Not all adiabatic vacua are physical states

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Abstract

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 four. Therefore, adiabatic vacua are physically reasonable only if their order is at least four.

A certain non-local 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 regularisation.

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1 Introduction

The semiclassical theory of quantised 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 renormalisation [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. The 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 Roberts and Lüders [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 behaviour 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

$$G_{\mu\nu} = -8\pi G \langle T_{\mu\nu} \rangle.$$  \hspace{2cm} (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
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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. (3.5) below) develops an initial singularity, i.e. the limit $\eta \to \eta_0$ does not exist ($\eta$ 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 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 four 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 admissible only if their order is four at least.

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

In the derivation of the condition on the adiabatic order we employ a non-local large momentum expansion of the conformal-like mode functions (see the appendix) that has 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 regularisation 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 section 2 we review the basic elements of scalar field quantisation in Robertson-Walker spaces including adiabatic regularisation as far as necessary and give the definition of adiabatic states following [6]. In section 3 we show that the adiabatic order of the state must not be less than four 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 $g_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ and we use units such that $\hbar = c = 1$.

2 Quantum fields on Robertson-Walker spaces

The Robertson-Walker metric is given by

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

(2.1)

where $h_{ik}$ denotes the metric of a 3-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
\[
\varphi(x) = \frac{1}{a(\eta)} \int d\tilde{\mu}(k) \left[ f_k(\eta) \Phi_k(x) a_k + f_k^*(\eta) \Phi_k^*(x) a_k^\dagger \right], \tag{2.3}
\]
where the creation and annihilation operators \(a_k^\dagger, a_k\) obey the usual commutation relations. The \(\Phi_k(x)\) are the eigenfunctions of the Laplace-Beltrami operator on the 3-space of constant curvature
\[
\Delta^{(3)} \Phi_k(x) = - \left( k^2 - \kappa \right) \Phi_k(x) \tag{2.4}
\]
and \(d\tilde{\mu}(k)\) is the measure on 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
\[
\Omega_k^2(\eta) = k^2 + a^2 \left( m^2 - \Delta \xi R \right) \overset{\text{def}}{=} \omega_k^2 - q(\eta) \overset{\text{def}}{=} k^2 + M^2(\eta) \tag{2.6}
\]
with \(\omega_k^2 = k^2 + m^2 a^2\) and \(\Delta \xi = 1/6 - \xi\). A complete set of mode solutions to eq. (2.3) 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 (2.3) leads to the following equation for the frequency \(W_k\):
\[
W_k^2 = \Omega_k^2 - \frac{1}{2} \left[ \frac{W_k''}{W_k} - \frac{3 W_k'^2}{2 W_k^2} \right]. \tag{2.8}
\]
This equation can be solved iteratively
\[
W_k^{(N+1)^2} = \omega_k^2 - \Delta \xi a^2 R - \frac{1}{2} \left[ \frac{W_k^{(N)''}}{W_k^{(N)}} - \frac{3 W_k^{(N)'^2}}{2 W_k^{(N)^2}} \right] \tag{2.9}
\]
with \(W_k^{(0)^2} = \omega_k^2\) in the sense that for a finite time interval and sufficiently large \(k\) the RHS of eq. (2.3) 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 \( N \)th iterative solution \( W_k^{(N)} \) is of adiabatic order \( 2N \). Substituting \( W_k^{(N)} \) back into (2.7) yields a so called approximate adiabatic mode \( \bar{f}_k^{(N)} \).

