{\tau} + \vec{\gamma} \cdot \overrightarrow{\nabla} + \frac{3a'}{2a} \gamma^0 + ima\right) \Psi = 0.$$
 (56)

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  $(D_{\vec{k}h} = B_{\vec{k}h})$  for Majorana spinors)

$$\psi(x) = \int d^3k \sum_{h} \left[ B_{\vec{k}h} u_{\vec{k}h}(x) + D_{\vec{k}h}^{\dagger} v_{\vec{k}h}(x) \right], \quad (57)$$

where the subindex h refers to the helicity, and where the umodes in the Dirac representation

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \qquad (58)$$

can be written as (we have re-expressed the results in [58,59] in terms of the conformal time, up to the above  $a^{-3/2}$  Weyl rescaling factor)

$$u_{\vec{k}h}(x) = \frac{e^{i\vec{k}\cdot\vec{x}}}{\sqrt{(2\pi)^3}} \begin{pmatrix} h_k^I(\tau)\xi_h(\vec{k}) \\ h_k^{II}(\tau)\frac{\vec{\sigma}\cdot\vec{k}}{\vec{k}}\xi_h(\vec{k}) \end{pmatrix}, \tag{59}$$

and where  $\xi_h$  is a constant and normalized two-component spinor  $\xi_h^{\dagger} \xi_{h'} = \delta_{h'h}$  that represent the helicity eigenstates.  $v_{\vec{k}h}(x)$  is obtained by the charge conjugation operation. The Dirac equation for the functions  $h_k^I(\tau)$  and  $h_k^{II}(\tau)$  is transformed into [we define again  $ma = \gamma \tau$ ]

$$h_k^{I} + ik h_k^{II} + i\gamma\tau h_k^{I} = 0,$$
 (60)

$$h_k^{II} + ik h_k^I - i\gamma\tau h_k^{II} = 0,$$
 (61)

together with the normalization condition

$$|h_k^I|^2 + |h_k^{II}|^2 = 1. (62)$$

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

$$h_k^I = C_{k,1} s_k^I(\tau) + C_{k,2} s_k^{II*}(-\tau),$$
 (63)

$$h_k^{II} = C_{k,1} s_k^{II}(\tau) + C_{k,2} s_k^{I*}(-\tau), \tag{64}$$

where

$$s_k^I = \frac{1}{\sqrt{2}} D_{-2i\kappa} \left( e^{\frac{i\pi}{4}} \sqrt{2\gamma} \tau \right),$$
  

$$s_k^{II} = e^{\frac{i\pi}{4}} \sqrt{\kappa} D_{-1-2i\kappa} \left( e^{\frac{i\pi}{4}} \sqrt{2\gamma} \tau \right),$$
 (65)

<sup>&</sup>lt;sup>4</sup>We use the conventions of [1,3].

and where again  $\kappa = \frac{k^2}{4\gamma}$ . The complex functions  $C_{k,1}$  and  $C_{k,2}$  defining the vacuum state are constrained by the normalization condition (62).<sup>5</sup>

It is important to note that the equations (60) and (61) for the time-dependent part of the field modes  $h_k^I$  and  $h_k^{II}$  remain unchanged under the transformation  $\tau \to -\tau$  and, simultaneously,  $h_k^I \to h_k^{II*}$  and  $h_k^{II} \to h_k^{I*}$ . Therefore, the vacuum will be CPT invariant if the chosen modes verify the relation

$$h_k^I(\tau) = h_k^{II*}(-\tau).$$
 (66)

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

$$h_k^I(0) = h_k^{II*}(0). (67)$$

Furthermore, we have also the normalization condition (62) at  $\tau = 0$  implying

$$|h_k^I(0)| = |h_k^{II}(0)| = \frac{1}{\sqrt{2}}.$$
 (68)

Therefore, the general  $(\tau = 0)$  solution to the conditions (67) and (68) can be written as

$$h_k^I(0) = \frac{e^{+i\Theta_k}}{\sqrt{2}}, \qquad h_k^{II}(0) = \frac{e^{-i\Theta_k}}{\sqrt{2}},$$
 (69)

where  $\Theta_k$  is an arbitrary trigonometric angle. In terms of  $\Theta_k$ , the constants  $C_{k,1}$  and  $C_{k,2}$  read

$$C_{k,1} = 2^{i\kappa} \sqrt{\pi} e^{\pi\kappa} \left( \frac{e^{i\Theta_k}}{\Gamma(\frac{1}{2} - i\kappa)} + \frac{\kappa^{\frac{1}{2}} e^{i\frac{j3\pi}{4}} e^{-i\Theta_k}}{\Gamma(1 - i\kappa)} \right), \quad (70)$$

 $C_{k,2} = C_{k,1}^*$ . Therefore, the *CPT*-invariant solution reads

$$h_k^{I;CPT} = C_{k,1} s_k^I(\tau) + C_{k,1}^* s_k^{II*}(-\tau), \tag{71}$$

$$h_k^{II;CPT} = C_{k,1} s_k^{II}(\tau) + C_{k,1}^* s_k^{I*}(-\tau), \tag{72}$$

and with  $C_{k,1}$  given above.

