

Choice of initial states in nonequilibrium dynamics

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Imposing initial conditions to nonequilibrium systems at some time t_0 leads, in renormalized quantum field theory, to the appearance of singularities in the variable $t-t_0$ in relevant physical quantities, such as energy density and pressure. These “initial singularities” can be traced back to the choice of initial state. We construct here, by a Bogoliubov transformation, initial states such that these singularities are eliminated. While the construction is not unique it can be considered a minimal way of taking into account the nonequilibrium evolution of the system prior to t_0 . [S0556-2821(98)04210-6]

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I. INTRODUCTION

Nonequilibrium dynamics in quantum field theory has become, during the last years, a very active field of research in particle physics [1–6] and in solid state physics [21]. The outline of typical computational experiments is as follows: a quantum field $\psi(\mathbf{x}, t)$ is driven by a classical field degree of freedom (Higgs, inflaton, condensate) $\phi(t)$ which takes an initial value away from a local or global minimum of the classical or effective action; the time development is then studied including the back reaction of the quantum field in one-loop, Hartree or large- N approximations. The initial state of the quantum field ψ is usually taken to be the vacuum state corresponding to a free field of some “initial mass” $m(t_0)$ or a thermal state built on such a vacuum state. In Friedmann-Robertson-Walker (FRW) cosmology [7–20] the usual initial quantum state is chosen to be the conformal vacuum, again corresponding to the initial mass $m(t_0)$. While such choices seem very natural, they are not necessarily appropriate; nevertheless, this point has received little attention up to now. The reason why we address this question is the occurrence, in some dynamically relevant physical quantities, of singularities in the time variable which are related to the choice of initial state. We will in fact show that these singularities can be removed by more appropriate choices.

The origin of these singularities can be traced back to a discontinuous switching on of the interaction with the external field $\phi(t)$. This interaction is given by a time-dependent mass term¹ $m^2(t) = m^2(0) + V(t)$ where, for the simplest case of a $\lambda\Phi^4$ theory [9,22],

$$V(t) = \frac{\lambda}{2} [\phi^2(t) - \phi^2(0)]. \quad (1)$$

In FRW cosmology the (conformal) time dependent mass term reads [7,19]

$$M^2(\tau) = a^2(\tau) \left\{ m^2 + \left(\xi - \frac{1}{6} \right) R(\tau) + \frac{\lambda}{2} \frac{\phi^2(\tau)}{a^2(\tau)} \right\}. \quad (2)$$

In this case $M^2(\tau)$ and therefore $V(\tau) = M^2(\tau) - M^2(0)$ also contain the scale parameter $a(\tau)$ and the curvature scalar $R(\tau)$.

A free field theory vacuum state corresponding to the mass $m(0)$ would be an appropriate equilibrium state if $V(t)$ stayed zero for all times. However, at $t=0$ the potential $V(t)$ changes in a nonanalytic way. This is unavoidable since at least the second derivative of $\phi(t)$ becomes nonzero on account of the equation of motion. As a result of these discontinuities relevant physical quantities develop singularities in the time variable t at $t=0$. In the case of $\lambda\Phi^4$ theory in Minkowski space such singularities only occur in the pressure. In FRW cosmology the problem becomes more acute. There, even the first derivative of $V(t)$ necessarily becomes nonzero at $t=0$; indeed, even with a constant external field ϕ the initial state could not be at equilibrium; this manifests itself by a nonvanishing first derivative of the scale parameter induced by the Friedmann equations. Furthermore, in this case both energy and pressure become singular; since they enter the Friedmann equations, this singular behavior also affects the dynamics.

Singularities arising from imposing initial conditions on quantum systems were noted for the first time by Stueckelberg [23], who called them “surface singularities”; they are briefly mentioned in the textbook of Bogoliubov and Shirkov [24]. The “Casimir effect” arising from initial conditions has been discussed by Symanzik [25]. In the context of nonequilibrium dynamics in FRW cosmology the occurrence of such singularities has been noted by Ringwald [7]. While he uses conformal time and the ensuing definition of the initial state, the use of comoving time leads to rather serious problems with renormalization, again related to the initial state [9,11]. In the following we will refer to these singularities as “initial singularities.”

Imposing an initial condition at some time t_0 does not mean, in most applications, that one assumes the system to have come into being at just this time. Rather, t_0 is usually chosen as a point in time at which one can make, on some physical grounds, plausible assumptions about the state of the system. Clearly, if the system is not at equilibrium after

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¹We choose $t_0=0$ for convenience.

t_0 , it will not have been so before. Therefore, the initial state should take into account, at least in some minimal way, the previous nonequilibrium evolution of the system. Such a minimal requirement is the vanishing of initial singularities. It is the aim of this paper to specify such initial states.

In order to avoid excessive algebra and to keep the presentation as transparent as possible we restrict our discussion to Φ^4 theory in the one-loop approximation. Clearly it also applies to the large- N approximation, to finite temperature systems and in particular to evolution in FRW cosmology where the problem of initial singularities is most stringent.

