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Entropy of the gravitational field

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We derive a formula for the nonequilibrium entropy of a classical stochastic field in terms of correlation functions of this field. The formalism is then applied to define the entropy of gravitational perturbations (both gravitational waves and density fluctuations). We calculate this entropy in a specific cosmological model (the inflationary Universe) and find that on scales of interest in cosmology the entropy in both density perturbations and gravitational waves exceeds the entropy of statistical fluctuations of the microwave background. The nonequilibrium entropy discussed here is a measure of loss of information about the system. We discuss the origin of the entropy in our cosmological models and compare the definition of entropy in terms of correlation functions with the microcanonical definition in quantum statistical mechanics.

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I. INTRODUCTION

The concept of entropy plays an important role in all branches of physics. Hence, it is no surprise that entropy can also be defined in general relativity and cosmology. The most famous application of entropy in general relativity is to black holes. Bekenstein's [1] realization that the area of a black hole behaves like an entropy led to the discovery of black-hole radiation [2]. Other important applications of entropy in cosmology relate to the characterization of the initial state of the Universe [3] and to the study of the post-bounce state in bouncing cosmologies.

Entropy expresses the loss of information about the system under consideration [4]. Quite a long time ago, Jaynes [4] argued that entropy expresses the extent of human ignorance about a system and is therefore an anthropomorphic concept. One can uniquely define entropy only after having specified the position of the observer with respect to the system.

Once we accept that entropy measures the loss of information about a system, it becomes important to ask whether there is a natural "coarse graining"; i.e., can it be uniquely specified which part of the information about a system is lost? The problem of defining the entropy becomes the task of determining the correct coarse graining.

We wish to address this question in order to define the entropy of the gravitational field. From a naive point of view, gravitational instability, which is responsible for the formation of structure in the Universe, should lead to an increasing entropy—in agreement with the second law of thermodynamics. In the initial state in which the gravitational field is (almost) uniform, the gravitational entropy (almost) vanishes. In contrast, the later state of the gravitational field which results from gravitational instability can be viewed as a particular realization of some stochastic process producing density perturbations and gravitational waves. Hence, there should be an associated entropy which characterizes the naturalness of the occurrence of the given distribution or, more quantitatively, measures the probability of the distribution.

To characterize the measure of a state of gravitational radiation or density perturbations in a quantitative manner, we need a well-defined and well-justified notion of entropy of gravitational perturbations. Since the states we are interested in are far from thermal equilibrium, our task will be to define an entropy for nonequilibrium systems in cosmology.

There already exists a considerable body of work on the definition of nonequilibrium entropy; in particular, in the context of cosmology. For example, Smolin [5] derived a formula for the entropy of a "quantum field" state of gravitational radiation and applied it to estimate the entropy of some astrophysical sources of gravitational radiation.

In a series of papers, Hu and Pavòn [6], Kandrup [7,8], and Hu and Kandrup [9] have discussed the entropy of particles produced in an expanding universe. They gave a definition of entropy based on the single-particle distribution function (density matrix) and showed that this entropy increases in time (if the initial state is free of correlations) as a result of particle production. This definition of entropy (and, in particular, the role of coarse graining

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and loss of correlations) was further discussed by Habib and Kandrup [10].

Some interesting speculations about the entropy S_g of the gravitational field have been made by Penrose [3] and Hu [11], who propose that S_g is proportional to the integral of the Weyl tensor squared C^2 over space. This definition expresses the expectation that metric fluctuations should give rise to entropy. With this formulation, Penrose's initial condition criterion [3] $C=0$ for the Universe is equivalent to the assumption that the Universe starts in a state of vanishing gravitational entropy.

In this paper we use two quite different approaches to define the nonequilibrium entropy of cosmological perturbations. One of them is based on the microcanonical ensemble [12] of quantized gravitational perturbations while the other is a formula for entropy which can be associated with the stochastic distribution which describes the state of the classical gravitational field. We show that these two definitions are in agreement and discuss the physical meaning of the entropy of gravitational fluctuations. Then, we apply our definitions to estimate the entropy of gravitational waves and linear density inhomogeneities produced by inflation [13]. We also indicate how to apply our methods to other cosmological models, e.g., those based on phase transitions [14].