As for the scalar field case, it is also possible to find solutions that are not *CPT* invariant. In particular, at late times there is a preferred solution for the field modes

$$\begin{split} &\frac{e^{\pi\kappa}}{2} \left( |C_{k,1}|^2 + |C_{k2}|^2 \right) + \frac{2\sqrt{\kappa} \; \sinh \; \left( 2\pi\kappa \right)}{\sqrt{\pi}} \\ &\times \text{Re}[e^{-i\frac{\pi}{4}} C_{k,1} C_{k,2}^* \Gamma(-2i\kappa)] = 1. \end{split}$$

given by the leading-order adiabatic expansion (positive-frequency solution)

$$h_k^{I(+)}(\tau) \sim \sqrt{\frac{\omega + ma}{2\omega}} e^{-i\int_{\tau} \omega(u)du} \sim e^{-i\left(\frac{\gamma}{2}\tau^2 + \kappa \ln(2\gamma\tau^2)\right)},$$
 (73)

$$h_{k}^{II(+)}(\tau) \sim \sqrt{\frac{\omega - ma}{2\omega}} e^{-i\int_{\tau} \omega(u)du} \sim \frac{\sqrt{\kappa}}{\sqrt{\gamma}\tau} e^{-i\left(\frac{\gamma}{2}\tau^{2} + \kappa \ln(2\gamma\tau^{2})\right)},$$
(74)

that leads to

$$C_{k,1} = \sqrt{2}e^{-\frac{\pi\kappa}{2}}, \qquad C_{k,2} = 0.$$
 (75)

This solution is not *CPT* invariant since  $C_{k,1} \neq C_{k,2}^*$ . For completeness, we also give the form of the preferred solution at early times  $(\tau \to -\infty)$ . Again, the solution is fixed by imposing the late-times negative-frequency behviour

$$h_{k}^{I(-)}(\tau) \sim \sqrt{\frac{\omega + ma}{2\omega}} e^{-i\int_{\tau} \omega(u)du} \sim -\frac{\sqrt{\kappa}}{\sqrt{\gamma}\tau} e^{+i\left(\frac{\nu}{2}\tau^{2} + \kappa \ln(2\gamma(-\tau)^{2})\right)},$$
(76)

$$h_k^{II(-)}(\tau) \sim \sqrt{\frac{\omega - ma}{2\omega}} e^{-i\int_{\tau} \omega(u)du} \sim e^{+i\left(\frac{\gamma}{2}\tau^2 + \kappa \ln(2\gamma(-\tau)^2)\right)}. \tag{77}$$

From this condition we get  $C_{k,1}=0$  and  $C_{k,2}=\sqrt{2}e^{-\frac{\pi\kappa}{2}}$ .

## A. Ultraviolet regularity of the *CPT*-invariant vacuum states

As happens with the scalar field case, it becomes fundamental to study the ultraviolet regularity of the *CPT*-invariant vacuum states. For cosmological backgrounds and for spin- $\frac{1}{2}$  fields it means that for large k, the behavior of the modes  $h_k^I(\tau)$  and  $h_k^{II}(\tau)$  should be dictated by their adiabatic expansion. 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 (59) for the modes, by

$$h_{k}^{I}(\tau) \sim \sqrt{\frac{\omega + ma}{2\omega}} (1 + F_{k}^{(1)} + F_{k}^{(2)} + \cdots) e^{-i\int^{\tau} \Omega_{k}(\tau')d\tau'},$$

$$h_{k}^{II}(\tau) \sim \sqrt{\frac{\omega - ma}{2\omega}} (1 + G_{k}^{(1)} + G_{k}^{(2)} + \cdots) e^{-i\int^{\tau} \Omega_{k}(\tau')d\tau'},$$
(78)

where again  $\omega^2 = k^2 + m^2 a^2$ , and  $\Omega_k(\tau) = \omega + \omega_k^{(1)} + \omega_k^{(2)} + \cdots$ . The recursive algorithm is displayed in

<sup>&</sup>lt;sup>5</sup>In terms of  $C_{k,1}$  and  $C_{k,2}$  the normalization condition reads

[58–61]. Note that (78) provides the adiabatic condition for spin- $\frac{1}{2}$  fields: for large k the behavior of the modes  $h_k^{I,II}$  should follow this expansion at all orders. This is the analogous adiabatic condition for scalar fields defined in Eqs. (21) and (22). Again, in order to find the desired asymptotic behavior for the trigonometric phase  $\Theta_k$  it is enough to evaluate the adiabatic expansion at  $\tau = 0$ . At this limit we obtain a well-defined large k asymptotic expansion

$$h_k^I(0) \sim \frac{1}{\sqrt{2}} \left( 1 - i \frac{\gamma}{4k^2} - \frac{\gamma^2}{32k^4} - i \frac{21\gamma^3}{128k^6} - \frac{85\gamma^4}{2048k^8} + \cdots \right),$$
(79)

