Not all adiabatic vacua are physical states

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Adiabatic vacua are known to be Hadamard states. We show, however, that the energy-momentum tensor of a linear Klein-Gordon field on Robertson-Walker spaces develops a generic singularity on the initial hypersurface if the adiabatic vacuum is of order less than 4. Therefore, adiabatic vacua are physically reasonable only if their order is at least 4. A certain nonlocal large momentum expansion of the mode functions has recently been suggested to yield the subtraction terms needed to remove the ultraviolet divergences in the energy-momentum tensor. We find that this scheme fails to reproduce the trace anomaly and therefore is not equivalent to adiabatic regularization. [S0556-2821(99)04604-4]

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I. INTRODUCTION

The semiclassical theory of quantized fields propagating on a curved (globally hyperbolic) spacetime does not provide a principle of how to choose a vacuum state. In the absence of isometries the vacuum state cannot be associated with such symmetries of the underlying spacetime. Instead, physically reasonable states (of linear fields) are required to be Hadamard states; i.e., the corresponding two-point functions have to possess the Hadamard singularity structure in order to allow for standard renormalization [1,2].

The proper choice of an initial state is not only essential for a consistent formulation of quantum field theory on curved spacetimes. In the context of concrete applications the dependence of the physical effects on the initial state becomes an equally significant aspect. This question arises, for example, in inflationary cosmology where particle creation and back reaction due to quantum fields play an important role. Interest in the consideration of these effects has recently been intensified in connection with the theory of reheating after inflation [3] (a discussion of Hadamard states in this case is appropriate because the quantum fluctuations satisfy linear equations of motion in the mean field approximation [4]).

The concept of adiabatic vacua was introduced by Parker in order to account for particle creation in an expanding universe [5]. The physical motivation behind the adiabatic particle picture is that it most closely resembles the particle concept of a static universe during an expansion. The notion of adiabatic vacuum states was put on a solid mathematical basis by Lüders and Roberts [6] who also suggested that adiabatic vacua and Hadamard states define the same class of physical states on the cosmologically relevant Robertson-Walker spaces. Indeed, both concepts are intimately related. Najmi and Ottewill [7] derived the leading asymptotic momentum behavior of a second-order adiabatic vacuum as a *necessary* condition for Hadamard states on a quasi-Euclidean space ($\kappa=0$). Using Fourier analysis, they compared the symmetric two-point function and its first derivative with the Hadamard series on the initial hypersurface. A related analysis can be found in [8]. Recently, Junker has succeeded in showing that in fact all adiabatic vacua are Hadamard states [9]. His proof exploits methods of the theory of pseudodifferential operators and wavefront sets on manifolds.

The expectation value of the energy-momentum tensor rather than the two-point function is the essential physical quantity to be considered because it determines the back reaction effect on the gravitational field via the semiclassical Einstein equations

$$G_{\mu\nu}=-8\pi G\langle T_{\mu\nu}\rangle. \tag{1.1}$$

The energy-momentum tensor involves second derivatives of the two-point function. However, the method of [7] could not be generalized to the case of a second derivative. So when considering the energy-momentum tensor one might expect to find further constraints on the physically admissible states.

It has recently been shown [10] that the expectation value of the energy-momentum tensor in a conformal-like initial state [see Eq. (3.4) below] develops an initial singularity, i.e., the limit $\eta\to\eta_0$ does not exist (η is the conformal time parameter). Since an initially singular energy-momentum tensor does not satisfy Wald's axioms [1], such states should not be considered physically reasonable.

In the present paper we are concerned with the question of whether adiabatic states of linear Klein-Gordon fields on Robertson-Walker spaces (with arbitrary spatial curvature) can lead to initial singularities as well. We show that the order of an adiabatic vacuum must not be less than 4 for the energy-momentum tensor to be finite on the initial hypersurface. As a primary new result, we find that even though *all* adiabatic vacua are Hadamard states [9], they are physically admissable only if their order is 4 at least.

In line with our result, the adiabatic particle picture developed in [11] shows that for adiabatic vacua of order 4 or higher the energy-momentum tensor splits naturally into a local part containing all the ultraviolet divergences and a finite, nonlocal piece that can be viewed as being due to particle production.

In the derivation of the condition on the adiabatic order, we employ a nonlocal large momentum expansion of the conformal-like mode functions (see the Appendix) that has

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similarly been used in [10,13,14]. We show that the subtraction of the leading terms of this expansion as suggested in [12] is not equivalent to adiabatic regularization on Robertson-Walker spaces because it fails to reproduce the trace anomaly. Besides, our proof reveals that the construction of states suggested in [10] effectively determines a fourth-order adiabatic vacuum.