Our analysis is based on the fact that the theory of gravitational waves and of linearized density perturbations in an expanding universe can be reduced [15] to the study of a real scalar field in an external classical background. Hence, we will investigate the more general question of how to define the entropy of a scalar field in a nonequilibrium state. We can either study the quantum theory of this field and use the microcanonical ensemble, or we can view the classical field as a stochastic process and determine its entropy.

The paper is organized in the following manner: After some general comments about nonequilibrium entropy in Sec. II, we give in Secs. III and IV the quantum and classical definitions of entropy. In Sec. V we show the equivalence of the two definitions when applied to situations when both are applicable. We also demonstrate that the entropy is a result of coarse graining. In Sec. VI we briefly review the gauge-invariant theory of cosmological perturbations upon which our definition of the entropy of the gravitational field is based. For a pedagogical introduction, the reader is referred to Ref. [16] for an extensive review of Ref. [15]. Section VII contains the main applications of our work: the evaluation of the entropy of gravitational waves and density perturbations in inflationary universe models.

We use units in which $\hbar=k_B=c=1$. Greek indices run over space-time variables, Latin indices only run over spatial variables.

II. NONEQUILIBRIUM ENTROPY

We will first develop a general definition of entropy for a system far from thermal equilibrium, based on the microcanonical ensemble [12]. Let us assume that the state of some physical system can be completely described by a set of discrete variables $J=\{I,i,j,\ldots\}$. If we know that the system is in a certain state J, then the information about the state of the system is complete and hence the entropy should be zero, as follows from the general definition of entropy in information theory according to which entropy means the loss of information. If, on the other hand, we only know the probability distribution P_J for the system, P_J being the probability to find the system in state J, then the associated entropy is [4,12]

$$S=-\sum_J P_J \ln P_J \ . \tag{1}$$

Now let us assume that we are not interested in or cannot measure the complete (fine grained) state of the system, but only some coarse grained characteristics, e.g., the value of the variable I. The coarse-grained state can be described by a distribution function P_I, and the associated entropy is given by the analogue of (1) where we sum only over the index I. This entropy characterizes the measure of solutions of the dynamical system which leads to the particular coarse-grained state.

If the variable J in (1) is continuous, some complications arise. If $\mathcal{D}J$ is the measure on the space of state, then a probability density $p(J)$ can be defined by

$$\mathcal{D}P(J)=p(J)\mathcal{D}J \ , \tag{2}$$

where $\mathcal{D}P(J)$ is the probability to find the system in the volume $\mathcal{D}J$ around the state J. For example, in a system of n particles with Cartesian coordinates $x_1,\ldots,x_n$ and momenta $p_1,\ldots,p_n$, we would have $J\equiv(x_1,\ldots,x_n,p_1,\ldots,p_n)$ and $\mathcal{D}J=\prod_{i=1}^{n}(dx_i dp^i)$. In a system with an infinite number of particles, $\mathcal{D}J$ becomes a measure in the space of functionals.

To derive the formula for the entropy of a system with continuous J starting from Eq. (1), we first divide phase space into sufficiently small cells $J_1,J_2,\ldots$ with volume elements $\Delta J_1,\Delta J_2,\ldots$. The probability to find the system in cell n is

$$P_{J_n}\simeq p(J_n)\Delta J_n \ , \tag{3}$$

and hence from (1) the entropy is

$$S=-\sum_n P_{J_n}\ln P_{J_n}$$
$$\simeq-\sum_n p(J_n)[\ln p(J_n)]\Delta J_n-\sum_n p(J_n)\ln(\Delta J_n)\Delta J_n \ . \tag{4}$$

This expression has no limit for $\Delta J_n\to 0$ because of the diverging second term which in general depends on $\{p(J_n)\}$. This term represents the information about the process of coarse graining.