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

$$\Theta_k \sim -\left(\frac{\gamma}{4k^2} + \frac{\gamma^3}{6k^6} + \frac{4\gamma^5}{5k^{10}} + \cdots\right).$$
(80)

This determines the appropriated rate for the decaying of  $\Theta_k$  when  $k \to \infty$  to have a *CPT*-invariant vacuum of infinite adiabatic order. A vacuum that satisfies the asymptotic condition above is an adiabatic vacuum state and hence ultraviolet regular or, equivalently, Hadamard.

### VI. STATES OF LOW ENERGY FOR FERMIONS

In this section, we extend the prescription to build states of low energy to spin- $\frac{1}{2}$  fields. We proceed here in analogy with the scalar field case. First, we consider a generic scale factor a, and then, we particularize the method for a radiation-dominated universe with CPT symmetry. Although we do not present here a formal proof that the states of low energy in a general FLRW are Hadamard, we check that the resulting CPT-invariant states of low energy considered here satisfy (80), and therefore are Hadamard/adiabatic states.

The starting point is again to fix a basis of solutions for the modes, namely,  $\{h_k^I, h_k^{II}\}$ . Any other set of modes can be parametrized in the form

$$t_k^I = \lambda_k h_k^I + \mu_k h_k^{II*}, t_k^{II} = \lambda_k h_k^{II} - \mu_k h_k^{I*}.$$
 (81)

From the normalization condition,  $\mu_k$  and  $\lambda_k$  should obey

$$|\lambda_k|^2 + |\mu_k|^2 = 1. (82)$$

The smeared energy density over a temporal window function  $f^2$  is given by (see Sec. III)

$$\mathcal{E}_k[f] \coloneqq \int \mathrm{d}\tau \sqrt{|g|} f^2 \rho_k, \tag{83}$$

where  $\sqrt{|g|} = a^4$ , and where the energy density  $\rho_k$  associated with the set of modes  $\{t_k^I, t_k^{II}\}$  reads

$$\rho_k(\tau) = \frac{2i}{a^4} \left( t_k^I \frac{\partial t_k^{I*}}{\partial \tau} + t_k^{II} \frac{\partial t_k^{II*}}{\partial \tau} \right). \tag{84}$$

We can choose  $\mu_k$  or  $\lambda_k$  to be real since  $\{e^{i\alpha}t_k^I,e^{i\alpha}t_k^{II}\}$  is also a solution of the system of equations. For future convenience, and following similar arguments than in the scalar case [23], we assume that  $\lambda_k$  is real and positive  $\lambda_k > 0$ . The smeared energy density can be written, as in the scalar case, in terms of two constants  $c_1 \equiv c_{k,1}$  and  $c_2 \equiv c_{k,2}$ , namely

$$\mathcal{E}_{k} = (1 - 2|\mu_{k}|^{2})c_{1} + 2|\mu_{k}|\operatorname{Re}(\mu_{k}^{*}c_{2})$$

$$\equiv (1 - 2|\mu_{k}|^{2})c_{1} + 2|\mu_{k}|\sqrt{1 - |\mu_{k}|^{2}}|c_{2}|$$

$$\times \cos(\operatorname{Arg}c_{2} - \operatorname{Arg}\mu_{k}), \tag{85}$$

where

$$c_1 = 2i \int d\tau f^2 \left( h_k^I \frac{\partial h_k^{I*}}{\partial \tau} + h_k^{II} \frac{\partial h_k^{II*}}{\partial \tau} \right), \tag{86}$$

$$c_2 = 2i \int d\tau f^2 \left( h_k^I \frac{\partial h_k^{II}}{\partial \tau} - h_k^{II} \frac{\partial h_k^I}{\partial \tau} \right). \tag{87}$$

From now on, we assume that the fiducial modes are such that  $c_1$  is a real, negative quantity. Note that this is the case for the standard mode solutions in Minkowski spacetime.

We find that  $\mathcal{E}_k$  is trivially minimized with respect to  $\text{Arg}\mu_k$  for  $\text{Arg}\mu_k = \text{Arg}c_2 + \pi$ . Therefore, the task now is to minimize

$$\mathcal{E}_k = (1 - 2|\mu_k|^2)c_1 - 2|\mu_k|\sqrt{1 - |\mu_k|^2|c_2|}.$$
 (88)

with respect to  $|\mu_k|$ . Taking  $\partial_{|\mu_k|}\mathcal{E}_k = 0$  we obtain four possible solutions. Only two of them are real and positive for  $\lambda_k$ ,

$$\lambda_{k} = \sqrt{\frac{1}{2} \mp \frac{c_{1}}{2\sqrt{c_{1}^{2} + |c_{2}|^{2}}}}, \quad |\mu_{k}| = \sqrt{\frac{1}{2} \pm \frac{c_{1}}{2\sqrt{c_{1}^{2} + |c_{2}|^{2}}}}.$$
(89)