The paper is organized as follows. In Sec. II we review the basic elements of scalar field quantization in Robertson-Walker spaces including adiabatic regularization as far as necessary and give the definition of adiabatic states following [6]. In Sec. III we show that the adiabatic order of the state must not be less than 4 to result in an initially well-behaved energy-momentum tensor. We conclude the paper with a brief summary and a technical appendix. Our metric convention is $g_{\mu\nu}=\mathrm{diag}(1,-1,-1,-1)$, and we use units such that $\hbar=c=1$.

II. QUANTUM FIELDS ON ROBERTSON-WALKER SPACES

The Robertson-Walker metric is given by

$$ds^2=a^2(\eta)[d\eta^2-h_{ik}dx^i dx^k], \tag{2.1}$$

where h_{ik} denotes the metric of a three-space of constant curvature $\kappa=-1,0,+1$ for an open, flat, and closed universe, respectively.

The free scalar field satisfies the Klein-Gordon equation

$$(\Box+m^2+\xi R)\varphi(x)=0. \tag{2.2}$$

The symmetry of the Robertson-Walker metric allows for separating variables in Eq. (2.2), and the scalar field can be decomposed as

$$\varphi(x)=\frac{1}{a(\eta)}\int d\tilde{\mu}(\mathbf{k})[f_k(\eta)\Phi_k(\mathbf{x})a_k+f_k^*(\eta)\Phi_k^*(\mathbf{x})a_k^\dagger], \tag{2.3}$$

where the creation and annihilation operators $a_k^\dagger, a_k$ obey the usual commutation relations. The $\Phi_k(\mathbf{x})$ are the eigenfunctions of the Laplace-Beltrami operator on the three-space of constant curvature,

$$\Delta^{(3)}\Phi_k(\mathbf{x})=-(k^2-\kappa)\Phi_k(\mathbf{x}), \tag{2.4}$$

and $d\tilde{\mu}(\mathbf{k})$ is the measure of the corresponding set of quantum numbers (for details, see [15]). The time-dependent part of the mode function satisfies the oscillatory equation

$$f_k''(\eta)+\Omega_k^2(\eta)f_k(\eta)=0. \tag{2.5}$$

The frequency $\Omega_k(\eta)$ is given by

$$\Omega_k^2(\eta)=k^2+a^2(m^2-\Delta\xi R)\overset{\mathrm{def}}{=}\omega_k^2-q(\eta)\overset{\mathrm{def}}{=}k^2+M^2(\eta), \tag{2.6}$$

with $\omega_k^2=k^2+m^2a^2$ and $\Delta\xi=1/6-\xi$. A complete set of mode solutions to Eq. (2.5) is specified by imposing initial conditions $f_k(\eta_0)$, $f_k'(\eta_0)$ on a Cauchy surface $\eta=\eta_0$. This corresponds to the choice of a homogeneous vacuum state.

We now give the definition of adiabatic vacua following [6]. Substituting the WKB ansatz

$$\tilde{f}_k(\eta)=\frac{1}{\sqrt{2W_k(\eta)}}\exp\left[-i\int_{\eta_0}^{\eta}d\eta' W_k(\eta')\right] \tag{2.7}$$

into Eq. (2.5) leads to the following equation for the frequency W_k:

$$W_k^2=\Omega_k^2-\frac{1}{2}\left[\frac{W_k''}{W_k}-\frac{3}{2}\frac{W_k'^2}{W_k^2}\right]. \tag{2.8}$$

This equation can be solved iteratively

$$W_k^{(N+1)^2}=\omega_k^2-\Delta\xi a^2R-\frac{1}{2}\left[\frac{W_k^{(N)''}}{W_k^{(N)}}-\frac{3}{2}\frac{W_k^{(N)'2}}{W_k^{(N)^2}}\right], \tag{2.9}$$

with $W_k^{(0)}=\omega_k$ in the sense that for a finite time interval and sufficiently large k the right-hand side (RHS) of Eq. (2.9) is strictly positive. Then $W_k^{(N)}$ can be continued to all values of k in such a way that it is a smooth function of time. As each iteration picks up two time derivatives, the Nth iterative solution $W_k^{(N)}$ is of adiabatic order $2N$. Substituting $W_k^{(N)}$ back into Eq. (2.7) yields a so-called approximate adiabatic mode $\tilde{f}_k^{(N)}$.

An adiabatic vacuum state of iteration order N is determined by a complete set of mode solutions $\{f_k, f_k^*\}$ to Eq. (2.5) satisfying initial conditions

$$f_k(\eta_0)=\tilde{f}_k^{(N)}(\eta_0),\quad f_k'(\eta_0)=\tilde{f}_k^{(N)'}(\eta_0); \tag{2.10}$$

i.e., an adiabatic mode coincides with an approximate mode $\tilde{f}_k^{(N)}$ on the initial Cauchy surface. With the particular form (2.7) of the approximate adiabatic modes, these initial conditions read, explicitly,

$$f_k(\eta_0)=\frac{1}{\sqrt{2W_k^{(N)}(\eta_0)}},$$

$$f_k'(\eta_0)=-\left(iW_k^{(N)}(\eta_0)+\frac{W_k^{(N)'}(\eta_0)}{2W_k^{(N)}(\eta_0)}\right)f_k(\eta_0). \tag{2.11}$$

According to this construction an adiabatic vacuum state depends on the initial time η_0, the order of iteration N, and the extrapolation of $W_k^{(N)}$ to small momenta k. In the following we simply write W_k instead of $W_k^{(N)}$ for the adiabatic frequency.