However, for a simple coarse graining with $\Delta J_1=\Delta J_2=\ldots$, the second term in (4) does not depend on the probability distribution $P(J)$ and can hence be neglected as some irrelevant additive constant $-\ln\Delta J$ to the entropy. Note that in a quantum dynamical system, there is a natural choice $\Delta J=(2\pi\hbar)^n$ due to the uncertainty principle. We conclude that in the case of a continuous probability distribution, the entropy is defined by coarse graining and depends on the measure in the phase space of the system. Dropping the second term in (4) and taking the continuum limit $\Delta J \to 0$ gives

$$S = -\int p(J) \ln p(J) \mathcal{D}J \ , \tag{5}$$

where $\mathcal{D}J$ is the functional measure for the variable J.

III. MICROCANONICAL DEFINITION OF ENTROPY FOR A QUANTIZED FIELD

Let us return to a system whose phase space is described by a set of discrete variables. Furthermore, we consider the case when the entire system consists of $\mathcal{N}$ identical subsystems (e.g., $\mathcal{N}$ photons), each characterized by a discrete set of variables $\{I, i, j, \dots\}$. We assume that there is some principal quantum number I which is completely distinguishable; i.e., any two states with different I can be experimentally distinguished, and that the other numbers $i, j, \dots$ correspond to different but experimentally indistinguishable states with the same values of I. As an example, for a gas of photons in a box we can take I to be the energy of a photon, and $i, j, \dots$ to correspond to different directions of motion.

The source of entropy in the above setup is the loss of information coming from the indistinguishability of states with identical I but different $i, j, \dots$. States labeled by I can be assigned a degeneracy g_I which equals the number of microphysical states with identical quantum number I.

Let us now assume that $\bar{n}_I$ subsystems have the same principal quantum number I. For the moment we assume that the spectrum of the system $\{\bar{n}_I\}$, i.e., the number $\bar{n}_I$ of subsystems with principal quantum number I (for all I), is fixed. Our goal is to calculate the number of possible microphysical states with a given spectrum which are in principle distinguishable. The calculation is done for systems with Bose statistics, e.g., photons, gravitons, or scalar-type cosmological perturbations.

The problem reduces to calculating the number of possible and distinguishable ways in which $\bar{n}_I$ subsystems can be distributed among g_I cells. This number is

$$W_{\bar{n}_I} = \frac{(g_I - 1 + \bar{n}_I)!}{\bar{n}_I!(g_I - 1)!} \ . \tag{6}$$

To obtain this expression, note that there are $(\bar{n}_I + g_I - 1)!$ ways of dividing $\bar{n}_I$ objects by $g_I - 1$ cell divisions. However, both the particles and the cell divisions are indistinguishable and hence we must divide by $\bar{n}_I!(g_I - 1)!$.

For a system of $\mathcal{N}$ subsystems with spectrum $\{\bar{n}_I\}$ (obeying $\sum_I \bar{n}_I = \mathcal{N}$), the phase volume (number of possible states) will be

$$\Gamma_{\{\bar{n}_I\}} = \prod\nolimits_I W_{\bar{n}_I} \ . \tag{7}$$

The next step is to assume that all possible states are equally probable. In this case, the probability for any state α with the given spectrum $\{\bar{n}_I\}$ is

$$P_{\{\bar{n}_I\}}(\alpha) = 1/\Gamma_{\{\bar{n}_I\}} \ . \tag{8}$$

From (1) it follows that the corresponding entropy of the system with definite spectrum $\{\bar{n}_I\}$ is

$$S = -\sum_\alpha P_{\{\bar{n}_I\}}(\alpha) \ln P_{\{\bar{n}_I\}}(\alpha) = \ln \Gamma_{\{\bar{n}_I\}} = \sum_I \ln W_{\bar{n}_I} \ , \tag{9}$$

taking into account the normalization condition

$$\sum_\alpha P_{\{\bar{n}_I\}}(\alpha) = 1 \ . \tag{10}$$

If $\bar{n}_I \gg 1$, then Stirling's formula can be applied to approximate $W_{\bar{n}_I}$ in (9). In this case, the entropy becomes

$$S = \sum_I g_I[(n_I + 1)\ln(n_I + 1) - n_I \ln n_I] \ , \tag{11}$$

where $n_I = \bar{n}_I / g_I$ are the occupation numbers.

