Entropy generation in cosmological particle creation and interactions: A statistical subdynamics analysis

B. L. Hu* and Henry E. Kandrup†
Center for Theoretical Physics, Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
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This paper applies a statistical-mechanics notion of nonequilibrium entropy to a quantum field in a cosmological setting. The key idea is to view the bosonic field as a collection of harmonic oscillators, with natural frequencies $\Omega(t)$, and to define a time-dependent entropy $S(t)$ which reflects correlations among the oscillators. The S so defined will be a constant of the motion in the absence of couplings, so that, e.g., there can be no entropy generation for a source-free linear field in a conformally static spacetime. If, however, interactions are induced by nonlinearities, material sources, or a more general dynamical background, S will exhibit a nontrivial time dependence. The form of this time dependence can be analyzed through the introduction of a "subdynamics," and one concludes that, at least in one limit, $dS/dt > 0$. Specifically, in addition to the "stimulated" changes in entropy, which reflect the choice of initial conditions and which can be either negative or positive, there will also be a "spontaneous" change in S induced by the dynamics which, at least for short times, is necessarily positive. The subdynamics analysis can also be applied to the phenomenon of particle creation, and one concludes that, here as well, there is a "natural" decomposition into a "spontaneous" particle creation induced by the dynamics, which leads to the net generation of quanta and a "simulated" change in particle number reflecting the choice of initial conditions, which is of indeterminate sign. The "spontaneous" contributions to particle creation can in turn be decomposed into two positive contributions: one, reflecting the effects of correlations, which is connected with spontaneous entropy generation, and another, induced by the time dependence of the Ω's, which reflects instead a type of "phase mixing."

I. INTRODUCTION

The general goal of this and related earlier work[1,2] has been to understand the statistical properties of quantum fields in curved space. Specifically, we are interested here in the conditions and assumptions underlying the definition and usage of entropy associated with quantum processes such as particle creation and interaction[3,4] in dynamical spacetimes. The relevance of this investigation with ongoing research in general relativity, quantum field theory, and statistical physics is at least twofold: (1) physical problems related to quantum-statistical processes in the early Universe and black holes and (2) theoretical issues related to the statistical nature of fields and geometry, both classical and quantum.

Cosmological particle production occurring in the Planck area at $\sim 10^{-43}$ sec after the big bang has been shown to be capable of playing a major role in determining the matter content and influencing the later evolution of the Universe.[5-7] This production is also believed to be a major source of entropy generation which may account for, among other observations, the age of the Universe.[8] Pair creation and interaction in strong or time-varying gravitational fields is an intrinsically nonlocal, nonequilibrium quantum-statistical process.[9] Recently we see the beginning of attempts to develop techniques and formalisms for treating nonequilibrium quantum processes in curved space.[10-12] An understanding of how entropy is to be defined and measured for quantum fields is essential to these developments.

The Bekenstein-Hawking result on black-hole quantum radiance[13] is perhaps the foremost example of how the behavior of quantum systems in curved space lends itself forcefully to a thermodynamic interpretation.[14] It is tempting to ask similar theoretical questions for more general curved spacetimes. However, while a geometric meaning of entropy is relatively well defined for spacetimes possessing event horizons, the more general case of cosmological spacetimes are more difficult to analyze, since in addition to global geometric factors, dynamics enters in an essential way. In the test-field approximation, where the background metric is assumed fixed, one is interested in entropy generation associated with the creation and interaction of particles from the vacuum or other quantum states with specified phase information. In the self-consistent treatment, where the back reaction of matter fields is included in the consideration, one would be interested also in how quantum-statistical effects of matter fields can influence the dynamics and geometry of spacetime.[5-7] Through this one hopes to deduce some statistical measures or criteria for the realization of certain geometries as physical spacetimes. If spacetime has some well-defined entropy, e.g., the gravitational entropy of Penrose,[15] then this may provide a thermodynamic description of Einstein's geometrodynamics. It has also been suggested[16] that the entropy of matter creation from the vacuum may provide some measure of the entropy of geometry and its dynamics. However, a viable definition of gravitational entropy is hitherto lacking. It is with the aim of understanding these issues concerning matter geometry and particle fields that a study of the statistical properties of the quantum fields may prove fruitful. The present work aims to provide a few threads for knitting a web of interconnections for these ideas.

As in the analysis of the entropy associated with black-hole radiance, several basic aspects enter into the consideration of entropy generation in cosmological spacetimes: the gravitational curved-spacetime aspect, the quantum-field aspect, and the statistical-mechanics aspect. The mechanisms for particle creation in black-hole and cosmological spacetimes are qualitatively different: the former is a result of infinite red-shift near event horizons, whereas the latter is related to the backscattering of waves. Cosmological particle production can be understood as the nonadiabatic parametric amplification of vacuum fluctuations,[3,4,17] a process similar in nature to pair creation in a strong external field. Here the coupling of the system with the external source or driving force, the interaction of modes, the phase relation of initial states, the change of correlations in time, the geometry of the spacetime, and the evolutionary history of the system all enter in entropy considerations. As suggested in Ref. 1 entropy generation can be considered in accordance with the nature of particle production and interaction as occurring in three stages: (1) creation from the vacuum or from n-particle states, (2) particle interaction, and (3) nonadiabatic red-shifting. These are not necessarily chronological stages, but should instead be viewed as different interconnected and overlapping factors. For example, with free fields, particles can be created from the vacuum (spontaneous production) or from an initial n-particle state with nontrivial phase information (stimulated production), the latter causing either an enhancement or depletion of the former, depending on the phase relation of the states and the spin-statistics of the particles. For interacting fields there could be additional contributions from multiparticle production. In spacetimes with lesser symmetry, where the fields do not admit a "natural" normal-mode decomposition, modes can also be coupled via the dynamics of spacetime over and above the coupling associated with explicit interactions.[17] In a changing background like the expanding Universe the created particles are constantly red-shifted. The nonadiabatic changes of the modes is an additional source of entropy generation, albeit one which is classical in nature and well understood. Analyzing entropy generation from particle production needs a better understanding of the origin and nature of the particle production processes—creation through spontaneous and stimulated excitation, extrinsic and intrinsic mode couplings and interactions, and nonadiabatic red-shifting. One also needs a viable framework to define entropy under these specific conditions.

Three earlier studies[1,18,19] sought to formulate the problem in a way understandable in simpler terms. Reference 1 used finite-temperature theory to derive the viscosity functions associated with the nonadiabatic red-shifting of modes in the classical (late times) regime. Reference 18 attempted a phenomenological description of the exact results from detailed back-reaction calculations of particle production in sample cosmological spacetimes with curved-space quantum-field-theory techniques. Using an imperfect-fluid formulation, Ref. 18 derived the viscosity functions associated with dissipations of the background dynamics from vacuum particle creation in the quantum regime. From the nature of the approximations used, we may call this a thermodynamic entropy.[20] Extending the ideas of Ref. 1, Ref. 19 analyzed the problem of vacuum creation in closer detail by studying a system of parametric oscillators and explored the rationale for regarding the number of particles produced spontaneously as a measure of entropy in such processes.

On the other hand, as already noted in Ref. 1, in a strict statistical-mechanics sense, where entropy is regarded as a measure of correlations or the lack thereof, the time-reversal invariance of the classical or quantum-mechanic laws governing the system suggests that one should expect no entropy change between an initial vacuum state and a final state consisting of particle pairs. In particular, the pair is produced with exact correlations, albeit at a spatial separation. As with any closed system, entropy appears only when one divides the whole system into a part that is of interest to the observer (the system) and the rest (the "bath") whose detailed correlation and evolution one does not need or want to know. This is the idea behind a statistical "subdynamics" analysis.[21–25] The introduction of a suitable notion of "coarse graining" which entails a "loss of information" lies at the heart of a statistical definition of entropy, and underlies the basic approach adopted in this paper.[2,26,27] From this point of view, it is easy to see that entropy generation can arise from the interaction, scattering, and decay of particles but not from the creation of particles, i.e., entropy can be generated in the second and third stages in the description of Ref. 1, but not in the first stage. Of course, in realistic situations, the normal modes of a system are usually coupled through interactions or dynamics, and thus the two processes of creation and interaction are necessarily interlinked. Given that "particle creation" generally refers to all of these processes combined, the entropy generation deduced here from a statistical mechanics definition and viewpoint is consistent with the thermodynamic viewpoint,[1,18] since the latter is premised upon the existence of strong interaction among the particles.

This paper is organized as follows. In Sec. II we give an elementary description of particle creation in dynamic spacetimes, starting with the Lagrangian of a free quantum field and ending with the Hamiltonian for a set of time-dependent coupled harmonic oscillators. We will use this coupled-oscillator system to model particle creation and discuss how to define the entropy of dynamical fields. We first show how vacuum particle production is related to parametric amplification. Using canonical quantization we derive an expression for the number density and the energy density of the produced particles. We indicate how the choice of the initial state—zero (vacuum) or n-particle states, including the stipulation of phase relations, leads to spontaneous and stimulated production of particles. We then use a $\lambda\phi^4$ theory to show that interaction of modes can lead to particle production. Finally we illustrate with a more general class of spacetime (the mixmaster universe) how mode coupling can also arise from the dynamics of the background spacetime without explicit interactions. These are the most relevant factors in particle creation which enter into the consideration of entropy generation. Section III introduces the statistical-mechanical view of entropy and its application to classical and quantum fields.[2] We review some of the basic notions of entropy, discuss the meaning of "coarse graining," and construct a "subdynamics" by projection operator techniques. We then discuss the properties of statistical entropy and show that it obeys some of the well-known properties. In Sec. IV we apply the method introduced in Sec. III to the consideration of entropy generation in particle creation processes as described in Sec. II. We discuss the effect of interaction and correlation and present results for entropy generation associated with spontaneous and induced particle creation. Section V ends with a discussion of the concepts used and elicited in this paper.

II. COSMOLOGICAL PARTICLE CREATION AND INTERACTION

This section gives a simplified but self-contained description of particle creation and interaction via the canonical quantization of fields in cosmological backgrounds.[3] The aim is to enable those readers unfamiliar with the methods of quantum field theory in curved spacetime[28] to understand the physical origin of these processes in quantum-mechanical language.

A. Free fields

Consider a massive (m) scalar field Φ coupled arbitrarily (ξ) with a background spacetime with metric $g_{\mu\nu}$ and scalar curvature R. Its dynamics is described by the Lagrangian density

$$L(x)=-\tfrac{1}{2}\sqrt{-g}\left[g^{\mu\nu}(x)\nabla_\mu\Phi\nabla_\nu\Phi - \left[m^2+(1-\xi)\frac{R}{6}\right]\Phi^2(x)\right] . \quad (2.1)$$

Here $\xi=0$ and 1 denotes, respectively, conformal and minimal coupling. The scalar field satisfies the wave equation

$$\left[\Box+m^2+(1-\xi)\frac{R}{6}\right]\Phi(x,t)=0 , \quad (2.2)$$

where $\Box=g^{\mu\nu}\nabla_\mu\nabla_\nu$ is the Laplace-Beltrami operator defined on the background spacetime.