The plan of the paper is as follows: in Sec. II we present the basic equations and formulate the problem for the case of a $\lambda\Phi^4$ theory; in Sec. III we discuss an appropriate choice of the initial quantum state such that the singular behavior in the time variable is removed; the modified renormalized equations for the nonequilibrium system are given in Sec. IV; we end with some concluding remarks in Sec. V.

II. FORMULATION OF THE PROBLEM

We consider a scalar $\lambda\Phi^4$ theory without spontaneous symmetry breaking. The Lagrangian density is given by

$$\mathcal{L} = \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 - \frac{\lambda}{4!} \Phi^4. \quad (3)$$

We split the field Φ into its expectation value ϕ and the quantum fluctuations ψ :

$$\Phi(\mathbf{x}, t) = \phi(t) + \psi(\mathbf{x}, t), \quad (4)$$

with

$$\phi(t) = \langle \Phi(\mathbf{x}, t) \rangle = \frac{\text{Tr } \Phi \rho(t)}{\text{Tr } \rho(t)}, \quad (5)$$

where $\rho(t)$ is the density matrix of the system which satisfies the Liouville equation

$$i \frac{d\rho(t)}{dt} = [\mathcal{H}(t), \rho(t)]. \quad (6)$$

The Lagrangian then takes the form

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1, \quad (7)$$

with

$$\mathcal{L}_0 = \frac{1}{2} \partial_\mu \psi \partial^\mu \psi - \frac{1}{2} m^2 \psi^2 + \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 - \frac{\lambda}{4!} \phi^4, \quad (8)$$

$$\mathcal{L}_1 = \partial_\mu \psi \partial^\mu \phi - m^2 \psi \phi - \frac{\lambda}{4!} \psi^4 - \frac{\lambda}{6} \psi^3 \phi - \frac{\lambda}{4} \psi^2 \phi^2 - \frac{\lambda}{6} \psi \phi^3. \quad (9)$$

The equation of motion for the field $\phi(t)$ is given by [9]

$$\ddot{\phi}(t) + m^2 \phi(t) + \frac{\lambda}{6} \phi^3(t) + \frac{1}{i} \frac{\lambda}{2} \phi(t) G^{++}(t, \mathbf{x}; t, \mathbf{x}) = 0. \quad (10)$$

Here G^{++} is the $++$ matrix element of the exact nonequilibrium Green function [26,27] in the background field $\phi(t)$. For a pure initial state $|i\rangle$ it can be written as

$$-iG^{++}(t, \mathbf{x}; t', \mathbf{x}') = \langle i | T \psi(t, \mathbf{x}) \psi(t', \mathbf{x}') | i \rangle. \quad (11)$$

If the classical field is spatially uniform, the equation of motion for the field $\psi(t, \mathbf{x})$ is given by

$$\left[\frac{\partial^2}{\partial t^2} - \Delta + m^2 + \frac{\lambda}{2} \phi^2(t) \right] \psi(t, \mathbf{x}) = 0. \quad (12)$$

We introduce the notation

$$m^2(t) = m^2 + \frac{\lambda}{2} \phi^2(t), \quad (13)$$

$$\omega_k(t) = [\mathbf{k}^2 + m^2(t)]^{1/2}, \quad (14)$$

and

$$\omega_{k0} = [\mathbf{k}^2 + m_0^2]^{1/2}. \quad (15)$$

We will discuss the choice of m_0 below. We define the ‘‘potential’’ $V(t)$ as

$$V(t) = \omega_k^2(t) - \omega_{k0}^2. \quad (16)$$

We further introduce the mode functions for fixed momentum $U_k(t) \exp(i\mathbf{k} \cdot \mathbf{x})$ which satisfy the evolution equation²

$$\left[\frac{\partial^2}{\partial t^2} + \omega_k^2(t) \right] U_k(t) = 0; \quad (17)$$

we choose the initial conditions

$$U_k(0) = 1, \quad \dot{U}_k(0) = -i\omega_{k0}. \quad (18)$$

The field ψ can now be expanded as

$$\psi(t, \mathbf{x}) = \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} [a(\mathbf{k}) U_k(t) e^{i\mathbf{k} \cdot \mathbf{x}} + a^\dagger(\mathbf{k}) U_k^*(t) e^{-i\mathbf{k} \cdot \mathbf{x}}], \quad (19)$$

where the operators $a(\mathbf{k})$ satisfy

$$[a(\mathbf{k}), a^\dagger(\mathbf{k}')] = (2\pi)^3 2\omega_{k0} \delta^3(\mathbf{k} - \mathbf{k}'). \quad (20)$$

If the initial state $|i\rangle$ is chosen as the vacuum state corresponding to the operators $a(\mathbf{k})$, i.e., as satisfying $a(\mathbf{k})|i\rangle = 0$, we obtain the Green function $G^{++}(t, t'; \mathbf{x} - \mathbf{x}')$ as

$$G^{++}(t, t'; \mathbf{x} - \mathbf{x}') = \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} [U_k(t) U_k^*(t') \theta(t - t') + U_k(t') U_k^*(t) \theta(t' - t)] e^{i\mathbf{k}(\mathbf{x} - \mathbf{x}')}. \quad (21)$$