All that was assumed in the above considerations is that the spectrum $\{\bar{n}_I\}$ is well defined. At no point was thermodynamic equilibrium invoked. Hence, (11) gives a formula for the entropy of a statistical system with definite spectrum which is valid both in and far out of thermodynamical equilibrium.

The simplest application of this formula for the entropy is to a blackbody spectrum of photons with

$$n_k = 2/(e^{\beta k} - 1) \tag{12}$$

with $\beta = 1/T$ and $k = |k|$. In this case, each photon is a subsystem. The principal quantum number I is the energy k, and the other quantum numbers $i, j, \dots$ correspond to the directions of photon propagation. The degeneracy g_k of level $I = k$ is

$$g_k = (4\pi/3) V k^2 dk \ , \tag{13}$$

where V is the volume of space. Substituting (12) and (13) into (11) we obtain the entropy density of the blackbody background

$$s = (S/V) \sim (4\pi/3) T^3 \ . \tag{14}$$

In the above example, the origin of the entropy is the absence of information about the direction of propagation of the photons.

If the spectrum $\{\bar{n}_I\}$ is not well known, there is an additional source of entropy. Let us assume a probability distribution $P(\{\bar{n}_I\})$ for different spectra. Note that even the total number $\mathcal{N}$ of subsystems need not be fixed. In this case, the space of all possible states is the direct sum of states for the different spectra $\{\bar{n}_I\}$. The probability to find the system in a state $\alpha_{\{\bar{n}_I\}}$ with spectrum $\{\bar{n}_I\}$ is

$$P(\alpha_{\{\bar{n}_I\}}) = P(\{\bar{n}_I\})[1/\Gamma(\{\bar{n}_I\})] \ , \tag{15}$$

and [from (1)] the entropy will be

$$S = -\sum_{\{\bar{n}_I\}} \sum_{\alpha\{\bar{n}_I\}} P(\alpha_{\{\bar{n}_I\}}) \ln P(\alpha_{\{\bar{n}_I\}}) = \sum_{\{\bar{n}_I\}} P(\{\bar{n}_I\}) \ln \Gamma(\{\bar{n}_i\}) - \sum_{\{\bar{n}_I\}} P(\{\bar{n}_I\}) \ln P(\{\bar{n}_I\}) \ , \tag{16}$$

where $\sum_{\{\bar{n}_i\}}$ stand for summation over all possible spectra $\{\bar{n}_I\}$. If the spectrum is completely specified, then $P(\{\bar{n}_I\})=1(0)$ for

$$\{\bar{n}_I\}=\{\bar{n}_I^0\}(\{\bar{n}_I\}\neq\{\bar{n}_I^0\})$$

and (16) reduces to (9). In the general case, there are two contributions to the entropy. The first term in (16) is due to the absence of information about the nonprincipal quantum numbers of the system for a fixed spectrum, the second comes from our ignorance of the precise spectrum.

In the case of cosmological perturbations, the distribution function $P(\{\bar{n}_I\})$ for the spectrum is well localized at a particular spectrum $\{\bar{n}_I^0\}$ and hence

$$S\simeq\ln\Gamma(\{\bar{n}_I^0\}) . \tag{17}$$

However, there are examples where the second term in (16) gives the main contribution to the entropy. For example, in the case of a black hole it is impossible to have information about the spectrum of the configuration making up the hole, since this information is hidden behind the horizon. If W is the number of possible different spectra for a black hole of fixed mass, and if we assume that all of these spectra have equal probability, then, neglecting the first term in (16), we get

$$S\simeq\ln W . \tag{18}$$

If the black hole is quantized, then W is finite. In fact, counting the number of spectra of a black hole with fixed mass gives a formula for the entropy in agreement with the classical result [17].