In the canonical quantization approach, one assumes a foliation of spacetime into dynamically evolving, time-ordered, spacelike hypersurfaces Σ, expands the field on Σ in normal modes, imposes canonical commutation relations on the time-dependent expansion functions now regarded as creation and annihilation operators, defines the vacuum state, and then constructs the Fock space. In flat space, Poincaré invariance guarantees the existence of a unique global Killing vector ∂_t orthogonal to all constant-time spacelike hypersurfaces, an unambiguous separation of the positive- and negative-frequency modes, and a unique and well-defined vacuum. In curved spacetime, general covariance precludes any such privileged choice of time and slicing. There is no natural mode decomposition and no unique vacuum. At any constant-time slice, one can expand the field Φ in terms of a complete set of (spatial) orthonormal modes $u_i(\mathbf{x})$ (Refs. 3 and 28)

$$\Phi(x)=\sum_k [\psi_k(t)u_k(\mathbf{x})+\psi_k^\dagger(t)u_k^*(\mathbf{x})] . \quad (2.3)$$

After second quantization, the fields Φ and their amplitudes ψ_k become operator-valued functions. Write

$$\psi_k(t)=a_k(t)\phi_k(t) , \quad (2.4)$$

where a_k are the annihilation operators and the (c-number) functions $\phi_k(t)$ obey the wave equation derived from (2.2). The canonical commutation rules on Φ imply these conditions on a_k and $a_j^\dagger$, i.e.,

$$[a_k,a_j]=[a_k^\dagger,a_j^\dagger]=0 \text{ and } [a_k,a_j^\dagger]=\delta_{kj} . \quad (2.5)$$

Assume that initially at $t=t_0, a_k=A_k$ and ϕ_k has only a positive-frequency component, then one can define a vacuum state $|0\rangle$ at t_0 by

$$A_k\,|0\rangle_{t_0}=0 , \quad (2.6)$$

and construct a Fock space from the n-particle states by the action of the creation operators. At a later time, say $t_1=t_0+\Delta t$, however, the vacuum state defined at t_0 will no longer be vacuous, since the annihilation operator $a_k(t_1)$ at t_1 is not equal to $A_k(t_0)$. In general, they are related by a set of Bogoliubov transformations

$$a_j(t_1)=\sum_k [\alpha_{jk}(t)A_k+\beta_{jk}^\dagger(t)A_k^\dagger] . \quad (2.7)$$

A new vacuum state $|0)$ at t_1 can be defined by

$$a_j\,|0)_t=0 \quad (2.8)$$

and from this a new Fock space can be constructed. One can easily see that $A_i\,|0)\neq 0$. The two vacuua are different by the coefficients α,β, whose time dependence are determined by the amplitude functions $\phi_k(t)$. In particular, any ϕ_k with only a positive-frequency component initially at t_0 will acquire a negative-frequency component at t_1. The new vacuum at t_1 now contains

$$S_j=(0\,|\,N_j\,|\,0)=\sum_k |\beta_{jk}|^2 \quad (2.9)$$

particles, where

$$N_j\equiv a_j^\dagger a_j \quad (2.10)$$

is the particle number operator. From (2.7) one sees that β_{jk} measures the negative-frequency component generated by dynamics. In curved space the inequivalence of Fock representation due to the lack of a global timelike Killing vector makes the constant separation of positive- and negative-frequency modes in general impossible. The mixing of positive- and negative-frequency modes in second-quantized form leads to vacuum particle creation. Particle creation may arise from topological, geometrical, or dynamical causes. In cosmological spacetimes the inequivalence of vacua appears at different times of evolution, and thus cosmological particle creation is by nature a dynamically induced effect. Note that we are dealing here with a free-field: particles are not produced from interactions, as in chemical reactions, but rather from the excitation of vacuum fluctuations by the changing background gravitational field.

1. Vacuum creation

For spacetimes with certain symmetries, some natural mode decomposition may present itself. For example, in the class of conformally static spacetimes (e.g., Robertson-Walker universe), where the metric is conformally related to a static spacetime (e.g., the Minkowski metric),

$$g_{\mu\nu}(x)=a^2(\eta)\eta_{\mu\nu} , \tag{2.11}$$

where a is the conformal factor, there exists a global conformal Killing vector ∂_η, where $\eta=\int dt/a(t)$ is the conformal time. Thus the vacuum defined by the mode decomposition with respect to ∂_η is a globally well-defined one, known as the conformal vacuum. For conformally invariant fields [e.g., a scalar field with $\xi=0$ in (2.1)] in conformally static spacetimes, it is easy to see that there is no particle creation.[3] Thus any small deviation from these conditions, e.g., small m,ξ, can be treated perturbatively from these states. For definiteness, we may want to use the Robertson-Walker universes as examples of our background spacetime, as they possess these special properties which make the field theory well defined with respect to the conformal vacuum. Consider the spatially flat case with metric

$$ds^2=a^2(\eta)(d\eta^2-d\mathbf{x}^2) . \tag{2.12}$$

The scalar fields can be separated into modes

$$\Phi(\eta,\mathbf{x})=\sum_k \phi_k(\eta)e^{i\mathbf{k}\cdot\mathbf{x}} , \tag{2.13}$$

where ϕ_k are the amplitude functions of the kth mode. Define new field variables $a(\eta)\phi_k(\eta)=\chi_k(\eta)$. From the wave equation (2.2) for the kth mode $\chi_k(\eta)$ satisfies

$$\chi_k''(\eta)+[k^2+(m^2-\xi R/6)a^2]\chi_k(\eta)=0 . \tag{2.14}$$

One sees that, for massless ($m=0$) conformally coupled ($\xi=0$) fields, χ_k admits solutions

$$\chi_k(\eta)=Ae^{-i\Omega\eta}+Be^{i\Omega\eta} , \tag{2.15}$$

which are of the same form as traveling waves in flat space. Since $\Omega=k=\text{const}$, the positive- and negative-frequency components remain separated and there is no particle production. More generally, the wave equation for each mode has a time-dependent natural frequency given by

$$\Omega_k{}^2(\eta)=k^2+\left[m^2-\frac{\xi R}{6}\right]a^2\equiv\omega^2a^2 . \tag{2.16}$$

The negative-frequency modes can thus be excited by the dynamics of the background through $a(\eta)$ and $R(\eta)=a''/a$ (a prime denotes $d/d\eta$). In analogy with the time-dependent Schrödinger equation, one can view the $(m^2-\xi R/6)a^2$ term in (2.16) as a time-dependent potential $V(\eta)$ which can induce backscattering of waves. The number of created particles in the kth mode is given in terms of χ' and χ by[5,17]

$$s_k=|\beta_k|^2=\frac{1}{2\Omega_k}(|\chi_k'|^2+\Omega_k{}^2|\chi_k|^2)-\tfrac{1}{2} . \tag{2.17}$$

The energy density associated with these particles is given by the expectation value of the 00 component of the conformal energy-momentum tensor (the Hamiltonian $H=\Lambda_0^0$) with respect to the conformal vacuum:

$$\begin{aligned}\rho_0&=\langle 0|\Lambda_0^0|0\rangle\\ &=\frac{1}{a^4}\int\frac{d^3k}{2(2\pi)^3}(|\chi_k'|^2+\Omega_k{}^2|\chi_k|^2)\\ &=\frac{1}{a^4}\int\frac{d^3k}{(2\pi)^3}(2s_k+1)\frac{\Omega_k}{2} .\end{aligned} \tag{2.18}$$

The analogy with parametric oscillators is formally clear: the energy density of vacuum particle creation comes from the amplification of vacuum fluctuations $\hbar\Omega_k/2$ by the factor $\mathscr{A}_k=2s_k+1$. In a Hamiltonian description of the dynamics of a finite system of oscillators, the Hamiltonian is simply

$$H_0(t)=\tfrac{1}{2}\sum_k(\pi_k{}^2+\Omega_k{}^2q_k{}^2)=\sum_k(N_k+\tfrac{1}{2})\Omega_k , \tag{2.19}$$

where one can identify $|\chi_k|^2$ and $|\chi_k'|^2$ with the canonical coordinates $q_k{}^2$ and moment $\pi_k{}^2$, the eigenvalue of H_0 being the energy $E_k=(N_k+\frac{1}{2})\Omega_k$. One can also identify the number operator N_k as s_k in (2.17):

$$N_k=\frac{1}{2\Omega_k}(\pi_k{}^2+\Omega_k{}^2q_k{}^2)-\tfrac{1}{2} . \tag{2.20}$$

2. n-particle creation

Equation (2.18) gives the vacuum energy density of particles produced from an initial vacuum, a pure state. If the initial state at t_0 is a statistical mixture of pure states, each of which contains a definite number of particles, then an additional mechanism of particle creation enters. This is categorically known as induced creation. In particular, as already pointed out in the original paper by Parker,[3] if the statistical density matrix μ is diagonal in the representation whose basis consists of the eigenstates of the number operators $A_k^\dagger A_k$ at time t_0 (for example, if the system has reached equilibrium by t_0, μ could be a function of the initial Hamiltonian which is diagonal in the t_0 representation), then for bosons, this process increases the average number of particles (in mode k in a unit volume) at a later time t_1 over the initial amount:

$$\begin{aligned}\langle N_k(t)\rangle&=\mathrm{Tr}\mu a^\dagger(t)a_k(t)\\ &=\langle N_k(t_0)\rangle\\ &\quad+|\beta_k(t)|^2[1+2\langle N_k(t_0)\rangle] ,\end{aligned} \tag{2.21}$$

where $\langle N_k(t_0)\rangle\rangle=\mathrm{Tr}\mu A_k^\dagger A_k$. For fermions it decreases the initial number.

The above result can be understood in the parametric oscillator description as the amplification of particles $s_k(0)$ already present, i.e.,

$$s_k(t)=s_k(0)+\mathscr{A}_k s_k(0) \quad (2.22)$$

by a factor

$$\mathscr{A}_k=1+2\,|\beta_k(0)|^2 .$$

The corresponding energy density ρ is given by[29] [cf. (2.18)]

$$\rho=\frac{1}{a^4}\int\frac{d^3k}{(2\pi)^3}(\,|\chi_k'|^2+\Omega_k{}^2|\chi_k|^2)\langle A_k^\dagger A_k\rangle, \quad (2.23)$$

where $\langle A_k^\dagger A_k\rangle\equiv\langle N_k(t_0)\rangle=\mathrm{Tr}\mu A_k^\dagger A_k$. Under the same assumption for μ, one sees that the energy density of the enhanced particles in the kth mode corresponds to the amplification of $\langle N_k\rangle\hbar\Omega_k$ by the amplification factor $\mathscr{A}$, where N_k is the number of particles originally present at t_0. The combined energy density of particles created from the vacuum and the n-particle state with a diagonal density matrix is

$$\rho_k(t)=\rho_k(0)+\mathscr{A}_k\rho_k(0) . \quad (2.24)$$

For the special but important case where μ is thermal at temperature $T=\beta^{-1}$, $\langle N_k\rangle$ obeys the Bose-Einstein distribution function for scalar fields. The magnification of the n-particle thermal state gives the finite-temperature contribution of particle creation, with energy density

$$\rho_T=\frac{1}{a^4}\int\frac{d^3k}{(2\pi)^3}(2s_k+1)\Omega_k/(e^{\beta\Omega_k}-1) . \quad (2.25)$$

For a massless conformal field, this yields the familiar Stefan-Boltzmann relation

$$\rho_T=\frac{\pi^2}{30}T^4 . \quad (2.26)$$

Finite-temperature particle creation and the related entropy generation problem have been discussed in Ref. 10.

For a more general density matrix the behavior of the induced creation could be very different: it can increase or decrease, depending on the correlation and phase relation of the initial state. We shall call those parts which always give an increase in particle number spontaneous creation, and those which may not, stimulated creation. Both are important factors in the consideration of entropy generation processes. These will be discussed in Sec. IV.