From the above solution, one can easily check that the one that minimizes the smeared energy density  $\mathcal{E}_k$  is

$$\lambda_{k} = \sqrt{\frac{1}{2} - \frac{c_{1}}{2\sqrt{c_{1}^{2} + |c_{2}|^{2}}}}, \quad |\mu_{k}| = \sqrt{\frac{1}{2} + \frac{c_{1}}{2\sqrt{c_{1}^{2} + |c_{2}|^{2}}}}.$$
(90)

and the minimum value of the smeared energy density  $\mathcal{E}_k$  is  $\mathcal{E}_k = -\sqrt{c_1^2 + |c_2|^2}$ .

As a final remark, we note that, in contrast to the analysis for scalar fields, it is here possible to find a maximal value for  $\mathcal{E}_k$ . If we take now  $\mathrm{Arg}\mu_k = \mathrm{Arg}c_2$  in (85) and then compute  $\partial_{|\mu_k|}\mathcal{E}_k = 0$  we find again (89). Now, inserting them into  $\mathcal{E}_k$  again, we find that it takes its maximum value for the opposite solution (+ for  $\lambda_k$  and – for  $\mu_k$ ), that gives  $\mathcal{E}_k = \sqrt{c_1^2 + |c_2|^2}$ . This renders a nonphysical state.

### A. CPT-invariant states of low energy

We can repeat the above analysis imposing *CPT* invariance. In this case, we can choose a convenient fiducial solution given by

$$h_k^I = h_k^{I;CPT}(\tau,\Theta_k = 0), \qquad h_k^{II} = h_k^{II;CPT}(\tau,\Theta_k = 0), \eqno(91)$$

with  $h_k^{I;CPT}$  and  $h_k^{II;CPT}$  given in Eqs. (71) and (72) for  $\Theta_k = 0$ . Therefore, the modes  $t_k^{I,II}$  read

$$t_k^I = \cos(\Theta_k) h_k^I + i \sin(\Theta_k) h_k^{II*}, \tag{92}$$

$$t_k^{II} = \cos(\Theta_k) h_k^{II} - i \sin(\Theta_k) h_k^{I*}. \tag{93}$$

Therefore,

$$\mathcal{E}_{k} = \cos(2\Theta_{k})c_{1} + \sin(2\Theta_{k})\operatorname{Im}(c_{2}), \tag{94}$$

and the minimization equation  $\partial_{\Theta_k} \mathcal{E}_k = 0$  becomes

$$-\sin(2\Theta_{k})c_{1} + \cos(2\Theta_{k})\operatorname{Im}(c_{2}) = 0, \tag{95}$$

therefore

$$\tan(2\Theta_k) = \frac{\operatorname{Im}(c_2)}{c_1}.$$
(96)

The solution for the angle then reads

$$\Theta_k = \frac{1}{2}\arctan\left(\frac{\operatorname{Im}(c_2)}{c_1}\right) + \frac{n\pi}{2}.\tag{97}$$

For n even we have a state of low energy, while for n odd we obtain a state of high energy, which has to be discarded. Up to irrelevant global phases (97) characterize a single low-energy state, CPT invariant, depending only on the smearing function  $f^2$ .

## 1. An example: CPT-invariant vacuum of low energy at late times

We can also compute the particle creation for an initial vacuum state characterized by  $\Theta_k$ . The vacuum  $|0\rangle$  is

perceived at late times as a collection of particles, defined as quantum excitations of the adiabatic out-vacuum  $|0_+\rangle$ . We find<sup>6</sup>

$$n_{k,h} = |\beta_{k,h}|^2 = \frac{1}{2} - \frac{e^{-\pi\kappa} \sinh(2\pi\kappa)\sqrt{\kappa}}{4\pi} \left( e^{-2i\Theta_k} e^{i\frac{\pi}{4}} \right) \times \Gamma(i\kappa) \Gamma\left(\frac{1}{2} - i\kappa\right) + e^{2i\Theta_k} e^{-i\frac{\pi}{4}} \Gamma(-i\kappa) \Gamma\left(\frac{1}{2} + i\kappa\right),$$

$$(98)$$

where  $\kappa = \frac{k^2}{4\gamma}$ . As for the case of scalar fields, and in agreement with the results of [32,33], the above expression can be rewritten as

$$|\beta_{k,h}|^2 = \frac{1}{2} (1 - \cos(2\eta_k)\cos(\Lambda_k)), \tag{99}$$

where  $\cos(\Lambda_k) = \sqrt{1 - e^{-4\pi\kappa}}$  and

$$2\eta_k = 2(\Theta_k^{\text{late}} - \Theta_k) \tag{100}$$

with

$$\Theta_k^{\text{late}} = \frac{\pi}{8} + \frac{1}{2} \operatorname{Arg} \left[ \Gamma \left( \frac{1}{2} - i\kappa \right) \Gamma(i\kappa) \right]. \tag{101}$$