Let us return to the discussion of the formula (11) for the entropy of a quantum system with fixed spectrum. In the classical limit $n_I \gg 1$, the equation simplifies to

$$S\simeq\sum_I g_I \ln n_I . \tag{19}$$

In order to apply this formula, the notion of particles (which is required to be able to determine n_I) must be well defined. However, when considering quantum fields in some external field (e.g., cosmological perturbations in an expanding background space-time), the notion of particles is not always well defined. It is hence desirable to have a formalism which generalizes the definition of entropy to situations where the number representation is not well defined.

For large occupation numbers n_I, the classical limit should give a good description of the dynamics of the system. It is therefore convenient to derive a formula for the entropy directly in terms of the classical field. In the cases when occupation numbers can be defined for this field, the new definition should reduce to (19).

In the next section, we will give a definition of entropy of a classical field based on the theory of stochastic processes and show that in the region where both definitions of entropy are applicable they agree.

IV. ENTROPY OF A CLASSICAL FIELD

Formulas (11) and (19) for the entropy of a field are only applicable if the spectrum of occupation numbers is well defined. In order for this to be the case, there must be a well-defined notion of particles for the field under consideration.

As will be shown in Sec. VI, the description of cosmological perturbations and gravitational waves in the Universe can be reduced to the study of a scalar field $\varphi(\mathbf{x},t)$ with a time-dependent effective mass [15,16]:

$$\varphi''-c_s^2\Delta\varphi-(z''/z)\varphi=0 . \tag{20}$$

Here, c_s is the speed of propagation of perturbations. For gravitational waves $c_s=1$, whereas for cosmological perturbations in a universe with hydrodynamical matter c_s is the speed of sound. The time-dependent function z depends on the system and on the background. For gravitational waves $z=a$, whereas z is a complicated function of the background parameters in the case of cosmological perturbations (for details see Ref. [15] and Sec. VI). In the above equation a prime denotes differentiation with respect to conformal time η.

The quantization of a scalar field obeying (20) is equivalent to the quantization of a scalar field in some external classical field. If $z''/z=0$ and $c_s^2=\text{const}\neq0$, then there is no coupling and the quantum theory for this field (in particular, the notion of particle) is well defined. As will be shown in Sec. VI, this applies for both cosmological perturbations and gravitational waves in a radiation-dominated universe. However, this is not the general case. The ratio z''/z can be nonvanishing and c_s^2 may be zero. For example, for cosmological perturbations in a matter-dominated universe $c_s=0$. In this case the solutions of (20) do not have oscillatory character and it is not possible to define the notion of particles. Hence it is not possible to define occupation numbers and Eqs. (11) and (19) are inapplicable.

However, if the perturbations are sufficiently large, the scalar field φ can be treated classically (in the case when occupation numbers *are* defined, the condition for classicality is $n_I \gg 1$). In order to define a notion of entropy valid in this case, we address the more general question of defining the entropy of a classical scalar field with an action which is quadratic in field variable and canonical momentum (see also Ref. [18]).

The source of the entropy is in this case the ignorance about the exact field configuration. A state of the system at some time t is specified by the values of the field $\varphi(\mathbf{x},t)$ and its canonical momentum $\pi(\mathbf{x},t)$ at all points $\mathbf{x}$ in space. We assume that all we know is the probability distribution $P(\varphi(\mathbf{x}),\pi(\mathbf{x}))$ of the field and its canonical momentum; i.e., we view $\varphi(\mathbf{x})$ as a stochastic classical field.

The above situation is realized in many situations of interest in cosmology. For example, in inflationary universe models, the amplification of scalar field fluctuations during the period of exponential expansion of the Universe and the nontrivial transition of quantum fluctuations to classical ones leads to a squeezed state [19,20] for the scalar field starting from the vacuum state at the beginning of inflation. The Gaussian random state is characterized by definite correlation functions $\langle\varphi(\mathbf{x},t)\varphi(\mathbf{y},t)\rangle$, $\langle\pi(\mathbf{x},t)\pi(\mathbf{y},t)\rangle$, and $\langle\varphi(\mathbf{x},t)\pi(\mathbf{y},t)\rangle$, where $\langle q\rangle$ stands for the ensemble average of the quantity q (which coincides with the space average of q for a spatially homogeneous stochastic process).