B. Interacting fields

It is clear from the above discussion that pair production from free fields corresponds to the mixing of positive- and negative-frequency components. If interactions are present among the modes, there could also be multiparticle production which, in general, can enhance the amount over that of the free fields.

1. Extrinsic (nonlinear) interactions

Consider a self-interacting scalar field with Lagrangian density[30]

$$L=L_0+L_I , \quad (2.27)$$

where L_0 is that of a massless conformal scalar field (2.1) and $L_I=-\lambda\Phi^4$. For simplicity, take the background spacetime to be that of a spatially flat Robertson-Walker universe (2.11) and use the interaction picture to describe the dynamics of the fields. The state vector $|\psi\rangle$ satisfies the Schrödinger equation

$$H_I\,|\psi\rangle=i\partial_\eta\,|\psi\rangle , \quad (2.28)$$

where H_I is the interaction Hamiltonian

$$H_I=\frac{\lambda}{4!}\int\sqrt{-g}\,d^3x\,\Phi^4 . \quad (2.29)$$

Assume that H_I is adiabatically switched off in the remote past $\eta=-\infty$ and future $\eta=+\infty$, whereupon Φ becomes a free field denoted by $\Phi_{\rm in},\Phi_{\rm out}$, respectively, and the in$|0\rangle_-$ and out$|0\rangle_+$ vacua are well defined as in the free-field theory. Impose the same canonical quantization conditions on Φ as in the free field theory. The in and out annihilation operators, $A_{\mathbf{k}}$ and $a_{\mathbf{k}}$, of the same mode $\mathbf{k}$ are related by (2.7)

$$a_{\mathbf{k}}=\alpha_{\mathbf{k}}A_{\mathbf{k}}+\beta_{\mathbf{k}}^*A_{-\mathbf{k}}^\dagger . \quad (2.30)$$

After formulating this problem in this way, one can use the S-matrix theory to treat particle creation from self-interaction. For small $|\lambda|\ll 1$, the S matrix is given to lowest order in λ by

$$S=1-i\int_{-\infty}^{\infty}H_I\,d\eta . \quad (2.31)$$

The interaction can produce particles in pairs or quartets. The amplitude for the creation of a quartet is

$$S_4={}_{\rm in}\langle\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4\,|\,S\,|\,0\rangle_{\rm in} . \quad (2.32)$$

This is similar to the scattering of a pair of particles. Whereas scattering of particle pairs may occur in flat spacetime, the creation process is possible only in a curved spacetime, where the conservation of field energy is no longer required. The pair creation process has amplitude

$$S_2={}_{\rm in}\langle\mathbf{k}_1\mathbf{k}_2\,|\,S\,|\,0\rangle_{\rm in} . \quad (2.33)$$

It contains divergences and need be renormalized. At $\eta\to 0$, the state of the system is a sum of vacuum, two-particle, and four-particle terms:

$$|\psi\rangle=|0\rangle_{\rm in}+|2\rangle+|4\rangle , \quad (2.34)$$

where

$$|2\rangle=\tfrac{1}{2}\int d^3\mathbf{k}_1d^3\mathbf{k}_2S_2\,|\mathbf{k}_1\mathbf{k}_2\rangle_{\rm in} ,$$

$$|4\rangle=\tfrac{1}{4}\int d^3\mathbf{k}_1d^3\mathbf{k}_2d^3\mathbf{k}_3d^3\mathbf{k}_4S_4\,|\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4\rangle_{\rm in} ,$$

with an appropriate normalization constant.

The energy of created particles is

$$E=\langle\psi\,|H_0|\,\psi\rangle , \quad (2.35)$$

where

$$H_0=\int d^3k\;\Omega_k a_k^\dagger a_k . \quad (2.36)$$

Expressing $(a_k^\dagger, a_k)$ in terms of $(A_k^\dagger, A_k)$, the in state, and evaluating the integral of the matrix elements, one gets[30]

$$\rho=\rho_0+\rho_2+\rho_4+\rho_{02}+\rho_{24} \ , \tag{2.37}$$

where ρ_0 denotes contribution from free fields, ρ_2 and ρ_4 that from 2-particle and 4-particle creation and ρ_{02} and ρ_{24} are the interference terms proportional to $\langle 0 | H_0 | 2\rangle$ and $\langle 2 | H | 4\rangle$, etc. Just as for free fields, the interacting field theory can be described and formulated in the analog of coupled oscillators via a Hamiltonian:

$$H=H_0+H_I \ , \tag{2.38}$$

where H_0 is that of the free field given by (2.19) and

$$H_I=\frac{\lambda}{4!}\sum_k q_k{}^4 \tag{2.39}$$

for a quartic interaction. Categorically, there can also be interaction among different modes in the bilinear form

$$H_I=\tfrac{1}{2}\sum_{k\neq k'} c_{kk'}q_k q_{k'} \ , \tag{2.40}$$

or other forms involving higher products.

There are two distinct features in the quantum-field-theory treatment of interacting particle creation in the above example. (1) The term ρ_{02} is of linear order in λ as it arises from the interaction with the vacuum. In the analogous quantum-mechanical description the lowest-order term would be λ^2. (2) For massless, conformal fields coupled via $\lambda\phi^4$ interaction, there is no particle production in the Robertson-Walker spacetime. This is in conformity with Parker's theorem,[3] as the $\lambda\phi^4$ theory is conformally invariant and the RW universe is conformally static. The discussion of entropy generation in Secs. III and IV is based on the quantum mechanics of coupled oscillators with Hamiltonian [in the form of (2.38)]. The first point above therefore indicates where a possible discrepancy may arise, i.e., there are quantum field processes which may not be included in such descriptions. More important is the second point. Since the entropy defined in Sec. III deals with the statistical correlation of the states of the system, the presence of interactions as in the $\lambda\phi^4$ theory can introduce entropy, albeit without particle creation. This shows the distinction between these two processes, and the difference in concepts adopted in describing them, which is the main theme of our later discussion. We now turn to another mechanism which can bring about interaction among modes even in a free field theory.

2. *Dynamical (linear) interactions*

In Ref. 17 particle creation for a free field in a mixmaster universe was studied. The lesser symmetry of the space does not allow for a "natural" mode decomposition in terms of simple basis functions. The eigenmodes are linear combinations of the characteristic functions $w_K(x)$ with time-dependent expansion coefficients. This leads to coupling between modes through the dynamics of the background. Write the complete wave functions as

$$X(\mathbf{x},\eta)=\sum_{K=-J}^{J}\chi_K(\eta)w_K(\mathbf{x}) \ , \tag{2.41}$$

where $\mathbf{x}$ denotes Euler angle variables (ψ,θ,ϕ) and $w_K=D^J_{\rm KM}$ are the symmetric top wave function. The wave equation for each mode amplitude then has the general form

$$\chi_K''(\eta)+(\Omega_{KK'}{}^2+Q\delta_{KK'})\chi_{K'}=0 \ , \tag{2.42}$$

where

$$\Omega_{KK'}{}^2=a^2(E_{KK'}+m^2) \ ,$$
$$Q(\eta)=a^2R/6-a''/a \ ,$$
$$a^3=l_1l_2l_3 \ ,$$

and the $E_{KK'}$'s are the eigenvalues of the Helmholtz operator on the mixmaster space with principal curvature radii l_i and scalar curvature R. The natural frequency matrix elements in (2.42) are the eigenvalues of the Hamiltonian operator

$$H=-{}^{(3)}\Delta+R/6+m^2 \tag{2.43}$$

with respect to the characteristic function w_k. One can factor out the part diagonal in H, call it H_0, and treat the nondiagonal part as the interacting Hamiltonian H_I. In the parametric oscillator analogy, H_0 would be of the form (2.19) and H_I would be of the form (2.40) with time-dependent coupling constants $C_{KK'}(\eta)$. This example illustrates how the modes of a free field could be coupled via the dynamics of spacetime. We see that this arises from the lack of a preferred choice of mode decomposition in curved spacetime and the lack of special symmetry in the space to warrant any special choice of eigenfunctions. We will use the form (2.40) as a model for particle creation and interaction in our later considerations of entropy generation in cosmological spacetimes. The overall qualitative features do not depend on the exact form of the interaction assumed.

III. THE "STATISTICAL" ENTROPY OF A QUANTUM FIELD

A. What is meant by the entropy?

By way of illustration consider this question first for a collection of N distinguishable quantum particles characterized by an N-particle density matrix μ whose evolution is governed by a quantum Liouville equation

$$\partial_t\mu=-[H,\mu]_-\equiv -L\mu \ . \tag{3.1}$$

Here ∂_t and $[\ ,\ ]_-$ denote, respectively, a time derivative and a commutator, and H is the Hamiltonian from which the dynamics derives. Given such a system, one is wont to introduce an "entropy"

$$\mathscr{S}[\mu]\equiv -{\rm Tr}\mu\ln\mu \ , \tag{3.2}$$

where Tr denotes a trace over the degrees of freedom of the system. The presumption then is that this $\mathscr{S}$ admits to a probabilistic or information-theoretic interpretation. Statistically probable mixed states are assumed to have large $\mathscr{S}$, whereas states which are somehow improbable are assumed to have a small $\mathscr{S}$. The special case of a pure state corresponds to a vanishing $\mathscr{S}$. If, moreover, the Hamiltonian is time independent, so that a static equilibrium state can be defined, one believes that $\mathscr{S}$ will be maximized by the thermal density matrix $\mu_{eq} \propto \exp(-\beta H)$, toward which the system is presumed to evolve.

The problem, however, is that such an interpretation is inconsistent with the linearity of the Liouville equation. It seems reasonable intuitively to argue that the evolution induced by the dynamics will lead to a more "random" or generic state, but it is obvious that $\mathscr{S}$ can provide no information about this randomization. It follows as a trivial consequence of the Liouville equation that $d\mathscr{S}/dt \equiv 0$. The entropy $\mathscr{S}$, like any functional of μ, must be conserved absolutely.

Historically, this difficulty led to the concept of a "coarse-grained averaging," namely, the notion that the microscopic entropy really is conserved, and that a true H theorem expressing entropy increase can only obtain in some quasimacroscopic average sense. This idea seems attractive, at least superficially, but it also leads to a serious problem. Even if one could construct an explicit algorithm to implement the desired averaging—which has not yet been done for any realistic systems—one would be confronted with the formidable task of proving that the averaging is "canonical" in some natural sense. Otherwise, one would be led to the conclusion that the existence of a meaningful notion of entropy is not a fundamental property of the dynamics, but reflects instead the physicist's anthropomorphic interpretation of the evolution of the system. Indeed, once one accepts that no unique coarse graining exists, one appears forced ultimately toward the extreme viewpoint advocated by Jaynes,[23] namely, that "Entropy is a property, not of the physical system, but of the particular experiments you or I choose to perform on it."

This viewpoint, albeit extreme, does serve to stress an important question: namely, what is it that one actually measures when probing the state of the system? The answer to this would in fact seem quite obvious. One attempts, typically, to measure the reduced one-particle density matrices, or perhaps the comparatively simple correlations buried in the two- and three-particle reduced matrices, but one never presumes to probe the complex higher-order correlations encapsulated in the full N-particle μ. One might, therefore, argue that realistic measurements of the state of a system entail a type of "intrinsic coarse graining," predicated not upon a quasimacroscopic averaging, but reflecting instead an incomplete knowledge of the form of the higher-order correlations.