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

\[
\begin{align*}
  f_k(\eta_0) &= \bar{f}_k^{(N)}(\eta_0), \\
  f_k'(\eta_0) &= \bar{f}_k^{(N)'}(\eta_0),
\end{align*}
\]  

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

\[
\begin{align*}
  f_k(\eta_0) &= \frac{1}{\sqrt{2W_k^{(N)}(\eta_0)}}, \\
  f_k'(\eta_0) &= -\left(iW_k^{(N)}(\eta_0) + \frac{W_k^{(N)'}(\eta_0)}{2W_k^{(N)}(\eta_0)}\right)f_k(\eta_0).
\end{align*}
\]  

According to this construction an adiabatic vacuum state depends on

- the initial time \( \eta_0 \)
- the order of iteration \( N \),
- 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]

\[
T_{\mu\nu} = (1 - 2\xi)\partial_\mu \varphi \partial_\nu \varphi - 2\xi \varphi \nabla_\mu \nabla_\nu \varphi + (2\xi - \frac{1}{2})g_{\mu\nu} \partial^\rho \varphi \partial_\rho \varphi
\]

\[
+ 2\xi g_{\mu\nu} \Box \varphi - \xi G_{\mu\nu} \varphi^2 - \frac{1}{2} g_{\mu\nu} m^2 \varphi^2.
\]  

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

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

\[
\begin{align*}
  \langle T^\mu_\mu \rangle &\equiv T = \int \frac{d\mu(k)}{2\pi^2 a^4} \left[ (6\Delta \xi h' + m^2 a^2) |f_k|^2 + 6\Delta \xi h \left(|f_k|^2\right)' \right]
\end{align*}
\]
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\[ -6\Delta \xi \left( |f_k'|^2 - \Omega_k^2 |f_k|^2 \right), \quad (2.13) \]

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

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

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 renormalised. This task can be achieved by the method of adiabatic regularisation [15–17]. In this scheme the renormalised energy momentum tensor is obtained by subtracting from the mode integrals (2.13) their fourth order adiabatic expansion:

\[
\langle T_{\mu\nu} \rangle_{\text{ren}} \overset{\text{def}}{=} \langle T_{\mu\nu} \rangle - \langle T_{\mu\nu} \rangle^{(4)}. \quad (2.15)
\]

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

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

in order to correctly reproduce the trace anomaly. The explicit form of the subtraction terms \( \mathcal{T}_{\mu\nu}^{(4)} \) can be found, e.g., in [15, 17]. Also, adiabatic regularisation 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].

3 Initial states and the energy-momentum tensor

In this section we show that an adiabatic vacuum must be at least of order four 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 cancelled by the divergent
terms of the adiabatic expansion, i.e. by all terms of $\mathcal{T}_{\mu\nu}^{(4)}(\eta)$ up to $\omega_k^{-3}$. 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 $\omega_k$ 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 $\eta_0$ becomes:

$$
\varepsilon(\eta_0) = \int \frac{d\mu(k)}{2\pi^2 a_0^4} \left[ W_k \frac{\Omega_k^2}{W_k} + \frac{(W_k \delta^0)^2}{4W_k^3} + 6\Delta\xi h_0 \frac{W_k}{W_k^3} \right]
\begin{align*}
&\quad + 6\Delta\xi \left( h_0' + 2h_0^2 \right) \frac{1}{W_k^3}, \\
T(\eta_0) = \int \frac{d\mu(k)}{2\pi^2 a_0^4} \left[ \left( 6\Delta\xi h_0' + m^2 a_0^2 \right) \frac{1}{W_k} - 6\Delta\xi h_0 \frac{W_k'}{W_k^2} \right]
\begin{align*}
&\quad - 6\Delta\xi \left( W_k - \frac{\Omega_k^2}{W_k} + \frac{(W_k \delta^0)^2}{4W_k^3} \right), \tag{3.1}
\end{align*}
\end{align*}
$$

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

\begin{align*}
W_k &= \omega_k \left[ 1 - \frac{q}{2\omega_k^2} (1 - \delta_{N,0}) - \frac{M''}{8\omega_k^2} (1 - \delta_{N,0}) \right. \\
&\quad \left. + \frac{q''}{8\omega_k^2} (1 - \delta_{N,0} - \delta_{N,1}) + O(\omega^{-6}) \right]. \tag{3.2}
\end{align*}