If the initial state of the system is Gaussian, and if the Hamiltonian is quadratic, then time evolution will preserve the Gaussian character of the state. We will assume, as is the case for linear cosmological perturbations and gravitational waves, that the state is Gaussian at all times. Therefore, the probability distribution $P(\varphi(\mathbf{x}),\pi(\mathbf{x}))$ can be expressed in terms of the above two-point correlation functions. Hence, also the entropy of the system must be expressible in terms of two-point correlation functions.

In the following, we will derive a general expression for the entropy of a stochastic Gaussian field in terms of its two-point correlation functions.

Starting point of the analysis is formula (5) for the entropy in terms of the probability distribution. In our case, the continuous variable J stands for a point in phase space. To justify the choice of the measure in (5), we divide phase space (φ,π) at every point $\mathbf{x}$ in space into units of volume $2\pi\hbar$ (the smallest volume the fields can be localized in by the uncertainty principle) and calculate the probability ΔP that the fields lie in the bin Δ_J:

$$\Delta P_J=\int_{\Delta_J} P(\varphi(\mathbf{x}),\pi(\mathbf{x}))\mathcal{D}\varphi(\mathbf{x})\mathcal{D}\pi(\mathbf{x}) \ . \tag{21}$$

Here, the integration ranges over fields $\varphi(\mathbf{x})$ and $\pi(\mathbf{x})$ which lie in bin Δ_J and $\mathcal{D}\varphi(\mathbf{x})\ \mathcal{D}\pi(\mathbf{x})$ denotes the functional integral measure for a scalar field.

Thus, from the analysis of Sec. II we conclude that (apart from an irrelevant constant), the entropy of the stochastic classical field is given by

$$S=-\int P(\varphi(\mathbf{x}),\pi(\mathbf{x}))\ln P(\varphi(\mathbf{x}),\pi(\mathbf{x}))\mathcal{D}\varphi(\mathbf{x})\mathcal{D}\pi(\mathbf{x}) \ . \tag{22}$$

For a Gaussian state, the probability distribution is

$$P(\varphi,\pi)=\frac{1}{W}\exp\left[-\frac{1}{2}(\varphi_x A^{xy}\varphi_y+\pi_x B^{xy}\pi_y+2\varphi_x C^{xy}\pi_y)\right] , \tag{23}$$

where the normalization factor W, determined by

$$\int P(\varphi,\pi)\mathcal{D}\varphi\,\mathcal{D}\pi=1 , \tag{24}$$

is given by

$$W=\int \exp\left[-\frac{1}{2}(\varphi_x A^{xy}\varphi_y+\pi_x B^{xy}\pi_y+2\varphi_x C^{xy}\pi_y)\right]\mathcal{D}\varphi\,\mathcal{D}\pi \ . \tag{25}$$

Here, we have used the shorthand notation $\varphi(\mathbf{x})=\varphi_x$ and $A^{xy}=A(\mathbf{x},\mathbf{y})$, and the Einstein "summation" convention for repeated indices,

$$\rho_x A^{xy}=\int d\mathbf{x}\,\rho(\mathbf{x})A(\mathbf{x},\mathbf{y}) , \tag{26}$$

is implied. For a homogeneous Gaussian state, the kernals A^{xy}, B^{xy}, and C^{xy} depend only on the difference of the arguments:

$$A^{xy}=A(\mathbf{x},\mathbf{y})=A(\mathbf{x}-\mathbf{y})=A(\mathbf{y}-\mathbf{x}) \ . \tag{27}$$

The kernel of the operator A^{-1} inverse to A will be denoted by A_{xy}^{-1}. This is defined as usual by

$$A_{xz}^{-1}A^{zy}=\int d^3z\ A^{-1}(\mathbf{x},\mathbf{z})A(\mathbf{z},\mathbf{y})=\delta^3(\mathbf{x}-\mathbf{y}) \ .$$

Note that the kernel C does not in general vanish since in general φ and π are not statistically independent. A nonvanishing C reflects a correlation between φ and π.