Given this observation, the materialist might argue that the "physical" entropy should be constructed from the reduced one-particle density matrices, say $f(i)$, and, as such, he might propose tentatively an "entropy"

$$S \equiv \sum_{i=1}^{N} \operatorname*{Tr}_i f(i) \ln f(i) , \tag{3.3}$$

where Tr_i denotes a partial trace over the degrees of freedom of the ith particle. Given the demand that S be constructed solely from the $f(i)$'s, this is perhaps the most conservative possible choice; and, indeed, this S has a number of attractive properties.

(1) In that the $f(i)$'s are well defined, physically measurable quantities, one may argue that S has a concrete physical meaning.

(2) In the presence of couplings between degrees of freedom, S, unlike $\mathscr{S}$, will in general be time-dependent. Thus, e.g., for a collection of N identical particles interacting via a pair potential H^I_{ij}, it follows immediately that

$$\frac{dS}{dt} = N(N-1) \operatorname*{Tr}_i \operatorname*{Tr}_j \ln f(i) i [f_2(i,j), H^I_{ij}]_- , \tag{3.4}$$

where $f_2(i,j)$ is the reduced two-particle density matrix for particles i and j.

(3) In the absence of couplings between degrees of freedom, $dS/dt \equiv 0$. Changes in the entropy can occur only in the presence of interactions which induce correlations among the particles not reflected in the one-particle $f(i)$'s.

(4) This S is in fact the standard Boltzmann entropy, and, as such, one anticipates that an H-theorem inequality will obtain at least in a "weak coupling" or "dilute gas" approximation. It is well known that, in such a limit, a collection of N identical particles will satisfy the Landau, or collisional Boltzmann, equation, and it follows trivially from each of these equations that $dS/dt \geq 0$.

(5) Regardless of the form of the interactions, one can prove a rigorous H theorem in at least one simple case. Specifically, if, at some initial time t_0, the system is free of correlations, so that $\mu = \prod_i f(i)$, it follows rigorously that, an instant later, at time $t_0 + \Delta t$, the entropy will be increasing:[26]

$$dS(t_0 + \Delta t)/dt > 0! . \tag{3.5}$$

Evolving correlations induce at least an initial increase in entropy. This demonstrates, in particular, that even for periodic systems, in which a universal H theorem cannot hold, changes in S are intimately connected with evolving (or decaying) interparticle correlations.

Equation (3.4) illustrates the obvious fact that, quite generally, for arbitrary interparticle interactions, the time derivative of the one-particle entropy S can be expressed in terms of the two- and higher-particle reduced density matrices. This is nothing other than a simple manifestation of the standard Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equations. What makes the definition of S more fundamental mathematically is the fact that, by introducing an appropriate "subdynamics," dS/dt can instead be reexpressed as a nonlocal, nonlinear functional of the one-particle $f(i)$'s.

As discussed by many authors, and applied to field theory by Kandrup,[26] the idea behind a "subdynamics" is very simple: view the full N-particle density matrix μ as being a sum of two contributions, a "relevant" μ_R and an "irrelevant" μ_I, and extract from the full N-particle Liouville equation $\partial_t \mu = -L\mu$ an equation for $\partial_t \mu_R$ which contains no explicit reference to μ_I. For the system of interest here,

$$\mu_R = \prod_{i=1}^{N} f(i) \tag{3.6}$$

and the entropy

$$S[\mu_R] = -\mathrm{Tr}\mu_R \ln\mu_R \ . \tag{3.7}$$

The nontrivial fact then is that $dS(t)/dt$ can be reexpressed in terms of μ_R at retarded times $t-\tau$. The key to obtaining such a "subdynamics" is the observation that μ_R and $\mu_I \equiv \mu - \mu_R$ can be viewed as "orthogonal" in an appropriate function space, so that, as illustrated at the end of this section, the decomposition of $\mu = \mu_R + \mu_I$ can be implemented rigorously by means of projection operators.

This basic idea sounds so simple that it is important to stress that there is no guarantee that an arbitrary decomposition of μ into two pieces μ_1 and μ_2 can be implemented rigorously. The existence of such a closed subdynamics for specific choices of μ_R exploits in a deep and fundamental way the overall symmetries of the Liouville equation. The μ_R of Eq. (3.6) is especially simple and, as first illustrated by Willis and Picard,[24] admits to a comparatively simple subdynamics. If, alternatively, one were concerned instead with pair correlations rather than simply with the one-particle $f(i)$'s, the construction of an appropriate μ_R which satisfies a closed subdynamics becomes a far more complicated, albeit still soluble, problem.[24]

B. Abstract definition of "field entropy"

The object here is to construct an analogous definition of entropy for a quantum field by exploiting the mathematical fact that such a field is equivalent to an infinite collection of oscillators. As illustrated for the case of a scalar field Φ, the idea is in fact straightforward.

Start with the fundamental action $S[\Phi]$ from which the basic field equation derives. Implement a preferred splitting into space and time so as to extract a Lagrangian $L[\Phi]$. Now expand $\Phi(\mathbf{x},t)$ in terms of an appropriate orthogonal basis set of eigenfunctions $\psi_k(\mathbf{x},t)$ with time-dependent coefficients $q_k(t)$:

$$\phi(\mathbf{x},t) = \sum_k q_k(t)\psi_k(\mathbf{x},t) \ . \tag{3.8}$$

For the case of flat space, these ψ_k's are to be chosen as the plane-wave eigenfunctions of the spatial Laplacian which serves to define the notion of particle. In a more complicated spacetime, they will in general be something quite different. Thus, for example, in a mixmaster universe, the "natural" decomposition entails an expansion in generalized Wang functions.[17] By exploiting the orthogonality of the ψ_k's, one can reinterpret L as being a function of the q_k's and their time derivatives $\dot{q}_k$. Standard manipulations then permit one to construct a Hamiltonian H which depends upon the "coordinates" q_k and the canonically conjugate momenta π_k, and which can be interpreted as representing a collection of oscillators.

The object now is to treat these oscillators as if they were a collection of real particles and proceed in complete analogy with the program outlined in the first part of this section. Specifically, assume that this system can be characterized by a many-oscillator density matrix μ defined in an appropriate infinite-dimensional phase space, and suppose that its evolution is governed by a quantum Liouville equation $\partial_t\mu = -i[H,\mu]_- \equiv -L\mu$ which expresses probability conservation in that infinite-dimensional space. The natural geometric structure of this space is unfortunately less than obvious. However, as discussed, e.g., in Ref. 25, it suffices to proceed as if this phase space were a flat infinite-dimensional manifold constructed in the obvious way as a direct product of infinitely many one-oscillator phase spaces. The commutator in the Liouville equation is then reinterpreted by the implementation of the canonical commutation relations

$$[q_k, p_{k'}] = i\delta_{kk'} \ . \tag{3.9}$$

Given this structure, it is straightforward formally to define reduced density matrices by partial traces over all but some finite number of field degrees of freedom. Thus, e.g., in analogy with the case of a system of N particles, one can define a reduced density matrix for the kth oscillator

$$g(k) \equiv \prod_{l \neq k} \mathrm{Tr}_l\, \mu \tag{3.10}$$

so that the "relevant" contribution to the total density matrix μ takes the form

$$\mu_R = \prod_k g(k) \ . \tag{3.11}$$

The field entropy S is then defined by the obvious prescription

$$S = -\mathrm{Tr}\mu_R \ln\mu_R = -\sum_k \mathrm{Tr}_k\, g(k) \ln g(k) \ . \tag{3.12}$$

For a source-free linear field theory in flat space, the oscillators decouple and the field entropy is conserved absolutely: $dS/dt \equiv 0$. If, alternatively, couplings are introduced by nonlinearities (as in a $\lambda\Phi^p$ field theory), by the presence of material sources, or, as illustrated in Sec. IV, by a nontrivial background spacetime, S will instead exhibit a complicated time dependence.

At this point it is important to reiterate the two critical, and potentially ambiguous, steps involved in the definition of S, namely, the implementation of a preferred splitting into space and time and the choice of a particular set of basis functions ψ_k. The definition of dynamics requires the singling out of a preferred notion of time. The enumeration of the degrees of freedom requires a preferred decomposition into "oscillators." For certain physical systems of interest, there will exist a canonical notion of time and an obvious preferred decomposition into some appropriate analogue of spatial plane waves, but, in general, even these apparently innocuous preliminaries introduce a fundamental ambiguity (or at least observer dependence) into the basic field-theoretic description.

It should, however, be emphasized that these are not ambiguities associated specifically with the definition of entropy or even the formulation of a Liouville equation. These are instead ambiguities arising at the very foundations of general relativity (choice of time) and quantum field theory in curved space (mode decomposition), and, particularly, the definition of "particle." From this point of view, the field entropy (3.12) is as reasonable—or unreasonable—an object as is the notion of "particle."

In conventional relativistic kinetic theory, these problems of noncovariance are circumvented by replacing the ordinary notion of an entropy S by a locally defined entropy flux s^{μ}, a vector field living in the spacetime manifold. The notion of an H theorem is then captured by the local statement that the covariant divergence $\nabla_{\mu}s^{\mu}$ is non-negative (see, e.g., Ref. 31), and it is only by integrating over some arbitrary three-dimensional spacelike hypersurface that one can identify a total entropy S which increases monotonically: $dS/dt>0$. Such a covariant reinterpretation of the field entropy (3.12) seems, however, very difficult to realize. The field entropy S is defined not in the spacetime manifold, or even in the associated cotangent bundle, but, instead, in the abstract Hilbert space associated with the q's and π's. Indeed, the entropy S, like the density matrix μ, makes no explicit reference at all to the spatial coordinates $\mathbf{x}$, so that there is no obvious sense in which, at some instant of time, some "piece" of the total entropy can be associated with some region of space.

C. The time dependence of the entropy

The object now is to use the notion of a subdynamics to obtain an expression for the time derivative dS/dt which involves only the "relevant" density matrix μ_R. The construction of the desired subdynamics is considered in great detail by Kandrup,[26] and, as such, it suffices here to simply sketch the basic picture and then quote the final results.

The key idea is to introduce a linear projection operator $P(t)$ defined to satisfy the three requirements[21-23]

$$P\mu=\mu_R \, , \tag{3.13}$$

$$P(t_2)P(t_1)=P(t_2) \quad \text{for } t_2\geq t_1 \, , \tag{3.14}$$

and

$$P\partial_t\mu=\partial_t P\mu \, . \tag{3.15}$$

The first of these requirements ensures that the operator P serves to project out from the total μ the desired μ_R. The second guarantees that, at any instant of time, P is in fact idempotent, so that μ_R does lie in an "invariant" subspace. The third requirement ensures that the notions of projection and time evolution commute, at least when restricted to the fundamental many-oscillator μ.

Given such a P, an explicit realization of which is presented in Ref. 26, it follows immediately that the single quantum Liouville equation $\partial_t\mu=-L\mu$ is equivalent to the coupled system

$$\partial_t\mu_R+PL\mu_R=-PL\mu_I \tag{3.16}$$

and

$$\partial_t\mu_I+(1-P)L\mu_I=-(1-P)L\mu_R \, . \tag{3.17}$$

The first of these equations expresses the fact that the correlations buried in μ_I serve as a source for changes in μ_R. The second equation expresses the fact that μ_R back reacts to induce changes in μ_I. The net effect of this interplay is that $\partial_t\mu_R(t)$ will involve the form of μ_R at retarded times $t-\tau$.