The Green function at equal space and time points then reads

²Note that the functions $U_k(t)$ depend only on the absolute value of \mathbf{k} .

$$G_k^{++}(t, t; \mathbf{0}) = i \int \frac{d^3 k}{(2\pi)^3 2\omega_{k0}} |U_k(t)|^2. \quad (22)$$

The resulting equation of motion for the classical field $\phi(t)$ is

$$\dot{\phi}(t) + m^2 \phi(t) + \frac{\lambda}{6} \phi^3(t) + \frac{\lambda}{2} \phi(t) \mathcal{F}(t) = 0, \quad (23)$$

where we have introduced fluctuation integral

$$\mathcal{F}(t) \equiv \int \frac{d^3 k}{(2\pi)^3 2\omega_{k0}} |U_k(t)|^2. \quad (24)$$

It determines the back reaction of the fluctuations onto the classical field $\phi(t)$.

We further consider the energy density and the pressure. The energy density is given by

$$\mathcal{E} = \frac{1}{2} \dot{\phi}^2(t) + V(\phi(t)) + \frac{\text{Tr } \mathcal{H}\rho(0)}{\text{Tr } \rho(0)}. \quad (25)$$

Calculating the trace over the Hamiltonian for the same initial state we obtain

$$\begin{aligned} \mathcal{E} = & \frac{1}{2} \dot{\phi}^2(t) + \frac{1}{2} m^2 \phi^2(t) + \frac{\lambda}{4!} \phi^4(t) \\ & + \int \frac{d^3 k}{(2\pi)^3 2\omega_{k0}} \left\{ \frac{1}{2} |\dot{U}_k(t)|^2 + \frac{1}{2} \omega_k^2(t) |U_k(t)|^2 \right\}. \end{aligned} \quad (26)$$

Using the equations of motion it is easy to see that the time derivative of the energy density vanishes.

The pressure is given by

$$p = \dot{\phi}^2(t) + \int \frac{d^3 k}{(2\pi)^3 2\omega_{k0}} \left\{ |\dot{U}_k^+(t)|^2 + \frac{\mathbf{k}^2}{3} |U_k^+(t)|^2 \right\} - \mathcal{E}. \quad (27)$$

The expressions for the fluctuation integral, the energy density and the pressure are divergent and one has to discuss the renormalization of this theory. We have presented recently [22] a fully renormalized framework for nonequilibrium dynamics. The main technical ingredient of this analysis is the perturbative expansion of the functions $U_k(t)$ with respect to orders in the potential $V(t)$. We write the functions U_k as

$$U_k(t) = e^{-i\omega_{k0}t} [1 + h_k(t)] \quad (28)$$

and expand further in orders of the potential $V(t)$ as

$$h_k(t) = \sum_{n=1}^{\infty} h_k^{(n)}(t). \quad (29)$$

We also introduce the partial sums

$$h_k^{(\bar{n})}(t) = \sum_{l=n}^{\infty} h_k^{(l)}(t), \quad (30)$$

so that

$$h_k(t) \equiv h_k^{(\bar{1})}(t) = h_k^{(1)} + h_k^{(\bar{2})}(t). \quad (31)$$

The integral equation for the function $h_k(t)$ can be derived in a straightforward way from the differential equation satisfied by the functions $U_k(t)$; it reads

$$h_k(t) = \frac{i}{2\omega_{k0}} \int_0^t dt' (e^{2i\omega_{k0}(t-t')} - 1) V(t') [1 + h_k(t')]. \quad (32)$$

We obtain

$$h_k^{(1)} = \frac{i}{2\omega_{k0}} \int_0^t dt' (e^{2i\omega_{k0}(t-t')} - 1) V(t'). \quad (33)$$

Using integrations by parts this function can be analyzed with respect to orders in ω_{k0} via

$$\begin{aligned} h_k^{(1)}(t) = & \frac{-i}{2\omega_{k0}} \int_0^t dt' V(t') + \sum_{l=0}^n \left(\frac{-i}{2\omega_{k0}} \right)^{l+2} [V^{(l)}(t) \\ & - e^{2i\omega_{k0}t} V^{(l)}(0)] \\ & - \left(\frac{-i}{2\omega_{k0}} \right)^{n+2} \int_0^t dt' e^{2i\omega_{k0}(t-t')} V^{(n+1)}(t'), \end{aligned} \quad (34)$$

where $V^{(l)}(t)$ denotes the l th derivative of $V(t)$. For the energy density and pressure we need the expansion of $\dot{h}_k^{(1)}(t)$ as well. From Eq. (34) and the relation

$$\dot{h}_k^{(1)} = 2i\omega_{k0} h_k^{(1)} - \int_0^t dt' V(t') \quad (35)$$

we find

$$\begin{aligned} \dot{h}_k^{(1)}(t) = & \sum_{l=0}^n \left(\frac{-i}{2\omega_{k0}} \right)^{l+1} [V^{(l)}(t) - e^{2i\omega_{k0}t} V^{(l)}(0)] \\ & - \left(\frac{-i}{2\omega_{k0}} \right)^{n+1} \int_0^t dt' e^{2i\omega_{k0}(t-t')} V^{(n+1)}(t'). \end{aligned} \quad (36)$$