Varying the action with respect to the metric yields the energy-momentum tensor. For a real scalar field with arbitrary curvature coupling, one finds [15]

$$T_{\mu\nu}=(1-2\xi)\partial_\mu\varphi\partial_\nu\varphi-2\xi\varphi\nabla_\mu\nabla_\nu\varphi+\left(2\xi-\frac{1}{2}\right)g_{\mu\nu}\partial^\rho\varphi\partial_\rho\varphi+2\xi g_{\mu\nu}\varphi\Box\varphi-\xi G_{\mu\nu}\varphi^2-\frac{1}{2}g_{\mu\nu}m^2\varphi^2. \quad (2.12)$$

A mode sum representation of its (bare) expectation value is obtained by substituting the mode decomposition (2.3) into Eq. (2.12). We choose the energy density and the trace as the two independent components. They take the following form:

$$\langle T^0{}_0\rangle\equiv\varepsilon=\int\frac{d\mu(k)}{2\pi^2a^4}\left[3\Delta\xi(h'+2h^2)|f_k|^2-3\Delta\xi h(|f_k|^2)'+\frac{1}{2}(|f_k'|^2+\Omega_k^2|f_k|^2)\right],$$

$$\langle T^\mu{}_\mu\rangle\equiv T=\int\frac{d\mu(k)}{2\pi^2a^4}[(6\Delta\xi h'+m^2a^2)|f_k|^2+6\Delta\xi h(|f_k|^2)'-6\Delta\xi(|f_k'|^2-\Omega_k^2|f_k|^2)], \quad (2.13)$$

where the abbreviation $h=a'/a$ has been introduced. The measure $d\mu(k)$ implies integration over continuous and summation over discrete momenta:

$$\int d\mu(k)=\begin{cases}\int_0^\infty dk k^2 & \text{if} \quad \kappa=0,-1,\\ \sum_{k=1}^{\infty}k^2 & \text{if} \quad \kappa=+1.\end{cases} \quad (2.14)$$

We note that the dependence on the quantum state enters the expectation values (2.13) via the initial conditions satisfied by the modes f_k. As we are concerned with adiabatic states, the modes f_k satisfy the initial conditions (2.10).

The formal expressions (2.13) are divergent and need to be renormalized. This task can be achieved by the method of adiabatic regularization [15,16,17]. In this scheme the renormalized energy-momentum tensor is obtained by subtracting from the mode integrals (2.13) their fourth-order adiabatic expansion:

$$\langle T_{\mu\nu}\rangle_{\rm ren}\stackrel{\rm def}{=}\langle T_{\mu\nu}\rangle-\langle T_{\mu\nu}\rangle^{(4)}. \quad (2.15)$$

This subtraction is to be interpreted as a renormalization of the gravitational constant, the cosmological constant, and the coupling constant of the squared curvature term in the classical gravitational action. As was shown in [17], even for closed spatial geometry ($\kappa=+1$) the subtraction has to be performed with the continuum measure

$$\langle T_{\mu\nu}\rangle^{(4)}=\int_0^\infty dk\frac{k^2}{2\pi^2a^2}\mathcal{T}^{(4)}_{\mu\nu} \quad (2.16)$$

in order to correctly reproduce the trace anomaly. The explicit form of the subtraction terms $\mathcal{T}^{(4)}_{\mu\nu}$ can be found, e.g., in [15,17]. Also, adiabatic regularization has been shown to be equivalent to covariant point splitting [17,18] and thus results in an energy-momentum tensor satisfying Wald's axioms [1].

III. INITIAL STATES AND THE ENERGY-MOMENTUM TENSOR

In this section we show that an adiabatic vacuum must be at least of order 4 for the expectation value of the energy-momentum tensor to be nonsingular on the initial Cauchy surface. Before proceeding with the proof we wish to give an intuitive argument in order to illuminate the problem.

Obviously, the subtraction procedure (2.15) only makes sense if the ultraviolet divergences of the bare expressions are canceled by the divergent terms of the adiabatic expansion, i.e., by all terms of $\mathcal{T}^{(4)}_{\mu\nu}(\eta)$ up to ω_k^{-3}. As the subtraction terms are local, this cancellation has to occur at each instant of time. In other words, the bare expressions need to possess an asymptotic expansion for large momenta that reproduces the divergent terms of the adiabatic expansion *uniformly* with respect to time. This includes in particular the initial time where the bare expressions are directly given in terms of the initial conditions. The simple idea is now to compare the asymptotic expansion of the bare expressions for large ω_k with the divergent part of the adiabatic expansion *at the initial time*.