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

\begin{align*}
\varepsilon(\eta_0) &= \int \frac{d\mu(k)}{2\pi^2 a_0^4} \left\{ \frac{\omega_k}{2} \frac{q_0}{4\omega_k} - \frac{q_0^2}{16\omega_k^3} (1 - \delta_{N,0}) + 3\Delta\xi h_0 \frac{M_0''}{4\omega_k^3} \right. \\
&\quad \left. + 3\Delta\xi \left( h_0' + 2h_0^2 \right) \left[ \frac{1}{2\omega_k} + \frac{q_0}{4\omega_k^3} (1 - \delta_{N,0}) \right] + O(\omega_k^{-5}) \right\}, \\
T(\eta_0) &= \int \frac{d\mu(k)}{2\pi^2 a_0^4} \left\{ \left( 6\Delta\xi h_0' + m^2 a_0^2 \right) \left[ \frac{1}{2\omega_k} + \frac{q_0}{4\omega_k^3} (1 - \delta_{N,0}) \right] \\
&\quad - 3\Delta\xi \frac{q_0}{\omega_k} \delta_{N,0} - 3\Delta\xi \frac{M_0''}{2\omega_k^3} \right. \\
&\quad \left. + 3\Delta\xi \frac{M_0''}{4\omega_k^3} (1 - \delta_{N,0}) + 3\Delta\xi \frac{q_0''}{4\omega_k^3} \delta_{N,1} + O(\omega_k^{-5}) \right\}. \tag{3.3}
\end{align*}
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 four) only appears in the second and subsequent iterations in (2.9). So when subtracting the adiabatic expansion [13, 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 \( \eta_0 \)).

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 behaviour 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

\[
\begin{align*}
g_k(\eta_0) &= \frac{1}{\sqrt{2\Omega_k(\eta_0)}}, \quad g_k'(\eta_0) = -i\Omega_k(\eta_0)g_k(\eta_0). \quad (3.4)
\end{align*}
\]

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

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

The identity \( \cosh^2 \theta_k - \sinh^2 \theta_k = 1 \) ensures that the normalisation constraint \( f_k f_k^* - f_k^* f_k = i \) 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:

\[
\begin{align*}
\cosh 2\theta_k &= \frac{1}{2} \left[ \frac{\Omega_{k0}}{W_{k0}} + \frac{W_{k0}}{\Omega_{k0}} + \frac{W_{k0}'}{\Omega_{k0}} \left( \frac{W_{k0}'}{2W_{k0}^2} \right)^2 \right], \\
\sinh 2\theta_k \cos \delta_k &= \frac{1}{2} \left[ \frac{\Omega_{k0}}{W_{k0}} - \frac{W_{k0}}{\Omega_{k0}} - \frac{W_{k0}'}{\Omega_{k0}} \left( \frac{W_{k0}'}{2W_{k0}^2} \right)^2 \right], \\
\sinh 2\theta_k \sin \delta_k &= -\frac{W_{k0}'}{2W_{k0}^2}. \quad (3.6)
\end{align*}
\]

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:

\[
T = \int \frac{d\mu(k)}{2\pi^2 a^4} \left\{ (6\Delta \xi h' + m^2 a^2) \left[ \cosh 2\theta_k |g_k|^2 + \sinh 2\theta_k \Re \left( e^{-i\delta_k} g_k^2 \right) \right] \right\}
\]
\[-6\Delta \xi \left[ \cosh 2\theta_k \left( |g'_k|^2 - \Omega^2_k |g_k|^2 \right) + \sinh 2\theta_k \Re \left( e^{-i\delta_k} \left( g'_k^2 - \Omega^2_k g_k^2 \right) \right) \right]\]
\[+ 6\Delta \xi h \left[ \cosh 2\theta_k |g_k|^2 \left( |g'_k|^2 \right)' + \sinh 2\theta_k \Re \left( e^{-i\delta_k} (g_k^2)' \right) \right] \right]. \quad (3.7)