In terms of an initial condition at time t_0, the equation for $\partial_t\mu_I$ admits the solution

$$\mu_I(t)=\mathcal{G}(t,t_0)\mu_I(t_0)-\int_0^{t-t_0}d\tau\,\mathcal{G}(t,t-\tau)[1-P(t-\tau)]L(t-\tau)\mu_R(t-\tau) \, , \tag{3.18}$$

where

$$\mathcal{G}(t_2,t_1)\equiv T\exp\left[-\int_{t_1}^{t_2}d\tau[1-P(\tau)]L(\tau)\right] , \tag{3.19}$$

and T denotes a time-ordering operator. By inserting this formal solution back into Eq. (3.16), one then concludes that

$$\partial_t\mu_R(t)+P(t)L(t)\mu_R(t)=-P(t)L(t)\mathcal{G}(t,t_0)\mu_I(t_0)+\int_0^{t-t_0}d\tau\,P(t)L(t)\mathcal{G}(t,t-\tau)[1-P(t-\tau)]L(t-\tau)\mu_R(t-\tau) \, . \tag{3.20}$$

One has obtained an exact closed (albeit nonlocal) equation for the evolution of μ_R which contains explicit reference to the "irrelevant" contribution μ_I only through the propagation of an initial condition $\mu_I(t_0)$.

By exploiting the explicit realization of P presented in Ref. 26, it is then straightforward to work out more concretely the form of the equation for $\partial_t\mu_R$, and to use that equation to evaluate the time derivative of the entropy. One discovers thereby that the term $PL\mu_R$ has no effect on the evolution of S and that it is only the back reaction of the "irrelevant" μ_I which induces changes in the entropy:

$$\frac{dS(t)}{dt}=-\mathrm{Tr}(1+\ln\mu_R)\partial_t\mu_R(t)=+\mathrm{Tr}\ln\mu_R(t)P(t)L(t)\mu_I(t) \, . \tag{3.21}$$

By inserting into this equation the μ_I of Eq. (3.18), and observing that $(1-P)L\mu_R$ contains no explicit reference to the "free" piece of L involving only the uncoupled oscillators, one then concludes that

$$\frac{dS(t)}{dt}=-\mathrm{Tr}\ln\mu_R(t)P(t)L(t)\mathcal{G}(t,t_0)\mu_I(t_0)+\int_0^{t-t_0}d\tau\,\mathrm{Tr}\mu_R{}^{-1}(t)\zeta(t)\mathcal{G}(t,t-\tau)\zeta(t-\tau) \, , \tag{3.22}$$

where, in terms of a suitably defined "average" interaction Liouvillian $\{L^I\}$,

$$\Delta \equiv L^I - \{L^I\} , \tag{3.23}$$

and the quantity $\zeta \equiv \Delta\mu_R$. Note in particular that, in the absence of couplings between the oscillators, L^I and Δ vanish identically, so that $dS/dt \equiv 0$.

The form of the "average" $\{L^I\}$ will of course depend upon the details of the interaction Hamiltonian H^I connecting the oscillators. Consider, for example, an interaction H^I constructed as a sum of pair potentials H^I_{jk} involving couplings between oscillators j and k. In this case, the interaction Liouvillian L^I also degenerates into a sum of contributions L^I_{jk}, and, for any function ξ, the "average" $\{L^I_{jk}\}$ takes the form

$$\{L^I_{jk}\}\xi = i[\{H^I_{jk}\},\xi]_- , \tag{3.24}$$

where

$$\{H^I_{jk}\} \equiv \mathop{\mathrm{Tr}}_j H^I_{jk} g(j) + \mathop{\mathrm{Tr}}_k H^I_{jk} g(k) \tag{3.25}$$

denotes an average value defined with respect to the one-oscillator reduced density matrices.

A "short times" H theorem follows immediately from Eq. (3.22). In the limit that $\tau \rightarrow 0$, $\mathcal{G}(t,t-\tau) \rightarrow 1$, and thus, neglecting temporarily the contribution to dS/dt involving the initial condition $\mu_I(t_0)$, one concludes that, at time $t_0+\Delta t$,

$$dS(t_0+\Delta t)/dt = \Delta t \,\mathrm{Tr}\mu_R{}^{-1}(t) \,|\, \zeta^2(t) \,|\, > 0 . \tag{3.26}$$

If, at some time t_0, the system is free of correlations, $dS(t_0)/dt$ will vanish, but the subsequent evolution of the system, induced by couplings between the degrees of freedom, leads at least initially to a subsequent increase in the entropy. In this sense, one can speak of a "spontaneous generation of entropy" induced by the evolving dynamics.

If, alternatively, one allows for nontrivial initial conditions, one can also obtain "stimulated" changes in the entropy.[26] Thus, quite generally, one concludes that

$$dS(t_0)/dt = -\mathrm{Tr}\ln\mu_R(t_0)P(t_0)L(t_0)\mu_I(t_0) , \tag{3.27}$$

a quantity which, depending upon the detailed form of $\mu_I(t_0)$, could be either positive or negative. This indeterminacy in the sign of dS/dt illustrates the fact that the field entropy cannot satisfy a completely general H theorem for all times. One might naively claim that this means that S does not constitute a satisfactory notion of entropy. However, further reflection suggests that, at least in principle, one *should* be able to specify initial conditions which result in an initial decrease in the entropy.

What one really expects physically[26] is that, eventually, the effects of any nontrivial initial correlations may be ignored compared with the "systematic" correlations induced by the evolving dynamics. It is these systematic effects which are reflected in the "spontaneous" changes associated with the contribution to dS/dt that involves the form of μ_R at retarded times $t-\tau$.

In this regard, it is worth emphasizing that standard derivations of the Landau equation for an electrostatic plasma all entail an assumption of "molecular chaos" equivalent to the hypothesis that $\mu_I(t_0) \equiv 0$. If nontrivial initial conditions are important, that equation must be supplemented by an additional term involving $\mu_I(t_0)$, and, in that case, the standard H theorem satisfied by the Landau equation requires a careful reexamination.

IV. ENTROPY GENERATION AND PARTICLE CREATION

The object here is to use the notion of subdynamics considered in the preceding section to address the phenomenon of particle creation in the early Universe and, especially, to illustrate the sense in which particle creation correlates with the generation of entropy as defined by Eq. (3.12). As a concrete example, attention will focus upon a collection of oscillators described by the specific model Hamiltonian discussed in Sec. II [Eqs. (2.19) and (2.40)]:

$$\begin{aligned} H(t) &= \tfrac{1}{2}\sum_k ({\pi_k}^2 + {\Omega_k}^2 {q_k}^2) + \tfrac{1}{2}\sum_{k' \neq k} c_{kk'} q_k q_k \\ &\equiv \sum_k H_k + H_I \equiv H_0 + H_i , \end{aligned} \tag{4.1}$$

where $\Omega_k > 0$ and $c_{kk'} = c_{k'k}$ are arbitrary real functions of time t.

This is a useful Hamiltonian to consider for a number of reasons. (1) In the limit that $c_{kk'} \equiv 0$ and the Ω_k's are time-independent, this is the Hamiltonian appropriate for a Klein-Gordon field in Minkowski space. (2) More generally, by assuming that $c_{kk'} \neq 0$ but that Ω_k is in fact time dependent, one recovers the form appropriate for a Klein-Gordon field in a spatially flat Friedmann cosmology [see, e.g., Eqs. (2.12)—(2.14)]. (3) By allowing for nontrivial time-dependent $c_{kk'}$'s, one can mock realistically the evolution of a Klein-Gordon field in a mixmaster universe.[17] This is important both for practical and conceptual reasons. On the practical side is the observation that these mixmaster universes represent a very general class of solutions to the classical Einstein equation which are believed in certain respects to illustrate the generic behavior of a realistic cosmology at very early times as one approaches the initial singularity. On the conceptual side, this Hamiltonian illustrates the important fact that, in a nontrivial background spacetime, the "normal modes" for even a source-free linear field theory will not decouple from one another. Even the simplest sorts of linear theory can, in a dynamical background, evidence complicated interactions among the normal modes. Mathematically, as discussed in Ref. 17, the reason for this is that, if the spacetime is not (at least) conformally static, the "natural" generalization of the three-dimensional Laplacian, which generates the decomposition into modes, will itself evidence a time dependence; and this time dependence, when combined with the dynamics encapsulated in the field equation, will induce a time-dependent linear mode-mode coupling.

One might also like to allow in the model Hamiltonian for nonlinear couplings of the form which would, e.g., arise in a $\lambda\Phi^p$ field theory even in flat space, but as discussed in Ref. 26, these additional complications would not alter the principal conclusions established here.

Given the Hamiltonian (4.1), it is natural to introduce the "number operator"

$$N_k \equiv \frac{1}{2\Omega_k}(\pi_k{}^2+\Omega_k{}^2q_k{}^2)-\tfrac{1}{2} \ . \tag{4.2}$$

For free fields ($c_{kk'}\equiv 0$) in flat space, this N_k admits to an unambiguous interpretation as representing the "number of quanta in the kth mode." And, in the presence of interactions ($c_{kk'}\neq 0$), this interpretation remains valid if, in the usual way, one supposes an adiabatic switching on and off of the $c_{kk'}$'s in the asymptotic regions. In curved spaces, the physical interpretation is in general less obvious, but it is evident that the statistical expectation values of the N_k's still contain important information, for example, about how the total energy of the field is distributed.

Because the natural frequencies Ω_k are functions of time, N_k itself is a time-dependent operator:

$$\partial_t N_k = \frac{-\dot{\Omega}_k}{2\Omega_k{}^2}(\pi_k{}^2-\Omega_k{}^2q_k{}^2) \ . \tag{4.3}$$

This means that the statistical expectation value

$$\langle N_k\rangle \equiv \mathrm{Tr}\mu N_k \tag{4.4}$$

associated with the density matrix μ changes both by virtue of changes μ and by virtue of changes in the definition of particle:

$$\frac{d\langle N_k\rangle}{dt}=\mathrm{Tr}(\mu\partial_t N_k+N_k\partial_t\mu) \ . \tag{4.5}$$

The second term in Eq. (4.5) can be reexpressed in terms of $\mu(t)$, rather than its time derivative, by exploiting the quantum Liouville equation for μ, the cyclic trace identity, and the fact that $[H,H_k]=[H_I,H_k]$. The net result is that

$$\frac{d\langle N_k\rangle}{dt}=-\frac{\dot{\Omega}_k}{2\Omega_k{}^2}\langle \pi_k{}^2-\Omega_k{}^2q_k{}^2\rangle-\sum_{k'\neq k}\frac{c_{kk'}}{\Omega_k}\langle \pi_k q_{k'}\rangle \ . \tag{4.6}$$

It is clear from Eq. (4.6) that particle creation can be induced either from a time-dependent Ω_k or from couplings between degrees of freedom encapsulated in nonvanishing $c_{kk'}$'s. The former mechanism will be viable if $\langle \pi_k{}^2-\Omega_k{}^2q_k{}^2\rangle\neq 0$, i.e., if the system is not "at equipartition." The latter will be viable if $\langle \pi_k q_{k'}\rangle\neq 0$. Initial conditions for which one or both of these expectation values is nonvanishing lead to a "stimulated" change in the number of particles. If, alternatively, initial conditions are chosen so that these expectation values all vanish (as is, e.g., the case for the vacuum), there will be no immediate change in the particle number.