With the adiabatic initial conditions (2.11) the expectation value of the energy-momentum tensor (2.13) at the initial time η_0 becomes

$$\varepsilon(\eta_0)=\int\frac{d\mu(k)}{2\pi^2a_0^4}\frac{1}{4}\left[W_{k0}+\frac{\Omega_{k0}^2}{W_{k0}}+\frac{(W_{k0}{}')^2}{4W_{k0}{}^3}+6\Delta\xi h_0\frac{W_{k0}{}'}{W_{k0}{}^2}+6\Delta\xi(h_0'+2h_0^2)\frac{1}{W_{k0}}\right],$$

$$T(\eta_0)=\int\frac{d\mu(k)}{2\pi^2a_0^4}\frac{1}{2}\left[(6\Delta\xi h_0'+m^2a_0^2)\frac{1}{W_{k0}}-6\Delta\xi h_0\frac{W_{k0}{}'}{W_{k0}{}^2}-6\Delta\xi\left(W_{k0}-\frac{\Omega_{k0}^2}{W_{k0}}+\frac{(W_{k0}{}')^2}{4W_{k0}{}^3}\right)\right], \quad (3.1)$$

where the subscript 0 indicates that the time argument of the respective quantity is set equal to the initial time η_0, i.e., $a_0\equiv a(\eta_0)$, etc. The asymptotic expansion of the adiabatic frequency W_k for large ω_k can be inferred from Eq. (2.9) by induction in N:

$$W_k=\omega_k\left[1-\frac{q}{2\omega_k^2}(1-\delta_{N,0})-\frac{M^{2''}+q''+q^2}{8\omega_k^4}(1-\delta_{N,0})+\frac{q''}{8\omega_k^4}(1-\delta_{N,0}-\delta_{N,1})+O(\omega_k^{-6})\right]. \quad (3.2)$$

Then, the divergent terms of Eqs. (3.1) are readily found:

$$\varepsilon(\eta_0)=\int \frac{d\mu(k)}{2\pi^2 a_0^4}\Bigg\{\frac{\omega_{k0}}{2}-\frac{q_0}{4\omega_{k0}}-\frac{q_0^2}{16\omega_{k0}^3}(1-\delta_{N,0}) +3\Delta\xi h_0\frac{M_0^{2\prime}+q_0'\delta_{N,0}}{4\omega_{k0}^3}+3\Delta\xi(h_0'+2h_0^2) \times\left[\frac{1}{2\omega_{k0}}+\frac{q_0}{4\omega_{k0}^3}(1-\delta_{N,0})\right]+O(\omega_{k0}^{-5})\Bigg\},$$

$$T(\eta_0)=\int \frac{d\mu(k)}{2\pi^2 a_0^4}\Bigg\{(6\Delta\xi h_0'+m^2a_0^2) \times\left[\frac{1}{2\omega_{k0}}+\frac{q_0}{4\omega_{k0}^3}(1-\delta_{N,0})\right] -3\Delta\xi\frac{q_0}{\omega_{k0}}\delta_{N,0}-3\Delta\xi h_0\frac{M_0^{2\prime}+q_0'\delta_{N,0}}{2\omega_{k0}^3} +3\Delta\xi\frac{M_0^{2\prime\prime}}{4\omega_{k0}^3}(1-\delta_{N,0}) +3\Delta\xi\frac{q_0''}{4\omega_{k0}^3}\delta_{N,1}+O(\omega_{k0}^{-5})\Bigg\}. \tag{3.3}$$

We observe that the structure of the divergences in the energy density coincides with that of the adiabatic expansion if $N>0$. For the trace, however, this is only true if $N>1$ because the term proportional to q_0'' (being of adiabatic order 4) only appears in the second and subsequent iterations in Eq. (2.9). So when subtracting the adiabatic expansion [15,17] in the cases $N=0,1$, one is effectively introducing divergent terms that are not present at the initial moment and the momentum integrals do not exist (at the initial time η_0).