In the following we will need the real and imaginary parts of this expression; we introduce the following useful notation:

$$\mathcal{C}(f, t) = \int_0^t dt' f(t') \cos[2\omega_{k0}(t-t')], \quad (37)$$

$$\mathcal{S}(f, t) = \int_0^t dt' f(t') \sin[2\omega_{k0}(t-t')]. \quad (38)$$

We now insert the perturbative expansion into the fluctuation integral to obtain

$$\begin{aligned}
\mathcal{F}(t) &= \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \{1 + 2 \operatorname{Re} h_k(t) + |h_k(t)|^2\} \\
&= \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left\{ 1 - \frac{V(t)}{2\omega_{k0}^2} + \frac{V(0)}{2\omega_{k0}^2} \cos(2\omega_{k0}t) \right. \\
&\quad + \frac{\dot{V}(0)}{4\omega_{k0}^3} \sin(2\omega_{k0}t) + \frac{\dot{V}(t)}{8\omega_{k0}^3} - \frac{\dot{V}(0)}{8\omega_{k0}^3} \cos(2\omega_{k0}t) \\
&\quad \left. - \frac{1}{8\omega_{k0}^4} \mathcal{C}(\ddot{V}, t) + 2 \operatorname{Re} \overline{h_k^{(2)}} + |h_k|^2 \right\}. \quad (39)
\end{aligned}$$

The first two terms in the curly brackets of the second expression, i.e., 1 and $V(t)/2\omega_{k0}^2$, lead to divergent integrals which have to be absorbed by the renormalization procedure. This has been discussed in [22]. There, the mass m_0 was chosen to be the ‘‘initial’’ mass $m(0)$ [see Eq. (13)]. With this choice of initial mass $V(0)$ is zero and the fluctuation integral is nonsingular at $t=0$. Though, with this choice, the divergent integrals depend on m_0 it was shown that the renormalization counterterms can be chosen independent of the initial mass $m_0 = m(0)$.

If, on the other hand, we choose $m_0 = m$, it is obvious that the divergences are absorbed by the counterterms depending only on the renormalized mass m , but we are faced with an initial singularity arising from the third term via (see Appendix B)

$$\int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \frac{V(0)}{2\omega_{k0}^2} \cos(2\omega_{k0}t) \approx -\frac{1}{8\pi^2} \ln(2m_0 t)$$

as $t \rightarrow 0$. (40)

Of course, nobody has made such an ‘‘unnatural’’ choice of the initial mass; this initial singularity can be avoided trivially by choosing $m_0 = m(0)$. It is important to note, however, that the renormalization can be performed in a way independent of the initial condition in both cases. The difference between the two approaches is in the initial ‘‘vacuum’’ state. These different initial states are related by a Bogoliubov transformation (see also Appendix A). So Bogoliubov transformations can be used to avoid initial singularities. A similar improvement of initial state, a Bogoliubov transformation from the comoving time vacuum state to the conformal time vacuum state in FRW cosmology, has been discussed previously [11].

In Eq. (39) we have extended the expansion of $\operatorname{Re} h_k^{(1)}(t)$ to display also the terms of order ω_{k0}^{-4} which depend on

$\dot{V}(0)$ and $\ddot{V}(0)$. These terms do not lead to divergences in the fluctuation integral; however, in the energy and pressure they appear multiplied by ω_{k0}^2 and/or k^2 . While the energy stays finite the pressure behaves in a singular way via

$$\begin{aligned}
P_{\text{fluct, sing}} \sim \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left[-\omega_{k0}^2 + \frac{k^2}{3} \right] &\left\{ \frac{\dot{V}(0)}{4\omega_{k0}^3} \sin(2\omega_{k0}t) \right. \\
&\left. - \frac{\dot{V}(0)}{8\omega_{k0}^4} \cos(2\omega_{k0}t) \right\}. \quad (41)
\end{aligned}$$

The behavior of the momentum integrals is given in Appendix B; they result in a $1/t$ singularity proportional to $\dot{V}(0)$ and a logarithmic one proportional to $\ddot{V}(0)$. Therefore, these terms have to be removed as well.

III. REMOVING THE INITIAL SINGULARITY

We have seen in the previous section that nonzero initial values of $V(t)$ and its derivatives lead to initial singularities. The clue for dealing with these terms has already been indicated: the leading singularity can be removed by a Bogoliubov transformation from the perturbative vacuum to a vacuum corresponding to free quanta of the initial mass $m(0)$. We expect, therefore, that the other singular terms can be removed in this way as well.