What is, however, important to observe is that, even in the absence of such "stimulating" initial conditions, the evolving dynamics will lead to a "spontaneous creation of particles." That this is the case may be established straightforwardly in the context of a simple perturbation theory. Indeed, given initial conditions at some time t_0, it is simple but tedious to calculate the expectation value $d\langle N_k(t_0+\Delta t)\rangle/dt$ to first order in Δt. The principal conclusion of this computation is that $d\langle N_k(t_0+\Delta t)\rangle/dt$ can be decomposed into a sum of two terms which are intrinsically positive for an arbitrary state, and a remaining piece, of indeterminate sign, which vanishes identically for an initial eigenstate of the N_k's (and many other nontrivial initial states). The former contributions, which will always be present, may be defined as corresponding to "spontaneous particle creation" induced by the dynamics. The latter, which require specialized initial conditions, may be defined as corresponding instead to a "stimulated particle creation."

It is instructive to focus explicitly upon the origin of the two sources of "spontaneous particle creation."

(1) Because Ω_k is time dependent, the system cannot in general remain "at equipartition." The number operator $N_k(t_0+\Delta t)$ will contain a contribution proportional to

$$\Delta t\partial_t(\pi_k{}^2-\Omega_k{}^2q_k{}^2)=-2\Omega_k\dot{\Omega}_k q_k{}^2\Delta t \ , \tag{4.7}$$

where Ω_k and $\dot{\Omega}_k$ refer to conditions at time t_0, and this leads to a contribution to $d\langle N_k\rangle/dt$ of the form

$$\frac{d\langle N_k(t_0+\Delta t)\rangle_f}{dt}=\frac{\dot{\Omega}_k{}^2}{\Omega_k}\langle q_k{}^2\rangle\Delta t>0 \ , \tag{4.8}$$

where the subscript f denotes spontaneous creation of quanta arising even in the absence of interactions.

(2) Correlations buried in the evolving $\mu_I(t)$ necessarily induce a nontrivial expectation value for $\langle \pi_k q_{k'}\rangle$. Suppose that, initially, $\mu_I(t_0)\equiv 0$. It then follows from the discussion in Sec. III that the interactions induce a nonvanishing

$$\begin{aligned}\mu_I(t_0+\Delta t)&=-\Delta t(1-P)L\mu_R(t_0)\\&=-\Delta t\xi(t_0) \ ,\end{aligned} \tag{4.9}$$

and, given this expression, it is easy to see that the quantity $\mathrm{Tr}\mu_I(t_0+\Delta t)\pi_k q_{k'}\neq 0$. The net result is a contribution of $d\langle N_k\rangle/dt$ of the form[26]

$$\frac{d\langle N_k(t_0+\Delta t)\rangle_c}{dt}=\sum_{k\neq k'}\frac{c_{kk'}{}^2}{\Omega_k}(\langle q_{k'}{}^2\rangle-\langle q_{k'}\rangle^2)\Delta t>0 \ , \tag{4.10}$$

where the subscript c denotes spontaneous creation of quanta associated with correlations induced by interactions.

Equations (4.8) and (4.10) represent the spontaneous creation of quanta. Assuming, for simplicity, that $\mu_I(t_0)=0$, i.e., that no initial correlations are present, the remaining "simulated" contributions take the form

$$\frac{d\langle N_k(t_0+\Delta t)\rangle_{\rm st}}{dt}=\sum_{k'\neq k}\frac{c_{kk'}}{\Omega_k}\left\{-\langle p_k\rangle\langle q_{k'}\rangle\left[1+\left[\frac{\dot c_{kk'}}{c_{kk'}}-\frac{\dot\Omega_k}{\Omega_k}\right]\Delta t\right]-\Delta t[\langle\pi_k\rangle\langle\pi_{k'}\rangle-\Omega_k{}^2\langle q_k\rangle\langle q_{k'}\rangle-\sum_{l\neq k}c_{kl}\langle q_{k'}\rangle\langle q_l\rangle]\right\}$$
$$+\frac{\dot\Omega_k}{2\Omega_k{}^2}\left\{-\langle\pi_k{}^2-\Omega_k{}^2q_k{}^2\rangle\left[1+\left[\frac{\ddot\Omega_k}{\dot\Omega_k}-\frac{2\dot\Omega_k}{\Omega_k}\right]\Delta t\right]+\Delta t[2\Omega_k{}^2\langle\pi_kq_k+q_k\pi_k\rangle+2\sum_{l\neq k}c_{kl}\langle q_k\rangle\langle q_l\rangle]\right\}. \tag{4.11}$$

As noted already, this contribution has no fixed sign: by a judicious choice of initial conditions, one can stimulate either a net increase or decrease in particle number. Indeed, this stimulated contribution can be nonvanishing only for special initial conditions so chosen that $\langle q_k\rangle$, $\langle\pi_k\rangle$, $\langle\pi_k{}^2-\Omega_k{}^2q_k{}^2\rangle$, and/or $\langle\pi_kq_k+q_k\pi_k\rangle$ is itself nonvanishing.

To further justify the appelation "stimulated," it is useful to ask what sorts of initial conditions are in fact required if the expectation value in Eq. (4.11) is to be nonvanishing. The first point to observe is that this expectation value vanishes identically if one chooses as an initial state the vacuum or, indeed, any initial eigenstate of the N_k's. That this is the case is easy to see. By reexpressing the q's and π's in terms of the standard creation and annihilation operators

$$a^\dagger=(2\Omega)^{-1/2}(\Omega q-i\pi)$$

and (4.12)

$$a=(2\Omega)^{-1/2}(\Omega q+i\pi)\ ,$$

it becomes obvious that $\langle q_k\rangle$ and $\langle\pi_k\rangle$ must vanish for such an eigenstate. And, by observing that

$$\pi^2-\Omega^2q^2=-\Omega[(a^\dagger)^2+(a)^2]$$

and

$$q\pi+\pi q=i[(a^\dagger)^2-(a^2)]\ , \tag{4.13}$$

it is easy to see that the remaining expectation values must vanish as well.

Less obvious, but equally important, is the fact that $d\langle N_k\rangle_{\rm st}/dt$ also vanishes for some highly nontrivial mixed states. Thus, for example, one can verify directly that there is no "stimulated" change in the number of quanta for an initial "pseudothermal" density matrix

$$\mu_{\rm in}\propto\exp(-\beta H_0)\ . \tag{4.14}$$

Indeed, various simple model calculations lead one to the conclusion that, at least in the absence of couplings between degrees of freedom, so that $c_{kk'}\equiv 0$, stimulated contributions arise only for initial conditions which, in the sense described below, contain nontrivial "phase" information.

This observation is connected intimately with Zel'dovich's intuitive explanation[4] of why the spontaneous contribution arising from a time-dependent Ω_k are always positive regardless of the sign of $\dot\Omega_k$, i.e., whether the Universe is expanding or contracting. The key to his understanding of this fact is that quantum-mechanical phase and occupation number are complementary notions in the same sense as the q's and π's (Ref. 32). An initial eigenstate of the N_k's has completely indeterminate phase, but, as the field evolves away from this eigenstate, it tends toward a configuration with partially determined phase and number which necessarily entails an increase in the expectation value of the N_k's.

The spontaneous "correlational" particle creation evidenced by Eq. (4.10) also admits to a simple physical interpretation. As is clear from Eq. (4.6), $d\langle N_k\rangle/dt$ will always contain a contribution involving the product $\mu_I(t)c_{kk'}(t)$. The crucial point then is that, in the absence of an initial $\mu_I(t_0)$, a nontrivial $\mu_I(t)$ is generated only by the evolving correlations and, as such, must itself be proportional to the $c_{kk'}$'s. The net result is that, to lowest order in quantum-mechanical perturbation theory, the evolving correlations induce a rate of particle creation quadratic in the c's (see, however, the quantum field discussion in Sec. II B 2).

Turn now to the entropy generation induced by the dynamics. In the absence of initial correlations $dS(t_0+\Delta t)/dt$ will be given by Eq. (3.26) which, for the model Hamiltonian (4.1), reduces to

$$dS(t_0+\Delta t)/dt=\sum_{k'\neq k}c_{kk'}{}^2{\rm Tr}\mu_R{}^{-1}(t_0)\chi_{kk'}(t_0)^2\Delta t>0\ . \tag{4.15}$$

Here, in terms of the "fluctuating" coordinate

$$\delta_k\equiv q_k-\langle q_k\rangle\ , \tag{4.16}$$

the operator $\chi_{kk'}$ takes the form

$$\chi_{kk'}=i\delta_k[q_{k'},\mu_R]+i\delta_{k'}[q_{k'},\mu_R]$$
$$=-\delta_k\frac{\partial\mu_R}{\partial p_{k'}}-\delta_{k'}\frac{\partial\mu_R}{\partial p_k}\ . \tag{4.17}$$

There is an obvious connection between entropy generation and particle creation in the sense that $dS(t_0+\Delta t)/dt$, like the "correlational" particle creation $d\langle N_k(t_0+\Delta t)\rangle_c/dt$, is positive and scales as $|c_{kk'}|^2$. However, it is also clear that there can exist no direct one-to-one connection. After all, spontaneous particle creation will obtain even in the absence of correlations as a consequence of the time dependence of the Q_k's. What is, however, true is that the correlations which give rise to a nonvanishing dS/dt lead also to an enhancement in the rate of particle creation.

In this regard it is useful to pursue a simple analogy with ordinary particle kinetic theory. Specifically, if, in the spirit of a simple mean-field theory (self-consistent field approximation), along the lines of the Vlasov (i.e., collisionless Boltzmann) equation, one were to neglect the evolving correlations and assume that $\mu \simeq \prod_k g(k)$, one would conclude that dS/dt and $d\langle N_k\rangle_c/dt$ both vanish identically, but that the total $d\langle N_k\rangle/dt \neq 0$. The "mean field" equation

$$\partial_t \mu_R + PL\mu_R \simeq 0 , \tag{4.18}$$

unlike the full equation (3.20) for $\partial_t\mu_R$, is linear and reversible, containing no "dissipation" which could lead to a change in the entropy. Changes in quantities like $\langle N_k\rangle$ induced from this simpler equation must be interpreted, not as manifesting a fundamental irreversibility in the subdynamics of μ_R, but, rather, as reflecting a type of "phase mixing."

From this point of view, one may say that $d\langle N_k\rangle/dt$ contains two sorts of contributions: namely, (i) particle creation due to a type of "phase mixing" which has no connection with the entropy and which will be present even if one pretends that $\mu_I \equiv 0$ and (ii) particle creation induced by changes in μ_I which manifest a direct connection with the phenomenon of entropy generation.

The discussion hitherto has focused upon the short time evolution of the field in response to specific initial conditions. It remains to determine what can be said about the later time evolution, e.g., in the limit that $t\to\infty$. In general, not much is known about this more generic evolution, but at least in the limit that $c_{kk'}\equiv 0$, so that the oscillators decouple and $dS/dt \equiv 0$, some concrete results are known.

Thus, for example, such authors as Parker[3] and Zel'dovich[4] have considered so-called "statically bounded" situations, for which the natural frequencies take the form

$$\Omega_k(t) = \Omega_k^0[1+Q_k(t)] , \tag{4.19}$$

where Ω_0 is a constant and the dynamical function $Q_k(t)$ tends toward well-defined static asymptotic limits $Q_k^{\pm}$ as $t\to\pm\infty$. This is, for example, the form of Ω_k appropriate for a Klein-Gordon field in a conformally flat spacetime with metric $g_{\mu\nu}\equiv a^2(t)\eta_{\mu\nu}$ where $a\to a_{\pm}$ as the conformal time $t\to\pm\infty$. For such a "statically bounded" system, one anticipates that an initial density matrix μ_- will tend eventually toward a static end state μ_+ and, as $t\to\pm\infty$, the expectation value $\langle N_k\rangle$ has an unambiguous physical interpretation as the "number of quanta in the kth mode."