Even though this simple comparison shows the root of the problem, it only proves the necessity of the condition $N>1$ under the assumption that the adiabatic expansion yields all the divergences present in the theory and therefore has to be subtracted. In order to give a self-contained proof, we have to show that $N>1$ is necessary for the bare expressions to possess uniform (with respect to a finite time interval, containing the initial time) large momentum asymptotic behavior that reproduces the divergent structure of the adiabatic expansion. For this purpose we represent the adiabatic modes f_k in terms of a different set of mode solutions g_k, subject to the conformal-like initial conditions

$$g_k(\eta_0)=\frac{1}{\sqrt{2\Omega_k(\eta_0)}},\quad g_k'(\eta_0)=-i\Omega_k(\eta_0)g_k(\eta_0). \tag{3.4}$$

As both mode solutions correspond to a homogeneous state, they are related by a diagonal Bogoliubov transformation

$$f_k(\eta)=e^{i\phi_k}[\cosh\theta_k g_k(\eta)+e^{i\delta_k}\sinh\theta_k g_k^*(\eta)]. \tag{3.5}$$

The identity $\cosh^2\theta_k-\sinh^2\theta_k=1$ ensures that the normalization constraint $f_kf_k^{*\prime}-f_k^*f_k'=i$ is preserved. The Bogoliubov coefficients are determined by the initial conditions satisfied by the modes f_k and g_k. Their particular combinations appearing in the representation of the energy-momentum tensor are

$$\cosh 2\theta_k=\frac{1}{2}\left[\frac{\Omega_{k0}}{W_{k0}}+\frac{W_{k0}}{\Omega_{k0}}+\frac{W_{k0}}{\Omega_{k0}}\left(\frac{W_{k0}'}{2W_{k0}^2}\right)^2\right],$$

$$\sinh 2\theta_k\cos\delta_k=\frac{1}{2}\left[\frac{\Omega_{k0}}{W_{k0}}-\frac{W_{k0}}{\Omega_{k0}}-\frac{W_{k0}}{\Omega_{k0}}\left(\frac{W_{k0}'}{2W_{k0}^2}\right)^2\right],$$

$$\sinh 2\theta_k\sin\delta_k=-\frac{W_{k0}'}{2W_{k0}^2}. \tag{3.6}$$

The energy-momentum tensor (2.13) can now be expressed in terms of the modes g_k and the Bogoliubov coefficients. As the problem of the initial singularity is less severe in the energy density, we will show the following calculation only for the trace:

$$T=\int \frac{d\mu(k)}{2\pi^2a^4}\big((6\Delta\xi h'+m^2a^2)[\cosh 2\theta_k|g_k|^2+\sinh 2\theta_k\mathcal{R}(e^{-i\delta_k}g_k^2)]-6\Delta\xi\{\cosh 2\theta_k(|g_k'|^2-\Omega_k^2|g_k|^2) +\sinh 2\theta_k\mathcal{R}[e^{-i\delta_k}(g_k'^2-\Omega_k^2g_k^2)]\}+6\Delta\xi h\{\cosh 2\theta_k(|g_k|^2)'+\sinh 2\theta_k\mathcal{R}[e^{-i\delta_k}(g_k^2)]\}\big). \tag{3.7}$$

The next step consists in finding the large momentum behavior of Eq. (3.7). For this purpose we make use of an asymptotic expansion of the mode solutions g_k that has similarly been used in [10,13,14]. The mode functions g_k satisfy the oscillatory equation (2.5). Adding Ω_{k0}^2 on both sides yields

$$g_k''+\Omega_{k0}^2g_k=-(\Omega_k^2-\Omega_{k0}^2)g_k\equiv-\Delta\Omega^2 g_k. \tag{3.8}$$

The key point is that $\Delta\Omega^2$ is independent of k. Moreover, it vanishes at the initial time: $\Delta\Omega^2(\eta_0)=0$. The quantity Ω_{k0}^2 is strictly positive for sufficiently large momentum k so that Eq. (3.8) possesses the homogeneous solution $e^{-i\Omega_{k0}(\eta-\eta_0)}$. Then, with the help of the ansatz

$$g_k(\eta)=\frac{e^{-i\Omega_{k0}(\eta-\eta_0)}}{\sqrt{2\Omega_{k0}}}[1+\tilde{g}_k(\eta)] \tag{3.9}$$

and using the initial conditions (3.4), the mode equation (3.8) can be transformed into the following integral equation:

$$\tilde{g}_k(\eta)=\frac{i}{2\Omega_{k0}}\int_{\eta_0}^{\eta}d\eta'(e^{2i\Omega_{k0}(\eta-\eta')}-1)\Delta\Omega^2(\eta')\times[1+\tilde{g}_k(\eta')]. \tag{3.10}$$

This equation can be solved by iteration starting with $\tilde{g}_k^{(0)}\equiv 0$. As each iteration increases the power of Ω_{k0}^{-1} by 1 the iterative solution yields an expansion of $\tilde{g}_k$ in inverse powers of Ω_{k0} on the finite time interval $[\eta_0,\eta]$. The details of this expansion as well as the result for $\tilde{g}_k$ are displayed in the Appendix.