We define a general initial state by requiring that

$$[a(\mathbf{k}) - \rho_k a^\dagger(\mathbf{k})] |i\rangle = 0. \quad (42)$$

The Bogoliubov transformation to this state is given in Appendix A. If the fluctuation integral, the energy and the pressure are computed by taking the trace with respect to this state, the functions $U_k(t)$ are just replaced by

$$F_k(t) = \cosh(\gamma_k) U_k(t) + e^{i\delta_k} \sinh(\gamma_k) U_k^*(t), \quad (43)$$

where γ_k and δ_k are defined by the relation

$$\rho_k = e^{i\delta} \tanh(\gamma_k). \quad (44)$$

The fluctuation integral now becomes

$$\begin{aligned}
\mathcal{F}(t) &= \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} |F_k(t)|^2 \\
&= \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \{ \cosh[2\gamma_k(t)] |U_k(t)|^2 \\
&\quad + \sinh(2\gamma_k) \operatorname{Re}[e^{-i\delta_k} U_k^2(t)] \}. \quad (45)
\end{aligned}$$

Expanding as before we find

$$\begin{aligned}
\mathcal{F}(t) &= \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left\{ \cosh(2\gamma_k) \left[1 - \frac{V(t)}{2\omega_{k0}^2} + \frac{V(0)}{2\omega_{k0}^2} \cos(2\omega_{k0}t) + \frac{\dot{V}(0)}{4\omega_{k0}^3} \sin(2\omega_{k0}t) \right. \right. \\
&\quad \left. \left. + \frac{\dot{V}(t)}{8\omega_{k0}^4} - \frac{\dot{V}(0)}{8\omega_{k0}^4} \cos(2\omega_{k0}t) \right] \right. \\
&\quad \left. - \frac{1}{8\omega_{k0}^4} \mathcal{C}(\ddot{V}, t) + 2 \operatorname{Re} \overline{h_k^{(2)}} + |h_k|^2 \right\} + \sinh(2\gamma_k) \cos(\delta_k) \cos(2\omega_{k0}t) - \sinh(2\gamma_k) \sin(\delta_k) \sin(2\omega_{k0}t) \\
&\quad \left. + \sinh(2\gamma_k) \operatorname{Re} e^{-2i\omega_{k0}t - i\delta} (2h_k + h_k^2) \right\}. \quad (46)
\end{aligned}$$

Let us first discuss how to get rid of the most singular term, proportional to $V(0)$. Requiring this term to be compensated by the terms proportional to $\sinh(2\gamma_k)$ we find

$$\delta_k = 0, \quad (47)$$

$$\tanh(2\gamma_k) = -\frac{V(0)}{2\omega_{k0}^2}. \quad (48)$$

As explained in Appendix A the standard Bogoliubov transformation from the perturbative vacuum with mass m to the vacuum corresponding to quanta with the initial mass $m(0)$ is mediated by a function $\gamma'_k(k)$ satisfying

$$e^{\gamma'_k} = \left(\frac{m^2 + \mathbf{k}^2}{m^2(0) + \mathbf{k}^2} \right)^{1/4}, \quad (49)$$

which implies

$$\tanh(2\gamma'_k) = \frac{-V(0)}{2\omega_{k0}^2 + V(0)}. \quad (50)$$

We see that γ_k and γ'_k agree asymptotically to leading order in $1/\omega_{k0}$. So requiring that the most pronounced initial singularity vanish leads essentially to the usual choice for the initial state, namely $m_0 = m(0)$ and therefore $V(0) = 0$. The analysis of subleading terms in the difference between γ_k and γ'_k becomes somewhat cumbersome. After we have convinced ourselves that the Bogoliubov transformation is the right technique for getting rid of initial singularities we will therefore choose $m_0 = m(0)$ as everybody does and apply this technique to get rid of the remaining singularities. So from now on $V(0) = 0$ and $\omega_{k0} = [\mathbf{k}^2 + m^2(0)]^{1/2}$. Requiring that the terms proportional to $\dot{V}(0)$ and $\ddot{V}(0)$ vanish leads to the conditions

$$\tan(\delta_k) = 2\omega_{k0} \frac{\dot{V}(0)}{\ddot{V}(0)}, \quad (51)$$

$$\tanh(2\gamma_k) = \frac{1}{4\omega_{k0}^3} \left[\dot{V}^2(0) + \frac{\ddot{V}^2(0)}{4\omega_{k0}^2} \right]^{1/2}. \quad (52)$$

Using these functions we are now ready to formulate the renormalized equation of motion and the energy momentum tensor.