Arg(z) refers to the argument of z. As for the scalar case this state is the low-energy state associated to a smearing function  $f^2$  with support at  $|\tau| \sim \infty$ . It minimizes the smeared energy density  $\mathcal{E}_k$  at late times independently of  $f^2$ , and as expected, it is Hadamard. One can easily check this statement by evaluating the asymptotic large k expansion of  $\Theta_k^{\text{late}}$  and confirming that it agrees with the adiabatic expansion (80) at any order. This Hadamard and CPT-invariant state turns out to be equivalent to the one proposed in [32,33].

### VII. CPT-INVARIANT STATES OF LOW ENERGY AT $\tau = 0$ FOR FERMIONS

In this section, we study how to obtain a vacuum state with the SLE prescription using a smearing function with support around  $\tau=0$ . For this purposes, we use again the Gaussian function  $f_g^2$  defined in Eq. (48). It is interesting to note that the energy density decays as  $a^{-4}$  for  $\tau \to 0$ , this is a consequence that massless fermions enjoys conformal invariance. A similar behavior was found for massive scalars with  $\xi=1/6$ . It means that the term  $\sqrt{|g|}=a^4$  from the volume element makes the integral of the smeared energy density perfectly finite (see also the conformally coupled scalar case Appendix C). As in the scalar case, we study both the massless and the massive cases.

<sup>&</sup>lt;sup>6</sup>Note that the spectrum is indeed independent of the helicity h.

#### A. Massless case

In this case the fiducial solution (91) correspond to the conformal modes  $h_k^I = \frac{1}{\sqrt{2}} e^{-ik\tau}$  and  $h_k^{II} = \frac{1}{\sqrt{2}} e^{-ik\tau}$ . For the smearing function we choose  $f^2 = f_g^2$ . If we compute the integrals (86) and (87) we obtain

$$c_1 = -\frac{2k}{2} \int d\tau f_g^2 = -\frac{k}{2}, \qquad c_2 = 0.$$
 (102)

Therefore, from (96) we get the state of low energy

$$\Theta_k^{m=0} = 0. \tag{103}$$

This result is independent of the smearing function that we use. This is because  $\Theta_k = 0$  minimizes the energy density

$$\rho_k(\tau) = -\frac{2k}{a^4}\cos 2\Theta_k,\tag{104}$$

for all  $\tau$ . We note that  $\Theta_k^{m=0} = 0$  satisfies the adiabatic condition (80) at all orders (remember that m=0 implies  $\gamma = 0$ ). This is the same situation as for the conformally coupled massless scalar field (see Appendix C).

#### B. Massive case

Let us study now the massive case. We follow the same procedure as in the scalar case to obtain an approximated state of low energy by expanding the modes  $h_k^I$  and  $h_k^{II}$  around  $\tau \sim 0$ . We explicitly compute its large-k behavior and check that it satisfies the adiabatic condition (80) up to a given order, that increases as we improve the orders of the expansion in  $\tau$ .

The process is as follows. First, we expand the modes in  $c_1$  and  $c_2$  in powers of  $\tau$  around  $\tau = 0$ . We use the fiducial solution given in (91) and the Gaussian smearing function  $f^2 = f_q^2$ . The first orders of the expansion read

$$c_{1} = 2i \int d\tau f_{g}^{2} \left( h_{k}^{I} \frac{\partial h_{k}^{I*}}{\partial \tau} + h_{k}^{II} \frac{\partial h_{k}^{II*}}{\partial \tau} \right)$$
$$= \int d\tau f_{g}^{2} \left( -4\sqrt{\gamma \kappa} - \frac{2}{3} \gamma^{2} \sqrt{\gamma \kappa} \tau^{4} + \cdots \right), \quad (105)$$

$$c_2 = 2i \int d\tau f_g^2 \left( h_k^I \frac{\partial h_k^{II}}{\partial \tau} - h_k^{II} \frac{\partial h_k^I}{\partial \tau} \right)$$
$$= i \int d\tau f_g^2 \left( 4\sqrt{\gamma^3 \kappa \tau^2} - \frac{16}{3} \gamma^{5/2} \kappa^{3/2} \tau^4 + \cdots \right). \quad (106)$$

Then, we insert this integrals in (96) and obtain an approximated solution for the initial phase  $\Theta_k$ . We have computed these expressions up to  $O(\tau^{14})$ . Finally, we compute the large-k expansion of  $\Theta_k$ , obtaining

$$\begin{split} \Theta_k &= \frac{1}{2}\arctan\bigg(\frac{\mathrm{Im}(c_2)}{c_1}\bigg) \\ &\sim -\bigg(\frac{\gamma}{4k^2} + \frac{\gamma^3}{6k^6} + \frac{4\gamma^5}{5k^{10}} + O(k^{-14})\bigg), \end{split} \tag{107}$$

which fully agrees with the asymptotic expansion (80). As for the scalar case, these computations have also required the assistance of the *Mathematica* software. The more orders we consider in the  $\tau$  expansion the better is the coincidence with the adiabatic expansion. We have checked that for an expansion at order  $O(\tau^{14})$  we recover the adiabatic expansion to  $O(k^{-14})$ . This gives strong evidence that the prescription for the lowenergy states proposed here is consistent with the Hadamard/adiabatic condition for more general FLRW spacetimes.