It remains to derive the asymptotic expansion of the Bogoliubov parameters (3.6) for large Ω_{k0}. For this purpose we solve Eq. (2.8) iteratively starting with Ω_k instead of ω_k. By induction in $\tilde{N}$ ($\tilde{N}$ is the number of iterations with respect to Ω_k), we find

$$\begin{aligned}W_k^{(\tilde{N})}&=\Omega_k\left[1-(1-\delta_{\tilde{N},0})\frac{M^{2''}}{8\Omega_k^4}+O(\Omega_k^{-6})\right],\\&=\omega_k\left[1-\frac{q}{2\omega_k^2}-\frac{q^2+M^{2''}(1-\delta_{\tilde{N},0})}{8\omega_k^4}+O(\omega_k^{-6})\right],\end{aligned} \tag{3.11}$$

where the second line is obtained by means of $\Omega_k^2=\omega_k^2-q$. The frequency $W_k^{(\tilde{N})}$ yields all terms up to ω_k^{-3} of a fourth-order adiabatic frequency only if $\tilde{N}>0$ as can be seen by comparing Eq. (3.11) with Eq. (3.2).

With the help of relation (3.11) it is now straightforward to calculate the asymptotics of the Bogoliubov parameters (3.6):

$$\begin{aligned}\cosh 2\theta_k&=1+O(\Omega_{k0}^{-6}),\\ \sinh 2\theta_k\cos\delta_k&=(1-\delta_{\tilde{N},0})\frac{M_0^{2''}}{8\Omega_{k0}^4}+O(\Omega_{k0}^{-6}),\\ \sinh 2\theta_k\sin\delta_k&=-\frac{M_0^{2'}}{4\Omega_{k0}^3}+O(\Omega_{k0}^{-5}).\end{aligned} \tag{3.12}$$

Equipped with these expansions, we finally isolate the divergent terms in the trace of the energy-momentum tensor:

$$\begin{aligned}T(\eta)=\int\frac{d\mu(k)}{2\pi^2a^4}\Bigg\{&(6\Delta\xi h'+m^2a^2)\\&\times\left(\frac{1}{2\Omega_{k0}}-\frac{\Delta\Omega^2}{4\Omega_{k0}^3}\right)-3\Delta\xi h\frac{M^{2'}}{2\Omega_{k0}^3}+\frac{3\Delta\xi}{4\Omega_{k0}^3}\\&\times[M^{2''}-\delta_{\tilde{N},0}M_0^{2''}\cos 2\Omega_{k0}(\eta-\eta_0)]+O(\Omega_{k0}^{-4})\Bigg\}.\end{aligned} \tag{3.13}$$

The term proportional to $M_0^{2''}\cos 2\Omega_{k0}(\eta-\eta_0)$ does not vanish for $\tilde{N}=0$. Since the integral $\int d\mu(k)\Omega_{k0}^{-3}\cos 2\Omega_{k0}(\eta-\eta_0)$ diverges logarithmically in the limit $\eta\to\eta_0$, it leads to an initial singularity. All other divergent terms are indeed local and coincide with the divergence structure of the adiabatic expansion because we have

$$\frac{1}{\Omega_{k0}^3}=\frac{1}{k^3}+O(k^{-5}),\quad \frac{1}{\Omega_{k0}}-\frac{\Delta\Omega^2}{2\Omega_{k0}^3}=\frac{1}{k}-\frac{M^2}{2k^3}+O(k^{-5}). \tag{3.14}$$

We conclude, then, that the large momentum behavior of the divergent terms of the bare trace is uniform on the time interval $[\eta_0,\eta]$ only if $\tilde{N}>0$. In other words, an adiabatic vacuum state must be *at least of adiabatic order 4* for the renormalized energy-momentum tensor to be finite on the initial Cauchy surface. Therefore, only adiabatic states of order 4 or higher are reasonable physical states. Some remarks are in order.

As the term causing the initial singularity is proportional to $\Delta\xi$, the problem of the dependence on the order of the adiabatic vacuum only affects nonconformally coupled fields.

Since the expansion in inverse powers of Ω_{k0} reproduces the local divergences of the adiabatic expansion, one could ask, why not subtract the leading terms of this expansion instead of the adiabatic ones? The answer is that even though these subtractions are covariantly conserved, they fail to reproduce the trace anomaly. To see this we rewrite the renormalized energy-momentum tensor (2.15) according to

$$\langle T_{\mu\nu}\rangle_{\rm ren}=\langle T_{\mu\nu}\rangle-\langle T_{\mu\nu}\rangle_{\rm div}+\langle T_{\mu\nu}\rangle_{\rm div}-\langle T_{\mu\nu}\rangle^{(4)} \tag{3.15}$$

and calculate the finite difference (with now $\tilde{N}>0$)

$$\langle T_{\mu\nu}\rangle^{\rm diff}\equiv\langle T_{\mu\nu}\rangle_{\rm div}-\langle T_{\mu\nu}\rangle^{(4)}, \tag{3.16}$$

where $\langle T_{\mu\nu}\rangle_{\rm div}$ denotes all divergent terms of the inverse Ω_{k0} expansion (i.e., up to Ω_{k0}^{-3}). The result can be represented as