IV. THE RENORMALIZED EQUATIONS

We have given the bare equation of motion and energy momentum tensor in Sec II. The renormalization for the original initial state has been discussed in [22]. We have to ensure now that the scheme used there is not spoiled by the improved initial state. The main new feature in the fluctuation integral, the energy density and the pressure is the appearance of the factors $\cosh(2\gamma_k)$ and $\sinh(2\gamma_k)$. We will need their asymptotic behavior. Using Eq. (52) we have

$$\gamma_k \simeq \frac{k \rightarrow \infty |\dot{V}(0)|}{8\omega_{k0}^3}. \quad (53)$$

The factor $\cosh(2\gamma_k)$ is equal to 1 for $\gamma_k = 0$; we will need the difference

$$\cosh(2\gamma_k) - 1 = 2 \sinh^2(\gamma_k) \simeq \frac{k \rightarrow \infty \dot{V}^2(0)}{32\omega_{k0}^6}. \quad (54)$$

There are new terms proportional to $\sinh(2\gamma_k)$; this factor behaves as

$$\sinh(2\gamma_k) \simeq \frac{k \rightarrow \infty |\dot{V}(0)|}{4\omega_{k0}^3}. \quad (55)$$

The dimensionally regularized fluctuation integral (46) takes, after cancellation of the singular integrals induced by Eqs. (51) and (52), the form

$$\begin{aligned} \mathcal{F}_{\text{reg}}(t) = & -\frac{m_0^2}{16\pi^2}(L_0 + 1) - \frac{V(t)}{16\pi^2}L_0 \\ & + \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left\{ \sinh^2(\gamma_k) \left[1 - \frac{V(t)}{2\omega_{k0}^2} \right] \right. \\ & \left. + \cosh(2\gamma_k) \left[\frac{\ddot{V}(t)}{8\omega_{k0}^4} - \frac{1}{8\omega_{k0}^4} \mathcal{C}(\ddot{V}, t) + 2 \text{Re } h_k^{\overline{2}} \right] \right. \\ & \left. + |h_k|^2 \right\} + \sinh(2\gamma_k) \text{Re } e^{-2i\omega_{k0}t - i\delta} (2h_k + h_k^{\overline{2}}). \end{aligned} \quad (56)$$

Here we have introduced the abbreviation

$$L_0 = \frac{2}{\epsilon} + \ln \frac{4\pi\mu^2}{m_0^2} - \gamma. \quad (58)$$

Using the estimates (54) and (55), and using the fact that the mode function h_k behaves as ω_{k0}^{-1} we see that the momentum integral is convergent.

Introducing the counterterm Lagrangian

$$\mathcal{L}_{\text{c.t.}} = \frac{1}{2} \delta m^2 \Phi^2 + \frac{\delta\lambda}{4!} \Phi^4 \quad (59)$$

the fluctuation integral gets replaced, in the equation of motion (23) for $\phi(t)$, by

$$\mathcal{F}_{\text{fin}} = \mathcal{F}_{\text{reg}} + \frac{2\delta m^2}{\lambda} + \frac{\delta\lambda}{3\lambda} \phi^2(t). \quad (60)$$

With the standard choice

$$\delta m^2 = \frac{\lambda m^2}{32\pi^2}(L + 1), \quad (61)$$

$$\delta\lambda = \frac{3\lambda^2}{32\pi^2}L, \quad (62)$$

$$L = \frac{2}{\epsilon} + \ln \frac{4\pi\mu^2}{m^2} - \gamma, \quad (63)$$

\mathcal{F}_{fin} is indeed finite.

The calculation of the energy density proceeds in an analogous way. The fluctuation energy becomes, using dimensional regularization,

$$\begin{aligned} \mathcal{E}_{\text{fluct}} &= \frac{1}{2} \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \{ |\dot{F}_k(t)|^2 + [\omega_{k0}^2 + V(t)] |F_k(t)|^2 \} \\ &= -\frac{m_0^4}{64\pi^2} \left(L_0 + \frac{3}{2} \right) - m_0^2 \frac{V(t)}{32\pi^2} (L_0 + 1) - \frac{V^2(t)}{64\pi^2} L_0 + \frac{1}{2} \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left\{ 2 \sinh^2(\gamma_k) \left[2\omega_{k0}^2 + V(t) \left(1 - \frac{V(t)}{2\omega_{k0}^2} \right) \right] \right. \\ &\quad + V(t) \cosh(2\gamma_k) \left[\frac{\dot{V}(t)}{8\omega_{k0}^4} - \frac{\mathcal{C}(\ddot{V}, t)}{8\omega_{k0}^4} + 2 \operatorname{Re} h_k^{(2)} + |h_k|^2 \right] + V(t) \sinh(2\gamma_k) \operatorname{Re} e^{-2i\omega_{k0}t - i\delta_k} (2h_k + h_k^2) + \cosh(2\gamma_k) \\ &\quad \left. \times \left(|\dot{h}_k|^2 - \frac{V^2(t)}{4\omega_{k0}^2} \right) + \sinh(2\gamma_k) \operatorname{Re} e^{-2i\omega_{k0}t - i\delta_k} [\dot{h}_k^2 - 2i\omega_{k0}(1+h_k)\dot{h}_k] \right\}. \end{aligned} \quad (64)$$