### VIII. CONCLUSIONS AND FINAL COMMENTS

The concept of states of low energy appears to be a very useful prescription to single out a preferred state in FLRW cosmologies. One of the major virtues of the construction is that it guarantees the Hadamard condition for the selected vacuum state. The crucial point is the use of a smearing window in the time variable. The prescription was established in [23] for scalar fields. In this paper, we have extended the construction to spin- $\frac{1}{2}$  fields and applied it to the special case of a radiation-dominated universe. In this context a further symmetry condition can also be imposed. In conformal time  $\tau$ , the expansion factor for a radiationdominated universe is a linear function, which allows analytic continuation to negative values of the conformal time [32,33]. CPT symmetry at the big bang can be naturally required as an extra condition to impose on the low-energy states. A possible choice for the smearing function is to select it with support at  $|\tau| \to \infty$ . In this case, the resulting state is independent of the particular choice of the smearing function, since its support lies in an adiabatic region of the spacetime. However, this involves giving initial conditions by knowing the late-times behavior of the expanding universe. There is a more natural option that consists of choosing the window function around the big bang itself. Performing a careful analysis for the minimization of the smeared energy density, including the appropriate factors coming from the volume element, we have checked that this choice is fully consistent with physical requirements at the ultraviolet, namely, the adiabatic/Hadamard condition. Therefore, these states are then suitable candidates as effective big bang vacua from the quantum field theory viewpoint. The infrared behavior of these states is then sensitive to the smearing function chosen. This ambiguity could be naturally interpreted, at least heuristically, as encoding quantum gravity effects of a more fundamental theory.

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#### APPENDIX A: THE ADIABATIC EXPANSION

In this appendix we briefly review the adiabatic method for scalar fields. We follow [3], but we translate the notation and expression to work in conformal time. Consider a massive scalar field  $\phi$  propagating in a flat FLRW spacetime  $ds^2 = a^2(d\tau^2 - d\vec{x}^2)$ . As in the main text, we expand the quantized field in Fourier modes (3). From the Klein-Gordon equation, we can easily obtain the equation for the field modes

$$\phi_k'' + 2\frac{a'}{a}\phi_k' + \left(k^2 + a^2m^2 + 6\xi\frac{a''}{a}\right)\phi_k = 0.$$
 (A1)

As in the main text, it is convenient to work with the rescaled Weyl field  $\varphi \equiv a\phi$  and the rescaled modes  $\varphi_k(\tau) \equiv a(\tau)\phi_k(\tau)$ . And then, the mode equation results in

$$\varphi_k'' + \left(\omega^2 + (6\xi - 1)\frac{a''}{a}\right)\varphi_k = 0.$$
 (A2)

An unavoidable requirement that any suitable vacuum state must meet is that is has to be ultraviolet regular. It can be easily understood by requiring that the short distance behavior of the Feynman Green's function  $iG_F(x,x')$  and related quantities must be similar to that found in Minkowski space. This becomes necessary to guarantee the existence of finite vacuum expectation values after renormalization. For quantum states in FLRW spacetimes this criterion can be implemented by the adiabatic condition (see Sec. 3.1) [3]. In terms of field modes this means that, for large k, the field modes must behave as

$$\varphi_k(\tau) \sim \frac{1}{\sqrt{\Omega_k(\tau)}} e^{-i\int^{\tau} \Omega_k(\tau')d\tau'},$$
(A3)

where the function  $\Omega_k(\tau)$  admits an asymptotic adiabatic expansion in terms of the derivatives of  $a(\tau)$ 

$$\Omega_k = \omega_k^{(0)} + \omega_k^{(1)} + \omega_k^{(2)} + \omega_k^{(3)} + \omega_k^{(4)} + \cdots$$
 (A4)