Our goal now is to express the kernels A^{xy}, B^{xy}, and C^{xy} in terms of the two point correlation functions $\langle\varphi(\mathbf{x})\varphi(\mathbf{y})\rangle$, $\langle\pi(\mathbf{x})\pi(\mathbf{y})\rangle$, and $\langle\varphi(\mathbf{x})\pi(\mathbf{y})\rangle$. As a first step, it is convenient to rewrite the distribution function $P(\varphi,\pi)$ in terms of new variables which are independent:

$$\begin{aligned}\zeta_x&=\varphi_x+C^{zy}A_{yx}^{-1}\pi_z \ ,\\ \pi_x&=\pi_x \ .\end{aligned} \tag{28}$$

The Jacobian of this transformation is 1 and hence

$$\mathcal{D}\varphi\,\mathcal{D}\pi=\mathcal{D}\zeta\,\mathcal{D}\pi \ . \tag{29}$$

The probability distribution (23) in terms of the new variables ζ and π is

$$P(\zeta,\pi)=\frac{1}{W}\exp\left[-\frac{1}{2}(\zeta_x A^{xy}\zeta_y+\pi_x\Gamma^{xy}\pi_y)\right] , \tag{30}$$

where

$$\Gamma^{xy}=B^{xy}-C^{xu}A_{uv}^{-1}C^{vy} \ . \tag{31}$$

At this point, the correlation functions can be immediately expressed in terms of the kernels

$$\begin{aligned}\langle\zeta_x\zeta_y\rangle&=A_{xy}^{-1} \ ,\\ \langle\pi_x\pi_y\rangle&=\Gamma_{xy}^{-1} \ ,\\ \langle\zeta_x\pi_y\rangle&=0 \ .\end{aligned} \tag{32}$$

This can be seen either by direct functional integration, or by calculating the generating functional (characteristic functional)

$$\Phi(J^\zeta,J^\pi)=\int P(\zeta,\pi)\exp(-iJ_x^\zeta\zeta^x-iJ_x^\pi\pi^x)\mathcal{D}\zeta\,\mathcal{D}\pi \tag{33}$$

and taking second derivatives of it, e.g.,

$$\langle\zeta_x\zeta_y\rangle=-\left.\frac{\delta^2\Phi}{\delta J_x^\zeta\delta J_y^\zeta}\right|_{J^\zeta=J^\pi=0} . \tag{34}$$

Substituting ζ from (28) into (32) and solving the resulting set of equations we obtain

$$\begin{aligned}A_{xy}^{-1}&=\langle\varphi_x\varphi_y\rangle-\langle\varphi_x\pi_u\rangle\langle\pi_u\pi_v\rangle^{-1}\langle\pi_v\varphi_y\rangle \ ,\\ B_{xy}^{-1}&=\langle\pi_x\pi_y\rangle-\langle\pi_x\varphi_u\rangle\langle\varphi_u\varphi_v\rangle^{-1}\langle\varphi_v\pi_y\rangle \ ,\\ C_{xy}^{-1}&=\langle\varphi_x\pi_y\rangle-\langle\pi_x\pi_u\rangle\langle\varphi_u\pi_v\rangle^{-1}\langle\varphi_v\varphi_y\rangle \ .\end{aligned} \tag{35}$$

Deriving the above formulas we took into account that for a spatially homogeneous Gaussian process the correlation functions depend only on the difference of the arguments.