The divergent parts are cancelled by the counterterms

$$\mathcal{E}_{\text{c.t.}} = \delta\Lambda + \frac{1}{2} \delta m^2 \phi^2(t) + \frac{\delta\lambda}{4!} \phi^4(t) \quad (66)$$

with the ‘‘cosmological constant’’ counterterm

$$\delta\Lambda = \frac{m^4}{64\pi^2} \left(L + \frac{3}{2} \right). \quad (67)$$

Finally, we have to consider the pressure. We find, for the regularized fluctuation part,

$$\begin{aligned} p_{\text{fluct}} &= -\mathcal{E}_{\text{fluct}} - \frac{m_0^4}{96\pi^2} - \frac{V(t)}{48\pi^2} m_0^2 - \frac{\dot{V}(t)}{96\pi^2} \left(L_0 + \frac{1}{3} \right) + \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \left\{ \sinh^2(\gamma_k) \left[2\omega_{k0}^2 + \left(-\omega_{k0}^2 + \frac{k^2}{3} \right) \left(1 - \frac{V(t)}{2\omega_{k0}^2} + \frac{\dot{V}(t)}{8\omega_{k0}^4} \right) \right] \right. \\ &\quad + \cosh(2\gamma_k) V \left(-\omega_{k0}^2 + \frac{k^2}{3} \right) \left[-\frac{\mathcal{C}(\ddot{V}, t)}{8\omega_{k0}^4} + 2 \operatorname{Re} h_k^{(2)} + |h_k|^2 \right] + \cosh(2\gamma_k) |\dot{h}_k|^2 \sinh(2\gamma_k) \operatorname{Re} e^{-2i\omega_{k0}t - i\delta_k} \left[-\omega_{k0}^2 + \frac{k^2}{3} \right] \\ &\quad \left. \times (2h_k + h_k^2) + \dot{h}_k^2 - 2i\omega_{k0}(1+h_k)\dot{h}_k \right\}. \end{aligned} \quad (68)$$

In order to cancel the divergent term proportional to \dot{V} one introduces a counterterm for the energy momentum tensor,

$$\delta T_{\mu\nu} = A (g_{\mu\nu} \partial_\alpha \partial^\alpha - \partial_\mu \partial^\nu) \Phi^2, \quad (69)$$

which leads to a counterterm

$$p_{\text{c.t.}} = A \frac{d^2}{dt^2} \phi^2(t) = \frac{2A}{\lambda} \dot{V}(t) \quad (70)$$

in the pressure. We choose

$$A = -\frac{\lambda}{192\pi^2} L. \quad (71)$$

The remaining momentum integral is finite and nonsingular in t . For most of the terms this can be seen by inspection using Eqs. (54),(55), and the expansions (34) and (36). There are some internal cancellations which are, however, the same

as for the case $\gamma_k=0$ already discussed in [22]. The only new, potentially singular term is

$$\int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \sinh(2\gamma_k) \left(-\omega_{k0}^2 + \frac{k^2}{3} \right) \operatorname{Re} e^{-2i\omega_{k0}t} 2h_k. \quad (72)$$

The leading singular behavior is given by

$$\begin{aligned} \dot{V}(0) \int_0^t dt' V(t') \int \frac{d^3k}{(2\pi)^3 2\omega_{k0}} \frac{1}{4\omega_{k0}^4} \\ \times \left(-\omega_{k0}^2 + \frac{k^2}{3} \right) \cos(2\omega_{k0}t). \end{aligned} \quad (73)$$

While the momentum integral behaves as $\ln t$ as $t \rightarrow 0$ the time integral behaves as t^2 since $V(0)=0$. So the renormalized pressure is indeed nonsingular at $t=0$.

From the analysis of divergent integrals given in this section it is obvious that only the leading asymptotic behavior

of γ_k is relevant, more precisely, only the terms of order ω_{k0}^{-3} and ω_{k0}^{-4} . This means that any Bogoliubov transformation whose function γ_k has this leading asymptotic behavior is equally suitable for defining an appropriate initial state.

We have formulated our modified renormalized equations for $\lambda\Phi^4$ theory in flat space. The generalization to a scalar field in a flat Friedmann-Robertson-Walker universe is straightforward and the cancellation of singular terms in the energy density and the trace of the energy momentum tensor proceeds in the same way.

V. CONCLUSIONS

We have considered here the choice of initial states for a nonequilibrium system in quantum field theory. Our considerations arose from the problem that logarithmic and linear singularities in the variable $t-t_0$ appear in the energy momentum tensor and affect the dynamics of FRW cosmology. We consider such singularities—and their consequences—as unphysical, at least if t_0 is just some conveniently chosen point in time within a continuous evolution of the system. Most authors, including ourselves, have chosen initial states that correspond to equilibrium states of the system. We have constructed here improved initial states for nonequilibrium systems in such a way that the appearance of initial singularities is avoided. These states are obtained from the usual “vacuum” states by a Bogoliubov transformation. The essential part of this transformation is a Bogoliubov “rotation” of the creation and annihilation operators at large momentum. The construction presented here specifies a transformation of creation and annihilation operators at all momenta. It is not unique in the sense that it may be arbitrarily modified at small momenta. This nonuniqueness is, however, nothing else as the freedom for choosing an “arbitrary,” pure or mixed, initial state. Our construction can be considered as formulating a minimal requirement for choosing such states in the sense that it specifies the initial state of the high momentum quantum modes.