The coefficient  $\omega_k^{(n)}$  depends on derivatives of  $a(\tau)$  up to and including the order n. The leading order of the expansion is  $\omega_k^{(0)} \equiv \omega = \sqrt{k^2 + a^2 m^2}$  and the next-to-leading orders are obtained, by systematic iteration, from the relation

$$\Omega_k^2 = \omega^2 + (6\xi - 1)\frac{a''}{a} + \frac{3}{4}\frac{(\Omega_k')^2}{\Omega_k^2} - \frac{1}{2}\frac{\Omega_k''}{\Omega_k},$$
 (A5)

derived from the mode equation (A2). Inserting the adiabatic expansion in the equation above, and grouping terms with the same adiabatic order, it is possible to obtain the *n*th coefficient from the lower ones once the leading term is defined. It can be proved that the terms with odd adiabatic order are zero, i.e.,  $\omega_k^{(2n+1)} = 0$ . The first next-to-leading-order terms can be found, for example, in [3]. From the adiabatic expansion of the field modes, one can easily build the adiabatic expansion of the Feynman Green's function at coincidence

$$iG_F(x,x)_{Ad} = \int \frac{\mathrm{d}^3 k}{2(2\pi)^3 a^2} \sum_{n=0}^{\infty} (\Omega_k^{-1})^{(n)}.$$
 (A6)

In Refs. [43–45] it was checked that the first orders of this expansion, when expressed at separated points, coincide with the deWitt-Schwinger expansion of the two point function in four spacetime dimensions. As stated above, in FLRW universes the Hadamard condition translates to require for the field modes  $\varphi_k$  a large momentum behavior dictated by (21) at all orders. A state that satisfies this requirement is called a state of infinite adiabatic order (or just an adiabatic state). We demand the physical admissible states to be adiabatic states (of infinite adiabatic order) and hence equivalent to be Hadamard states.

## APPENDIX B: LARGE k EXPANSION AT A FIXED TIME

In this appendix, we give, for a radiation-dominated spacetime, the large-k expansion of the CPT-invariant two-point function in momentum space at a fixed time and for an arbitrary  $\theta_k$ , and compare it with its adiabatic expansion. Our goal here is to show that only if  $\theta_k$  satisfies the asymptotic condition given in (24), the field modes are compatible with the adiabatic condition, and therefore, the vacuum state is Hadamard.

From the CPT-invariant solution (17), and for an arbitrary value of  $\theta_k$ , we can compute the large k expansion of the square of the CPT-invariant modes at a fixed time  $\tau$ 

$$\begin{split} |\varphi_k^{CPT}|^2 &\sim \cosh(2\theta_k) \left(\frac{1}{k} - \frac{\gamma^2 \tau^2}{2k^3} + \frac{3\gamma^4 \tau^4}{8k^5} + \frac{\gamma^2}{4k^5} - \frac{\gamma^2 \cos(2k\tau)}{4k^5} + \mathcal{O}(k^{-6})\right) \\ &+ \sinh(2\theta_k) \left(-\frac{\gamma^2}{4k^5} + \frac{\cos(2k\tau)}{k} - \frac{\gamma^2 \tau^3 \sin(2k\tau)}{3k^2} - \frac{\gamma^4 \tau^6 \cos(2k\tau)}{18k^3} - \frac{\gamma^2 \tau^2 \cos(2k\tau)}{2k^3} + \mathcal{O}\left(\frac{\sin(2k\tau)}{k^4}\right)\right), \end{split} \tag{B1}$$

and compare this result with the asymptotic behavior dictated by the adiabatic expansion, namely

$$|\varphi_k|_{\mathrm{Ad}}^2 \sim \frac{1}{k} - \frac{\gamma^2 \tau^2}{2k^3} + \frac{\gamma^2}{4k^5} + \frac{3\gamma^4 \tau^4}{8k^5} + \mathcal{O}(k^{-6}).$$
 (B2)

If we now impose for the initial hyperbolic phase the asymptotic behavior given in (24), the oscillatory behavior in (B1) cancels out and we recover, order by order, the large k behavior required by the adiabatic expansion (B2) at any time  $\tau$ . Therefore, any  $\theta_k$  obeying (24) gives an adiabatic (Hadamard) CPT-invariant vacua.

## APPENDIX C: STATES OF LOW ENERGY FOR CONFORMALLY COUPLED SCALARS

For conformally coupled scalar fields  $\xi=1/6$  it is convenient to write the energy density  $\rho_k$  for the mode  $T_k$  in terms of the Weyl transformed mode  $\mathcal{T}_k$  (i.e.,  $\mathcal{T}_k=aT_k$ ) because it takes the simple form

$$\rho_k(\tau) = \frac{1}{4a^4} (|\mathcal{T}_k'|^2 + \omega^2 |\mathcal{T}_k|^2), \tag{C1}$$

with  $\omega^2 = k^2 + m^2 a^2$ . Note that all the divergent behavior at  $\tau \to 0$  is encapsulated in the term  $a^{-4}$ . The minimization prescription follows as in Sec. III. The smeared energy density to be minimized around the big bang takes the simple form

$$\mathcal{E}_{k}[f] \coloneqq \int d\tau \sqrt{|g|} f^{2} \rho_{k} = \frac{1}{4} \int d\tau f^{2} (|\mathcal{T}'_{k}|^{2} + \omega^{2} |\mathcal{T}_{k}|^{2}), \tag{C2}$$