The next step consists in finding the large momentum behaviour of (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 $\Omega^2_{k0}$ on both sides yields
\[g''_k + \Omega^2_{k0} g_k = - \left( \Omega^2_k - \Omega^2_{k0} \right) g_k \equiv - \Delta \Omega^2 g_k. \quad (3.8)\]
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 $\Omega^2_{k0}$ 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
\[g_k(\eta) = \frac{e^{-i\Omega_{k0}(\eta - \eta_0)}}{\sqrt{2\Omega_{k0}}} \left[ 1 + \tilde{g}_k(\eta) \right] \quad (3.9)\]
and using the initial conditions (3.4) the mode equation (3.8) can be transformed into the following integral equation
\[\tilde{g}_k(\eta) = \frac{i}{2\Omega_{k0}} \int_{\eta_0}^{\eta} d\eta' \left( e^{2i\Omega_{k0}(\eta - \eta')} - 1 \right) \Delta \Omega^2(\eta') \left[ 1 + \tilde{g}_k(\eta') \right]. \quad (3.10)\]
This equation can be solved by iteration starting with $\tilde{g}_k^{(0)} \equiv 0$. As each iteration increases the power of $\Omega_{k0}^{-1}$ by one the iterative solution yields an expansion of $\tilde{g}_k$ in inverse powers of $\Omega_{k0}$ 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 $\Omega_{k0}$. For this purpose we solve eq. (2.8) iteratively starting with $\Omega_k$ instead of $\omega_k$. By induction in $\tilde{N}$ ($\tilde{N}$ is the number of iterations with respect to $\Omega_k$) we find:
\[W^{(\tilde{N})}_k = \Omega_k \left[ 1 - (1 - \delta_{\tilde{N},0}) \frac{M^2}{8\Omega_k^2} + O(\Omega_k^{-6}) \right], \quad (3.11)\]
where the second line is obtained by means of $\Omega_k^2 = \omega_k^2 - q$. The frequency $W^{(\tilde{N})}_k$ yields all terms up to $\omega_k^{-3}$ of a fourth order adiabatic frequency only if $\tilde{N} > 0$ as can be seen by comparing (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)
\[\cosh 2\theta_k = 1 + O(\Omega_{k0}^{-6}), \quad (3.12)\]
\[ \sinh 2\theta_k \cos \delta_k = (1 - \delta \tilde{N}, 0) \frac{M_0''}{8 \Omega_{k0}^4} + O(\Omega_{k0}^{-6}) , \]
\[ \sinh 2\theta_k \sin \delta_k = -\frac{M_0''}{4 \Omega_{k0}^2} + O(\Omega_{k0}^{-5}) . \]  

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

\[ T(\eta) = \int \frac{d\mu (k)}{2\pi^2 a^4} \left\{ (6 \Delta \xi h' + m^2 a^2) \left( \frac{1}{2 \Omega_{k0}} - \frac{\Delta \Omega^2}{4 \Omega_{k0}^3} \right) - 3 \Delta \xi h \frac{M_0'}{2 \Omega_{k0}^2} + \frac{3 \Delta \xi}{4 \Omega_{k0}^3} \left[ M_0'' - \delta \tilde{N}, 0 M_0'' \cos 2 \Omega_{k0} (\eta - \eta_0) \right] + O(\Omega_{k0}^{-4}) \right\} . \]  

The term proportional to \( M_0'' \cos 2 \Omega_{k0} (\eta - \eta_0) \) 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 \( \eta \rightarrow \eta_0 \) 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

\[ \frac{1}{\Omega_{k0}^3} = \frac{1}{k^3} + O(k^{-5}) \quad \text{and} \quad \frac{1}{\Omega_{k0}} - \frac{\Delta \Omega^2}{2 \Omega_{k0}^3} = \frac{1}{k} - \frac{M_0'}{2 k^3} + O(k^{-5}) . \]

We conclude then, that the large momentum behaviour 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 four for the renormalised energy-momentum tensor to be finite on the initial Cauchy surface. Therefore, only adiabatic states of order four 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 non-conformally coupled fields.