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APPENDIX A: BOGOLIUBOV TRANSFORMATION

In this appendix we briefly recall some basic features of the Bogoliubov transformation (see, e.g., [28]). We start with a vacuum state defined by

$$a(\mathbf{k})|0\rangle=0. \quad (\text{A1})$$

We would like to obtain a new state $|\tilde{0}\rangle$ that is annihilated by $a(\mathbf{k})+\rho_k a^\dagger(\mathbf{k})$, where ρ_k is some complex function of k ; i.e. we require

$$[a(\mathbf{k})-\rho_k a^\dagger(\mathbf{k})]|\tilde{0}\rangle=0. \quad (\text{A2})$$

Such a state can be obtained from $|0\rangle$ by a Bogoliubov transformation

$$|\tilde{0}\rangle=\exp(Q)|0\rangle. \quad (\text{A3})$$

Using the general relations given in [28] one finds the explicit form of the operator Q as

$$Q=\frac{1}{2}\int\frac{d^3k}{(2\pi)^32\omega_{k0}}\gamma_k[e^{i\delta_k}a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})-e^{-i\delta_k}a(\mathbf{k})a(-\mathbf{k})]. \quad (\text{A4})$$

Here γ_k and δ_k are defined by the relation

$$\rho_k=e^{i\delta_k}\tanh\gamma_k \quad (\text{A5})$$

so that Eq. (A2) can also be written as

$$\tilde{a}(\mathbf{k})|\tilde{0}\rangle=[\cosh(\gamma_k)a(\mathbf{k})+e^{i\delta_k}\sinh(\gamma_k)a^\dagger(-\mathbf{k})]|\tilde{0}\rangle=0. \quad (\text{A6})$$

A special class of new “vacuum” states $|\tilde{0}\rangle$ is obtained when the new creation and annihilation operators refer to free particles with a different mass \tilde{m}_0 . In the field expansion (19) this means that the energy $\omega_{k0}=(\mathbf{k}^2+m_0^2)^{1/2}$ is replaced by $\tilde{\omega}_{k0}=(\mathbf{k}^2+\tilde{m}_0^2)^{1/2}$. In this case

$$\tilde{a}(\mathbf{k})=\sqrt{\frac{\tilde{\omega}_{k0}}{\omega_{k0}}}a(\mathbf{k})+\sqrt{\frac{\omega_{k0}}{\tilde{\omega}_{k0}}}a^\dagger(\mathbf{k}) \quad (\text{A7})$$

and therefore

$$\gamma_k=\frac{1}{2}\ln\frac{\omega_{k0}}{\tilde{\omega}_{k0}} \quad (\text{A8})$$

while $\delta_k=0$. For $k\gg m_0, \tilde{m}_0$ the function γ_k behaves as

$$\gamma_k\approx\frac{m_0^2-\tilde{m}_0^2}{4k^2}. \quad (\text{A9})$$

APPENDIX B: SOME SINGULAR INTEGRALS

The singular behavior in time arises from the following integrals:

$$I_1(t)=\int\frac{d^3k}{(2\pi)^32\omega_{k0}}\frac{1}{\omega_{k0}^2}\cos(\omega_{k0}t) \quad (\text{B1})$$

and

$$I_2(t)=\int\frac{d^3k}{(2\pi)^32\omega_{k0}}\frac{1}{\omega_{k0}}\sin(\omega_{k0}t). \quad (\text{B2})$$

The first integral can be rewritten as

$$\begin{aligned}
I_1(t) &= \frac{1}{4\pi^2} \int_m^\infty \frac{d\omega \sqrt{\omega^2 - m^2}}{\omega^2} \cos(2\omega t) \\
&= \frac{1}{4\pi^2} \int_m^\infty d\omega \left(\frac{1}{\sqrt{\omega^2 - m^2}} \cos(2\omega t) \right. \\
&\quad \left. - \frac{m^2}{\omega^2 \sqrt{\omega^2 - m^2}} \cos(2\omega t) \right). \quad (\text{B3})
\end{aligned}$$

The integral over the second term is nonsingular; the first term yields a Bessel function $Y_0(2mt)$, explicitly

$$I_1(t) = -\frac{1}{8\pi} Y_0(2mt) + O(t^2) \stackrel{t \rightarrow 0}{\approx} -\frac{1}{4\pi^2} \ln(2mt). \quad (\text{B4})$$

The integral $I_2(t)$ is simply given by

$$I_2(t) = -\frac{1}{2} \frac{d}{dt} I_1(t) \quad (\text{B5})$$

and therefore

$$I_2(t) \stackrel{t \rightarrow 0}{\approx} \frac{1}{8\pi^2 t}. \quad (\text{B6})$$

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