As we see in the above equation, conformally coupled scalar fields are less sensitive to the big bang singularity. The same behavior was found for spin- $\frac{1}{2}$  fields. We try to define a Hadamard state around  $\tau=0$  as we did in the above sections. The integrals which are left to compute are

$$c_1 \equiv c_{k,1} = \frac{1}{4} \int d\tau f^2(|\varphi_k'|^2 + \omega^2 |\varphi_k|^2),$$
 (C3)

$$c_2 \equiv c_{k,2} = \frac{1}{4} \int {\rm d}\tau \, f^2 (\varphi_k'^2 + \omega^2 \varphi_k^2). \eqno(C4)$$

where  $\{\varphi_k, \varphi_k^*\}$  are a pair of fiducial solutions of the Klein-Gordon equation. Any general mode is given by

$$\mathcal{T}_k(\tau) = \lambda_k \varphi_k(\tau) + \mu_k \varphi_k^*(\tau). \tag{C5}$$

For the massless case we can take the conformal vacuum  $\varphi_k(\tau) = \frac{e^{-ik\tau}}{\sqrt{k}}$  as the fiducial mode and obtain that  $c_2 = 0$  irrespectively of  $f^2$ . Therefore, using (34), we find  $\mu_k = 0$  and  $\lambda_k = 1$ , and we conclude that the conformal vacuum minimizes the energy density at any  $\tau$ . Therefore, this state is independent of the test function. One can also see this by computing the energy density for any CPT-invariant state parametrized by  $\theta_k$ . In this case one obtains  $\rho_k = \frac{k}{4a^4} \cosh(2\theta_k)$ . This quantity is minimized for  $\theta_k = 0$ , at any  $\tau$ .

For the massive case we can take Eq. (35) as the fiducial solution and build a state that minimizes the smeared energy density with  $f^2$  with support at  $\tau = 0$ . As for spin- $\frac{1}{2}$  fields, we do not need extra requirements for the smearing function. The resulting Hadamard state is also dependent on  $f^2$ .

### APPENDIX D: STATES OF LOW ENERGY IN MINKOWSKI FOR FERMIONS

Let us consider the minimization prescription described in Sec. VI for fermions in a Minkowski spacetime. A general mode  $\{t_k^I, t_k^{II}\}$  solution can be described by the following linear combination of fiducial solutions:

$$t_{k}^{I} = \lambda_{k} h_{k}^{I} + \mu_{k} h_{k}^{II*},$$
  

$$t_{k}^{II} = \lambda_{k} h_{k}^{II} - \mu_{k} h_{k}^{I*}.$$
 (D1)

We take the well-known postive and negative frequency solutions of Minkowski spacetime as the fiducial solutions.

$$h_k^I = \sqrt{\frac{\omega + m}{2\omega}} e^{-i\omega\tau}, \qquad h_k^{II} = \sqrt{\frac{\omega - m}{2\omega}} e^{-i\omega\tau}.$$
 (D2)

By minimizing the smeared energy density for a generic mode we obtain that only  $\lambda_k=1$  and  $\mu_k=0$  renders a minimum value for the smeared energy density  $\mathcal{E}_k$ , irrespective of the test function used. This solution as one can see from (D1) corresponds to the standard positive frequency mode in Minkowski spacetime. The calculation proceeds as follows. First one has to compute the coeficients  $c_1$  and  $c_2$  given in (86) and (87). By substituting with (D2) one arrives at

$$c_1 = -2\omega \int d\tau f^2 \qquad c_2 = 0.$$
 (D3)

Therefore, the two possible solutions that appears when minimizing  $\mathcal{E}_k$  [see Eq. (88)] are given by

$$\lambda_k = \sqrt{\frac{1}{2} \mp \frac{-\omega}{2\omega}}, \qquad |\mu_k| = \sqrt{\frac{1}{2} \pm \frac{-\omega}{2\omega}}.$$
 (D4)

From the above solutions, the one that minimizes the smeared energy density is given by

$$\lambda_k = 1, \qquad \mu_k = 0, \tag{D5}$$

which corresponds to the standard positive-frequency solution (D2). If we compute the energy density we obtain

$$\rho_k = 2i \left( h_k^I \frac{\partial h_k^{I*}}{\partial \tau} + h_k^{II} \frac{\partial h_k^{II*}}{\partial \tau} \right) = -2\omega.$$
 (D6)

In other words, this choice gives the well-know state of low energy in Minkowski spacetime. This is the state of lowest energy for fermions. As a curiosity, the other possible solution that we obtain when finding the extrema of  $\mathcal{E}_k$  corresponds to  $\lambda_k = 0$ ,  $\mu_k = 1$ . That correspond to negative frequencies, which renders a nonphysical state. In this case, the vacuum energy density results in  $\rho_k = +2\omega$ , which corresponds to its maximal value.

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