Since the expansion in inverse powers of \( \Omega_{k0} \) 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 renormalised energy-momentum tensor \(2.13\) according to

\[ \langle T_{\mu \nu} \rangle_{\text{ren}} = \langle T_{\mu \nu} \rangle - \langle T_{\mu \nu} \rangle_{\text{div}} + \langle T_{\mu \nu} \rangle_{\text{div}} - \langle T_{\mu \nu} \rangle^{(4)} \]  

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

\[ \langle T_{\mu \nu} \rangle_{\text{diff}} \equiv \langle T_{\mu \nu} \rangle_{\text{div}} - \langle T_{\mu \nu} \rangle^{(4)} , \]
where \( \langle T_{\mu\nu} \rangle_{\text{div}} \) denotes all divergent terms of the inverse \( \Omega_{k0} \) expansion (i.e. up to \( \Omega_{k0}^{-3} \)). The result can be represented as

\[
T^{\text{diff}} = T^{\text{Anomaly}} - \frac{1}{8\pi^2} \left( m^4 - m^2 \Delta \xi R + 3(\Delta \xi)^2 \nabla^\mu \nabla_\mu R \right) \ln \frac{ma}{M_0}
\]

\[
+ \frac{1}{a^2} \left( \frac{m^4}{4} g_{00} + m^2 \Delta \xi G_{00} - \frac{1}{2} (1) H_{00} \right) - \frac{3m^4}{4} + \frac{m^2}{36a^2} (1 - 18\Delta \xi) R
\]

\[
- \frac{1}{12} \Delta \xi \nabla^\mu \nabla_\mu R - \frac{1}{4} (\Delta \xi)^2 R^2 - \frac{\kappa}{6a^4} \left[ 6\Delta \xi h' + m^2 a^2 (1 - 36\Delta \xi) \right]
\]

\[
+ \frac{3}{a^2} (\Delta \xi)^2 \left[ 2(h' + h^2) R + h R' \right] + \frac{M_0^2}{2a^4} (6\Delta \xi h' + m^2 a^2) \right) .
\] (3.17)

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

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, \( T^{\text{diff}} \) contains the logarithmic terms which give rise to the so-called anomalous scaling as well as the renormalisation 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 renormalised energy-momentum tensor as it cannot reproduce the trace anomaly.

### 4 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 four. 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 four. 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 four.

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 polarisation) containing all the divergences which have to be subtracted and a non-local piece due to particle creation.

We have further shown that the subtraction of the divergent terms of the non-local large momentum expansion \[ (3.13) \] (cf. the appendix) as suggested in [12] does not result in the correct renormalised 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 \[ (3.17) \]. Only the remaining part needs to be calculated numerically.

Appendix

In this appendix we wish to derive an asymptotic expansion of the conformal-like mode functions \( g_k \) in inverse powers of \( \Omega k_0 \), i.e. for large momentum. The Volterra-type integral equation \[ (3.10) \] (which holds for sufficiently large \( k \)) serves as the starting point. The iteration procedure

\[
\tilde{g}_k^{(n+1)}(\eta) = \frac{i}{2\Omega k_0} \int_{\eta_0}^{\eta} d\eta' K_k(\eta, \eta') \left[ 1 + \tilde{g}_k^{(n)}(\eta') \right]
\]  

(A.1)

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

\[
K_k(\eta, \eta') \overset{\text{def}}{=} \left[ e^{2\Omega k_0 (\eta - \eta')} - 1 \right] \Delta \Omega^2(\eta').
\]  

(A.2)