$$\begin{aligned}T^{\rm diff}=T^{\rm anomaly}-\frac{1}{8\pi^2}\Bigg\{&(m^4-m^2\Delta\xi R+3(\Delta\xi)^2\nabla^\mu\nabla_\mu R)\\&\times\ln\frac{ma}{M_0}+\frac{1}{a^2}\left(\frac{m^4}{4}g_{00}+m^2\Delta\xi G_{00}-\frac{1}{2}{}^{(1)}H_{00}\right)\\&-\frac{3m^4}{4}+\frac{m^2}{36a^2}(1-18\Delta\xi)R-\frac{1}{12}\Delta\xi\nabla^\mu\nabla_\mu R\\&-\frac{1}{4}(\Delta\xi)^2R^2-\frac{\kappa}{6a^4}[6\Delta\xi h'+m^2a^2(1-36\Delta\xi)]\\&+\frac{3}{a^2}(\Delta\xi)^2[2(h'+h^2)R+hR']\\&+\frac{M_0^2}{2a^4}(6\Delta\xi h'+m^2a^2)\Bigg\}.\end{aligned} \tag{3.17}$$

Here $G_{\mu\nu}$ is the Einstein tensor, and the definition of ${}^{(1)}H_{\mu\nu}$ can be found, e.g., in [16]. Here $T^{\rm anomaly}$ is the anomalous trace [19]:

$$T^{\text{anomaly}} = \lim_{m\to 0}\langle T^{\mu}_{\mu}\rangle_{\text{ren}} - \left\langle\left(\lim_{m\to 0} T^{\mu}_{\mu}\right)\right\rangle_{\text{ren}}$$
$$= -\frac{1}{2880\pi^2}\bigg[R^{\mu\nu}R_{\mu\nu} - \frac{1}{3}R^2 + (30\xi-6)\nabla^{\mu}\nabla_{\mu}R + 90(\Delta\xi)^2R^2\bigg]. \tag{3.18}$$

The energy density $\varepsilon^{\text{diff}}$ is calculated likewise. The covariant conservation of $\langle T_{\mu\nu}\rangle^{\text{diff}}$ has explicitly been checked. Besides the trace anomaly, T^{diff} contains the logarithmic terms which give rise to the so-called anomalous scaling as well as the renormalization scale dependence [20].

So we see that even though $\langle T_{\mu\nu}\rangle_{\text{div}}$ is covariantly conserved and has the correct local singularity structure, its subtraction does not yield the correct renormalized energy-momentum tensor as it cannot reproduce the trace anomaly.

IV. CONCLUSIONS

Since all adiabatic vacua are Hadamard states [9], they are usually considered physically admissible quantum states of linear Klein-Gordon fields on Robertson-Walker spaces. However, we find that the corresponding energy-momentum tensor develops a generic singularity on the initial Cauchy surface if the order of the adiabatic state is less than 4. The divergent terms of the large momentum asymptotics of the energy-momentum tensor only coincide with those of the adiabatic expansion if the adiabatic vacuum is at least of order 4. As a result, an adiabatic vacuum state only results in an energy-momentum tensor satisfying Wald's axioms and thus is a *physically reasonable* state if it is *at least of order 4*.

This result is supported by the adiabatic particle picture developed in [11]. There, this restricted class of adiabatic vacua is shown to lead to a natural physical interpretation of the structure of the energy-momentum tensor. It splits into a local part (vacuum polarization) containing all the divergences which have to be subtracted and a nonlocal piece due to particle creation.

We have further shown that the subtraction of the divergent terms of the nonlocal large momentum expansion (3.13) (cf. the Appendix) as suggested in [12] does not result in the correct renormalized energy-momentum tensor of a scalar field on a Robertson-Walker space because it fails to reproduce the trace anomaly. Nevertheless, this expansion can be useful in practical calculations of the energy-momentum tensor as the difference $\langle T_{\mu\nu}\rangle^{\text{diff}}$ between the divergent terms (3.13) and the adiabatic subtractions has been calculated explicitly, Eq. (3.17). Only the remaining part needs to be calculated numerically.