For this special case, it is well known that an initial vacuum state, with $\langle N_k\rangle_- \equiv 0$, will evolve ultimately toward a final state $\langle N_k\rangle_+ = |\beta_k|^2$, where β_k is a calculable Bogoliubov coefficient. The real question is how the net change in quanta $\Delta\langle N_k\rangle \equiv \langle N_k\rangle_+ - \langle N_k\rangle_-$ will be affected by nontrivial initial conditions. The principal conclusion obtained to date is that an initial presence of particles will, at least in the case of bosonic fields, tend to enhance the overall rate of particle creation. Thus, for example, Parker[3] has showed that, for an arbitrary initial mixed state constructed as a superposition of eigenstates of N_k, the net generation of particles

$$\Delta\langle N_k\rangle = |\beta_k|^2(1+2\langle N_k\rangle_-) . \tag{4.20}$$

Equation (4.20) manifests an obvious connection with the short time $d\langle N_k\rangle_p/dt$ of Eq. (4.8). Thus, if one supposes that, initially, $\langle \pi_k^2 - \Omega_k^2 q_k^2\rangle = 0$, as is true for the situation considered by Parker,[3] he concludes that

$$\frac{d\langle N_k(t_0+\Delta t)\rangle_p}{dt} = \frac{\dot\Omega_k^2}{2\Omega_k^2}\Delta t[1+2\langle N_k(t_0)\rangle] . \tag{4.21}$$

For short times, $|\beta_k| = \dot\Omega_k\Delta t/2\Omega_k$. One obtains the spontaneous particle creation associated with the vacuum, amplified by a multiplicative factor $1+2\langle N_k(t_0)\rangle$ which reflects the number of particles already present.

A simple expression for β_k can be derived in the special limit that $Q_k\to 0$ in the limit that $t\to\pm\infty$, i.e., for a background spacetime which at early and late times approaches flat space with metric $g_{\mu\nu}=\eta_{\mu\nu}$. Thus, if one assumes that $|Q_k| \ll 1$ and that $|\dot Q_k|$ is small in an appropriate sense, he concludes that[4]

$$\beta_k \sim \int_{-\infty}^{\infty} dt\, \dot Q_k(t)\exp(-2\Omega_k^0 t) . \tag{4.22}$$

As a concrete example, suppose that

$$Q_k = Q_0(1+t^2/\tau^2)^{-1} , \tag{4.23}$$

where Q_0 and τ are constants. In this case, one concludes that

$$\beta_k \sim i\pi Q_0(2\Omega_k^0\tau)\exp(-2\Omega_k^0\tau) , \tag{4.24}$$

this corresponding to an overall particle creation proportional to $|Q_0|^2$ but modulated by the dimensionless product $\Omega_0\tau$. Here, the natural frequency Ω_k is invariant under time inversion $t\to -t$, and, as such, it is evident that the net creation of particles must be interpreted as a direct consequence of an asymmetry imposed by the initial conditions, rather than by an "arrow" of time induced by Ω_k.

Suppose, for instance, that at early times the system is "at equilibrium," so that

$$\mu_- \equiv \mu(t\to -\infty) \propto \exp[-\beta H(t\to -\infty)] . \tag{4.25}$$

In this case, the initial

$$\langle N_k\rangle_- = \tfrac{1}{2}\coth(\beta\Omega_k/2) \simeq (\beta\Omega_k)^{-1} , \tag{4.26}$$

the final approximate equality obtaining in the "semiclassical" limit that $\beta\Omega_k \ll 1$. This implies a net creation of particles

$$\Delta\langle N_k\rangle \simeq \frac{8\pi^2 Q_0{}^2(\Omega_k^0\tau)^2}{\beta\Omega_k^0}\exp(-4\Omega_k^0\tau) . \tag{4.27}$$

In a similar vein, one might hope to reach some concrete conclusions regarding the evolution of systems with nontrivial couplings $c_{kk'}$ in the limit that the Hamiltonian H is independent of time, so that the average energy is conserved. Here one is wont to suppose that an arbitrary $\mu_{\rm in}$ will converge toward a thermal density matrix $\mu_{\rm eq} \propto \exp(-\beta_{\rm eq}H)$, where the value of $\beta_{\rm eq}$ is determined by energy conservation. The problem, however, is that such an interpretation cannot be literally true: conservation of phase, as embodied in the Liouville equation, imposes a severe restriction on the allowed evolution of μ, so that, in general, $\mu_{\rm in}$ cannot converge pointwise toward $\mu_{\rm eq}$ (Refs. 26 and 33). There may perhaps be a convergence toward $\mu_{\rm eq}$ in some appropriate norm, or in some appropriate time-averaged sense, but a true pointwise convergence is simply impossible. What does, however, appear to be true (see, e.g., the plausibility arguments presented in Ref. 26) is that, for arbitrary initial conditions, (1) $S_{\rm eq} > S_{\rm in}$ and (2) $\langle N_k\rangle_{\rm eq} > \langle N_k\rangle_{\rm in}$.

For the Hamiltonian (4.1), this can be established rigorously for an initial pseudothermal density matrix (4.14), at least in the limit that the c_{kk}'s are sufficiently small that H is a positive quadratic form and $\mu_{\rm eq}$ is well defined.

By way of illustration, consider the case of two oscillators k_1 and k_2 in the classical limit ($\beta\Omega_k \ll 1$) that μ can be interpreted as an ordinary distribution function. Here energy conservation implies that the initial and final "temperatures" must be equal, i.e., that $\beta_{\rm eq}=\beta$, so that the normalized reduced one-oscillator distribution functions take the forms

$$g_{\rm in}(k)=(\beta\Omega_k/2\pi)\exp\left[-\frac{\beta}{2}(\pi_k{}^2+\Omega_k{}^2q_k{}^2)\right] \tag{4.28}$$

and

$$g_{\rm eq}(k)=(\beta\Omega_k\alpha/2\pi)\exp\left[-\frac{\beta}{2}(\pi_k{}^2+\Omega_k{}^2\alpha^2q_k{}^2)\right] , \tag{4.29}$$

where

$$\alpha^2=1-c_{k_1k_2}{}^2/\Omega_{k_1}{}^2\Omega_{k_2}{}^2 \equiv 1-A . \tag{4.30}$$

Provided that $c_{k_1k_2}{}^2 < \Omega_{k_1}{}^2\Omega_{k_2}{}^2$, α will be real and the equilibrium $g_{\rm eq}(k)$'s are well defined. One then concludes immediately that

$$\langle N_k\rangle_{\rm in}=(\beta\Omega_k)^{-1} \tag{4.31}$$

and

$$\langle N_k\rangle_{\rm eq}=\langle N_k\rangle_{\rm in}[(1+A/2)/(1-A)]\rangle\langle N_k\rangle_{\rm in} . \tag{4.32}$$

And, similarly, one verifies that

$$S_{\rm in}=2-\ln\frac{\beta\Omega_{k_1}}{2\pi}-\ln\frac{\beta\Omega_{k_2}}{2\pi} \tag{4.33}$$

and

$$S_{\rm eq}=S_{\rm in}-2\ln\alpha > S_{\rm in} . \tag{4.34}$$

For this simple example, it is also easy to see that $\mu_{\rm eq}$ could not have evolved from $\mu_{\rm in}$. As noted in Sec. III, it is clear that the ordinary "entropy" $\mathscr{S}=\mathrm{Tr}\mu\ln\mu$ must be conserved, but it is easy to verify explicitly that, in this case, $\mathscr{S}_{\rm eq}\neq\mathscr{S}_{\rm in}$. The initial $\mathscr{S}_{\rm in}$ is of course given by Eq. (4.33), whereas the equilibrium value

$$\mathscr{S}_{\rm eq}=\mathscr{S}_{\rm in}-\ln\alpha . \tag{4.35}$$

For an isolated system, it makes no sense *a priori* to suppose that, for example, all initial configurations with the same energy (and, perhaps, some other finite set of conserved quantities, such as linear and/or angular momentum) will converge toward the same final state. Only by allowing for a coupling with some external environment, which plays the role of a "bath" or "reservoir," can one relax the highly nontrivial constraints imposed by "conservation of phase."

V. DISCUSSION

By way of summarizing our results here we will make precise some of the concepts and terminology we employed which may differ from ordinary loose usage.

(A) The main emphasis of this work has been on the relationship between particle creation and entropy generation in dynamical spacetimes. We used a quantum field-theoretical formalism (Sec. II) to discuss *particle creation* and pointed out the following differences.

(1) The difference between particle creation in the absence of ($c_{kk'}=0$) and those in the presence of interactions ($c_{kk'}\neq 0$). The free part includes parametric amplification of vacuum fluctuations and from n-particle states [e.g., ρ_0 in (2.37)]. The interacting part includes those from the interactions among particles (accountable in a quantum-mechanical treatment) and those between the particle pairs and vacuum fluctuations [e.g., terms such as ρ_{02} in (2.37), which are distinct quantum-field effects].

The free part we have loosely called creation by "parametric amplification" and the interacting part, "correlational" particle creation. This should not, however, be mistaken to mean that parametric amplification acts only on free fields. There is also creation by parametric amplification for interacting fields. Particle creation by parametric amplification is present for all dynamic fields, except for conformally invariant fields in conformally static spacetimes.

(2) The difference between what we have called *extrinsic interaction* of modes (including self-interaction) and *intrinsic interaction* of modes due to the time dependence and the coupling of the expansion functions. The latter arises from the wide class of eigenfunctions associated with spaces of lesser symmetry. This dynamically induced linear coupling between modes in a free-field theory is quite different from that of nonlinear coupling externally introduced, but it generates "correlation entropy" just the same. Coupling of this nature serves to illustrate the breakdown of the apparent distinction between phenomena associated with free fields such as particle creation alone and those with interacting fields; both can introduce correlations and generate entropy. Note that there is no preferred choice of mode decomposition in curved

space—the corresponding vacuum state and the physical effects associated therewith could vary accordingly. It therefore is conceivable that an otherwise simple phenomenon for an observer associated with one set of eigenmodes (the "natural" one) may appear very complicated (e.g., with mode coupling) for another observer associated with an "unnatural" set of eigenmodes. This "naturalness" is of course a physically ill-defined concept. The mixmaster space is for us an interesting illustration of just this effect. If the nature of interaction depends on the choice of the observer, then the correlational entropy generated through these interactions may vary accordingly. One needs to stipulate a complete set of eigenstates to define the particle states, and the phenomena of particle creation, interaction, and entropy generation will be measured with respect to these states. This apparent ambiguity of course stems from the lack of a covariant description of these processes and is common in quantum field theory and statistical mechanics in curved spacetimes.