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

\[
\tilde{g}_k(\eta) = \sum_{n=1}^{\infty} \left( \frac{i}{2\Omega k_0} \right)^n \int_{\eta_0}^{\eta} d\eta_1 K_k(\eta, \eta_1) \cdots \int_{\eta_0}^{\eta_{n-1}} d\eta_n K_k(\eta_{n-1}, \eta_n).
\]  

(A.3)

The estimate

\[
|\tilde{g}_k(\eta)| \leq \exp \left\{ \frac{1}{\Omega k_0} \int_{\eta_0}^{\eta} d\eta' \left| \Delta \Omega^2(\eta') \right| \right\} - 1
\]  

(A.4)

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 \( \Omega k_0 \) can now be achieved by expanding each addend of the series \[ (A.3) \]. For this purpose we provide repeatedly integration by parts \( (\Delta \Omega^2, \text{i.e. } R(\eta) \text{ is assumed to be smooth}) \) to the most inner integral of the \( n \)th addend and find

\[
\int_{\eta_0}^{\eta_{n-1}} d\eta_n K_k(\eta_{n-1}, \eta_n) = - \int_{\eta_0}^{\eta_{n-1}} d\eta_n \Delta \Omega^2(\eta_n)
\]  

(A.5)
\[-\sum_{m=0}^{\infty} \left( \frac{-i}{2\Omega_{k0}} \right)^{m+1} \left[ \Delta \Omega^{2(m)}(\eta_{n-1}) - \Delta \Omega^{2(m)}(\eta_0) e^{2i\Omega_{k0}(\eta_{n-1}-\eta_0)} \right].\]

As all subsequent integrations have the same structure, they are treated likewise. The result is an asymptotic series for the \(n\)th addend of (A.3) 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 \(\Omega_{k0}^{-n}\) are contained in the first \(n\) addends of (A.3). If \(n = 4\) we find, for example,

\[
\Re \tilde{g}_k(\eta) = -\frac{1}{4\Omega_{k0}^2} \left[ \Delta \Omega^2 + \frac{1}{2} I_1^2 \right] + \frac{1}{8\Omega_{k0}^4} \Delta \Omega^{2''} \sin 2\Omega_{k0}(\eta - \eta_0)
+ \frac{1}{16\Omega_{k0}^4} \left[ \Delta \Omega^{2''} - \Delta \Omega^{2''} \cos 2\Omega_{k0}(\eta - \eta_0) + \Delta \Omega^{2''} I_1 + \frac{5}{2} (\Delta \Omega^2)^2 \right.
+ \Delta \Omega^{2''} I_1 \cos 2\Omega_{k0}(\eta - \eta_0) + \frac{1}{2} \Delta \Omega^2 I_1^2 + I_1 I_2 + \frac{1}{4!} I_1^4 \bigg] + O(\Omega_{k0}^{-5})
\]

\[
\Im \tilde{g}_k(\eta) = -\frac{1}{2\Omega_{k0}} I_1 + \frac{1}{8\Omega_{k0}^3} \left[ \Delta \Omega^{2'} - \Delta \Omega^{2'} \cos 2\Omega_{k0}(\eta - \eta_0) \right.
+ \Delta \Omega^{2'} I_1 + I_2 + \frac{1}{3!} I_3 \bigg] - \frac{1}{16\Omega_{k0}^4} \left[ \Delta \Omega^{2''} \sin 2\Omega_{k0}(\eta - \eta_0) \right.
- \Delta \Omega^{2''} I_1 \sin 2\Omega_{k0}(\eta - \eta_0) \bigg] + O(\Omega_{k0}^{-5}),
\]

where the abbreviation
\[
I_m = \int_{\eta_0}^{\eta} d\eta' \left[ \Delta \Omega^2(\eta') \right]^m
\]

has been used. Note that (A.6) already contains all terms contributing to the divergences of the trace (3.13).

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