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APPENDIX

In this appendix we wish to derive an asymptotic expansion of the conformal-like mode functions g_k in inverse powers of Ω_{k0}, i.e., for large momentum. The Volterra-type integral equation (3.10) (which holds for sufficiently large k) serves us as the starting point. The iteration procedure

$$\tilde{g}_k^{(n+1)}(\eta) = \frac{i}{2\Omega_{k0}}\int_{\eta_0}^{\eta} d\eta' K_k(\eta,\eta')[1+\tilde{g}_k^{(n)}(\eta')], \tag{A1}$$

with $\tilde{g}_k^{(0)}(\eta)\equiv 0$, converges uniformly on the time interval $[\eta,\eta_0]$ (for fixed k). According to Eq. (3.10), the kernel $K_k(\eta,\eta')$ is given by

$$K_k(\eta,\eta') \overset{\text{def}}{=} [e^{2i\Omega_{k0}(\eta-\eta')}-1]\Delta\Omega^2(\eta'). \tag{A2}$$

As a result of the iteration, the solution $\tilde{g}_k(\eta)$ has the series representation

$$\tilde{g}_k(\eta) = \sum_{n=1}^{\infty}\left(\frac{i}{2\Omega_{k0}}\right)^n \int_{\eta_0}^{\eta} d\eta_1 K_k(\eta,\eta_1)\cdots \times\int_{\eta_0}^{\eta_{n-1}} d\eta_n K_k(\eta_{n-1},\eta_n). \tag{A3}$$

The estimate

$$|\tilde{g}_k(\eta)| \leq \exp\left\{\frac{1}{\Omega_{k0}}\int_{\eta_0}^{\eta} d\eta' |\Delta\Omega^2(\eta')|\right\} - 1 \tag{A4}$$

shows that $\tilde{g}_k(\eta)$ remains bounded and goes to zero as $k\to\infty$. An asymptotic expansion of $\tilde{g}_k(\eta)$ in inverse powers of Ω_{k0} can now be achieved by expanding each addend of the series (A3). For this purpose we provide repeatedly integration by parts [$\Delta\Omega^2$: i.e., $R(\eta)$ is assumed to be smooth] to the most inner integral of the nth addend and find

$$\int_{\eta_0}^{\eta_{n-1}} d\eta_n K_k(\eta_{n-1},\eta_n) = -\int_{\eta_0}^{\eta_{n-1}} d\eta_n \Delta\Omega^2(\eta_n) - \sum_{m=0}^{\infty}\left(\frac{-i}{2\Omega_{k0}}\right)^{m+1} \times[\Delta\Omega^{2^{(m)}}(\eta_{n-1}) - \Delta\Omega^{2^{(m)}}(\eta_0)e^{2i\Omega_{k0}(\eta_{n-1}-\eta_0)}]. \tag{A5}$$

As all subsequent integrations have the same structure, they are treated likewise. The result is an asymptotic series for the nth addend of Eq. (A3) with leading term

$$\frac{1}{n!}\left(\frac{-i}{2\Omega_{k0}}\int_{\eta_0}^{\eta}d\eta'\Delta\Omega^2(\eta')\right)^n+O(\Omega_{k0}^{-(n+1)}).$$

Consequently, all terms contributing to $\tilde{g}_k(\eta)$ up to order Ω_{k0}^{-n} are contained in the first n addends of Eq. (A3). If $n=4$, we find, for example,

$$\begin{aligned}\mathcal{R}\tilde{g}_k(\eta)=&-\frac{1}{4\Omega_{k0}^2}\left[\Delta\Omega^2+\frac{1}{2}I_1^2\right]\\&+\frac{1}{8\Omega_{k0}^3}\Delta\Omega_0^{2\prime}\sin 2\Omega_{k0}(\eta-\eta_0)\\&+\frac{1}{16\Omega_{k0}^4}\left[\Delta\Omega^{2\prime\prime}-\Delta\Omega_0^{2\prime\prime}\cos 2\Omega_{k0}(\eta-\eta_0)\right.\\&+\Delta\Omega^{2\prime}I_1+\frac{5}{2}(\Delta\Omega^2)^2\\&+\Delta\Omega_0^{2\prime}I_1\cos 2\Omega_{k0}(\eta-\eta_0)\\&\left.+\frac{1}{2}\Delta\Omega^2I_1^2+I_1I_2+\frac{1}{4!}I_1^4\right]+O(\Omega_{k0}^{-5}),\end{aligned}$$

$$\begin{aligned}\mathcal{I}\tilde{g}_k(\eta)=&-\frac{1}{2\Omega_{k0}}I_1+\frac{1}{8\Omega_{k0}^3}\\&\times\left[\Delta\Omega^{2\prime}-\Delta\Omega_0^{2\prime}\cos 2\Omega_{k0}(\eta-\eta_0)\right.\\&\left.+\Delta\Omega^2I_1+I_2+\frac{1}{3!}I_1^3\right]\\&-\frac{1}{16\Omega_{k0}^4}[\Delta\Omega_0^{2\prime\prime}\sin 2\Omega_{k0}(\eta-\eta_0)\\&-\Delta\Omega_0^{2\prime}I_1\sin 2\Omega_{k0}(\eta-\eta_0)]+O(\Omega_{k0}^{-5}),\end{aligned}\tag{A6}$$

where the abbreviation

$$I_m=\int_{\eta_0}^{\eta}d\eta'[\Delta\Omega^2(\eta')]^m$$

has been used. Note that Eq. (A6) already contains all terms contributing to the divergences of the trace (3.13).

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