(3) The difference between *spontaneous* and *stimulated* creation. We have defined spontaneous creation [Eqs. (4.8) and (4.10)] as that part which has $d\langle N\rangle/dt\,|_{t_0}=0$ initially (at t_0) and stimulated creation [Eq. (4.11)] as that part which has $d\langle N\rangle/dt\,|_{t_0}\neq 0$. We have also shown that for spontaneous creation, at least for short times, the average particle number always increases. This spontaneous creation may come from parametric amplification [Eq. (4.8)] or from interactions [Eq. (4.10)]: the latter part which we call "correlational," also gives rise to entropy generation. For stimulated changes, the particle number may increase or decrease at $t_0+\Delta t$, depending on the phase relation of the initial state. For example, the stimulated contribution vanishes if the initial state is an eigenstate of the number operator. Two important cases are the vacuum (a pure state) and a thermal state (a special, mixed state), neither of which leads to stimulated creation. Spontaneous particle creation from the vacuum gives rise to the zero-temperature vacuum quantum energy density ρ_0,[29] while spontaneous creation from the thermal n-particle state gives rise to the finite-temperature energy density ρ_T (Ref. 10). In discussions of finite-temperature quantum field theory a distinction is usually made between vacuum and n-particle states. The latter refers to general mixed states containing n_i particles in k_i modes with an arbitrary form of the density matrix. Those described by a thermal density matrix are called thermal n-particle states. These states, when subjected to parametric amplification, give rise to finite-temperature particle creation in exactly the same way [Eq. (2.25)] as particle creation from the vacuum, both being spontaneous in nature. There should be corresponding stimulated production from initial states containing nontrivial phase information.

(B) For the discussion of *entropy generation* we used a subdynamics analysis first developed for classical and quantum fields in Ref. 26. Here we use this formalism as a criterion to define and quantify the notion of entropy in dynamical quantum systems. The central idea explained in Sec. III involves the division of the full N-particle density matrix μ into the sum of a relevant part μ_R and an irrelevant part μ_I. We used the model Hamiltonian of a system of time-dependent coupled harmonic oscillators to explicate these ideas. The relevant contribution to the total density matrix is defined as the product of the reduced density matrices for each oscillator, and the entropy S is defined by tracing μ_R [Eq. (3.12)]. In the absence of initial correlations the time rate of change of $S(t)$ involves only μ_R and the interaction Liouvillian [Eq. (3.26)] which depends on the interaction of the oscillators. We then apply these results to the analysis of particle creation and interaction. The usage and implication of the main ideas here are quite different from those applied to particle creation:

(4) The key idea for the discussion of entropy in this paper is that of *correlation.* A system of completely uncorrelated states will have $\mu_I=0$ identically and, in the absence of interactions, the entropy of the system cannot change with time. *Interactions* among the particles or normal modes can generate correlations and increase the entropy. Changes in entropy can also be classified into spontaneous and stimulated, similar to that for particle creation. For short times at least, just as in particle creation, the spontaneous contributions always lead to a net increase in entropy. The stimulated contributions, which involve a nontrivial initial μ_I, can either increase or decrease the entropy. Combining what we have learned about the different particle creation processes, we conclude that the presence of interaction leads to a net increase in both the particle number and entropy from an initially uncorrelated state. Thus, according to this statistical definition of entropy it is only the correlational part of particle creation which can generate entropy. It says nothing, however, about the effect of parametric amplification (cf. Ref. 19). The correlational entropy which is proportional to the product of $\mu_I(t)$ and $c_{kk'}(t)$ always increases in time.

(5) We suggested a statistical or wave mechanical explanation of the fact that spontaneous particle creation takes place for both the expanding and contracting phases of the Universe (i.e., regardless of the sign of Ω_k). This fact has been explained in a number of equivalent ways before (cf. Refs. 3, 4, and 16). This apparent irreversibility can be viewed as the result of the stipulation of some special initial state and the intrinsic simultaneous indeterminacy between occupation numbers N_k and phases θ_k (Ref. 32). It is well known that the number operator is an adiabatic invariant under slowly varying conditions.[3,4,17] Parametric amplification violates the adiabatic condition and gives rise to particle creation. We remarked earlier that all initial states which are eigenstates of the number operator N_k can only engender spontaneous creation. Such states have completely indeterminate phases θ_k. As the dynamics of spacetime drives the system away from this eigenstate, the phases become partially determinate, accompanied by an increase in the expectation value of N_k. The situation is analogous to the spreading of a wave packet with x and p_x playing the role of N and θ, in that both pairs obey an uncertainty relation. Thus, an initial δ function wave at $x=0$ provides complete information about its position but is totally indeterminate in momentum. As time evolves, it spreads into a Gaussian wave

packet, with increasing variance in its position. Dynamics of the background only serves to magnify this effect,[19] which remains intrinsically time-reversal invariant. This "spreading" is associated with a specially chosen initial state (δ function) and is the workings of the uncertainty principle intrinsic in wave mechanics (either classical or quantum). For the same reason, in particle creation processes, we can understand why there is always an increase in particle number for initial states which are superpositions of the eigenstates of the N_k's (such as the vacuum or the thermal state). This explains the apparent irreversible character of spontaneous particle creation. The phrase *phase mixing* is used loosely here to convey the phase-number duality relation. It is clearly different from that of *frequency mixing* on the one hand, which addresses the mixing of positive- and negative-frequency components of a mode leading to particle creation, and *mode mixing* on the other, which addresses couplings amongst different modes. More discussions on spontaneous creation can be found in Ref. 19.

(6) The short and long time behavior of statistical systems can be very different. For example, stimulated entropy generation can be a transient effect compared with the systematic effects of spontaneous generation (Sec. III). We also show that (detailed in Ref. 26) it makes no sense to suppose that an isolated time-dependent system always converge to an equilibrium state, or any single final state.

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*Present address: Institute for Advanced Study, Princeton, NJ 08540.

†Present address: Physics Department, Syracuse University, Syracuse, NY 13244.

[1]B. L. Hu, in *Cosmology of the Early Universe*, edited by L. Z. Fang and R. Ruffini (World Scientific, Singapore, 1984).

[2]H. Kandrup, Class. Quantum Gravit. **3**, L55 (1986).

[3]L. Parker, Phys. Rev. **183**, 1057 (1969); Phys. Rev. D **3**, 346 (1971); **7**, 976 (1973). For a lucid review, see L. Parker, in *Asymptotic Structures of Spacetime*, edited by F. Esposito and L. Witten (Plenum, New York, 1977).

[4]Ya. B. Zel'dovich, Pis'ma Zh. Eksp. Teor. Fiz. **12**, 443 (1970) [JETP Lett. **12**, 307 (1970)]; in *Physics of the Expanding Universe*, edited by M. Demiánski (Lecture Notes in Physics, Vol. 109) (Springer, New York, 1979).

[5]Y. B. Zel'dovich and A. A. Starobinsky, Zh. Eksp. Teor. Fiz. **61**, 2161 (1971) [JETP **34**, 1159 (1972)]; Pis'ma Zh. Eksp. Teor. Fiz. **12**, 443 (1970) [JETP Lett. **12**, 307 (1970)].

[6]B. L. Hu and L. Parker, Phys. Lett. **63A**, 217 (1977); Phys. Rev. D **7**, 933 (1978).

[7]J. B. Hartle and B. L. Hu, Phys. Rev. D **20**, 1772 (1979); **21**, 2756 (1980).

[8]For a discussion of how entropy content is related to the oldness and flatness problem, see, e.g., A. Guth, Phys. Rev. D **23**, 347 (1981). For a general description of thermal quantum gravitational processes see, e.g., B. L. Hu, Phys. Lett. **130B**, 331 (1981).

[9]For a discussion of the importance of incorporating quantum-statistical consideration in these problems, see B. L. Hu, in talk at the Santa Barbara Workshop on Cosmology and Particle Physics, May, 1982.

[10]B. L. Hu, Phys. Lett. **108B**, 19 (1982); **123B**, 189 (1983); L. F. Chen and B. L. Hu, *ibid.* **160B**, 36 (1985); B. L. Hu, R. Critchley, and A. Stylianopoulos, Phys. Rev. D **35**, 510 (1987), and references therein.

[11]E. Calzetta, and B. L. Hu (unpublished), and references therein.

[12]E. Calzetta, S. Habib, and B. L. Hu (unpublished).

[13]J. D. Bekenstein, Phys. Rev. D **7**, 2333 (1973); **12**, 3077 (1975); S. W. Hawking, Commun. Math. Phys. **43**, 199 (1975). For an introductory review on black-hole thermodynamics and related issues, see, e.g., P. C. W. Davies, Rep. Prog. Phys. **41**, 1313 (1978).

[14]D. W. Sciama, *Centenario di Einstein* (Editrice Giunti Barbara-Universitaria, 1979); P. Candelas and D. W. Sciama, Phys. Rev. Lett. **38**, 1372 (1977); D. W. Sciama, P. Candelas, and D. Deutsch, Adv. Phys. **30**, 327 (1981); E. Mottola, Phys. Rev. D **33**, 2136 (1986).

[15]R. Penrose, in *General Relativity: An Einstein Centenary Volume*, edited by S. W. Hawking and W. Israel (Cambridge University Press, NY, 1979).

[16]B. L. Hu, Phys. Lett. **97A**, 368 (1983).

[17]B. L. Hu, Phys. Rev. D **9**, 3263 (1974); Ph.D. thesis, Princeton University, 1972, Chaps. 2 and 3.

[18]B. L. Hu, Phys. Lett. **90A**, 375 (1982).

[19]B. L. Hu and D. Pavon, Phys. Lett. **180B**, 329 (1986).

[20]Other work on this problem include H. Kodama, Prog. Theor. Phys. **67**, 1415 (1982); M. Morikawa and M. Sasaki, Phys. Lett. **165B**, 59 (1985).

[21]The notion of using projection operators to define a subdynamics was first introduced by R. Zwanzig, in *Lectures in Theoretical Physics*, edited by W. E. Brittin, B. W. Downes, and J. Downes (Interscience, New York, 1961), pp. 106—141.

[22]The classic reference is R. Balescu and J. Wallenborn, Physica **54**, 477 (1971).

[23]For a more leisurely introduction, see R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics* (Wiley, New York, 1975); E. T. Jaynes, Am. J. Phys. **33**, 391 (1965).

[24]Alternative approaches to the construction of a subdynamics have been considered by C. R. Willis and R. H. Picard, Phys. Rev. A **9**, 1343 (1974); H. E. Kandrup and S. Hill Kandrup, Astrophys. J. **277**, 1 (1984).

[25]The notion of a subdynamics for a classical field in curved space was first introduced by H. E. Kandrup, J. Math. Phys. **26**, 2850 (1985).

[26]H. E. Kandrup, J. Math. Phys. (to be published).

[27]A similar approach exploiting similar techniques was used recently for studying the entropy of black holes by L. Bombelli *et al.*, Phys. Rev. D **34**, 373 (1986).

[28]For a general introduction, see, e.g., N. D. Birrell and P. C. W. Davies, *Quantum Fields in Curved Space* (Cambridge University Press, NY, 1982).

[29]S. A. Fulling, L. Parker, and B. L. Hu, Phys. Rev. D **10**, 3905 (1974).

[30]For a general discussion of interacting field theory see, e.g., Chap. 9 of Ref. 28; N. D. Birrell and L. H. Ford, Ann. Phys. (N.Y.) **122**, 1 (1979), whose treatment we follow here; T. S. Bunch, P. Panangadan, and L. Parker, J. Phys. A **13**, 901 (1980).

[31]See, e.g., W. Israel, in *General Relativity, Papers in Honour of S. L. Synge,* edited by L. O'Raifeartaigh (Clarendon, Oxford, 1972), pp. 201–241.

[32]This relation was first shown in maser theory by R. Serber and C. H. Townes, in *Quantum Electronics—A Symposium,* edited by C. H. Townes (Columbia University Press, New York, 1960). See also W. H. Louisell, A. Yariv, and A. E. Siegman, Phys. Rev. **124**, 1646 (1961).

[33]A. I. Akhiezer and S. V. Peletminskii, *Methods of Statistical Physics* (Pergamon, Oxford, 1981).