To calculate the entropy, we substitute (30) into the general formula (22) using the fact that the Jacobian of the transformation (28) is unity and obtain

$$\begin{aligned} S &= -\int P(\zeta,\pi)\ln P(\zeta,\pi)\mathcal{D}\zeta\,\mathcal{D}\pi \\ &= V\delta^3(0)+\ln W \\ &= V\delta^3(0)+\ln\int \exp\left[-\frac{1}{2}(\zeta_x A^{xy}\zeta_y+\pi_x\Gamma^{xy}\pi_{xy})\right] \\ &\qquad\times\mathcal{D}\zeta\,\mathcal{D}\pi \\ &= V\delta^3(0)+\frac{1}{2}\ln\det(A^{-1}\Gamma^{-1})\ , \end{aligned} \tag{36}$$

where V is the volume of space. Dropping the irrelevant constant contributions to the entropy and inserting (32) and (35) in the above, we get the following expression for the entropy in terms of correlation functions:

$$\begin{aligned} S &= \tfrac{1}{2}\ln\det(\langle\varphi_x\varphi_z\rangle\langle\pi_z\pi_y\rangle-\langle\varphi_x\pi_z\rangle\langle\pi_z\varphi_y\rangle) \\ &= \tfrac{1}{2}\ln\det\mathcal{D}^{xy}\ . \end{aligned} \tag{37}$$

Thus, the problem of calculating the entropy has been reduced to the evaluation of a determinant of the operator

$$\begin{aligned} \mathcal{D}^{xy}=\mathcal{D}(\mathbf{x}-\mathbf{y}) = \int [&\langle\varphi(\mathbf{x})\varphi(\mathbf{z})\rangle\langle\pi(\mathbf{z})\pi(\mathbf{y})\rangle \\ &-\langle\varphi(\mathbf{x})\pi(\mathbf{z})\rangle\langle\pi(\mathbf{z})\varphi(\mathbf{y})\rangle]d^3z\ . \end{aligned} \tag{38}$$

This determinant can be calculated by ζ function regularization (see the Appendix). The result is

$$\det\mathcal{D}\propto\exp\left[V\int d^3k\,\ln\mathcal{D}_k\right]\ , \tag{39}$$

where

$$\mathcal{D}_{\mathbf{k}}=\frac{1}{(2\pi)^3}\int d^3\mathbf{x}\,e^{-i\mathbf{k}\cdot\mathbf{x}}\mathcal{D}(\mathbf{x}) \tag{40}$$

is the spectral density of the operator $\mathcal{D}(\mathbf{x})=\mathcal{D}(\mathbf{x}-\mathbf{y})$. Substituting (39) in (37) we obtain the following expression for the entropy per unit volume:

$$\begin{aligned} s=S/V &= \int d^3\mathbf{k}\,\ln\mathcal{D}_k \\ &= \int d^3\mathbf{k}\,\ln(\langle|\varphi_{\mathbf{k}}|^2\rangle\langle|\pi_{\mathbf{k}}|^2\rangle-\langle|\varphi_{\mathbf{k}}|^2|\pi_{\mathbf{k}}|^2\rangle)\ . \end{aligned} \tag{41}$$

where we expressed the entropy in terms of the spectral density of correlation functions and omitted irrelevant contributions which do not depend on the spectrum of the scalar field.

Note that the key assumptions in deriving (41) were the reduction of the problem to that of a free scalar field, and the choice of a Gaussian initial state. Hence, our formalism is applicable also to the entropy of quantum matter fields in an expanding universe, a topic which has been analyzed in detail in past works [6–10]. However, to our knowledge the expression (41) for the entropy in terms of expectation values is new (the closest is the analysis of Ref. [10]). What is fundamentally new in our analysis is the application of nonequilibrium entropy considerations to calculate the entropy of gravitational perturbations by treating them as classical stochastic fields.

V. GENERAL COMMENTS

In this section we shall focus on two issues: The connection between the two definitions of entropy given in Secs. III and IV, and a further discussion of the origin of entropy. To concretize the analysis we consider a quantized free scalar field $\hat{\varphi}(\mathbf{x},\eta)$ with time-dependent effective mass. The field is assumed to start out in its initial vacuum state. As is well known, this state evolves into a squeezed state [19,20]. Such a state is highly excited in the sense that the expectation value of the number operator is large.

If the mass is constant at the beginning and at the end, then the notion of particles is well defined for the in state and for the out state, and in the corresponding time intervals the field operator $\hat{\varphi}$ can be expanded either in terms of in creation and annihilation operators $\hat{a}^+$ and $\hat{a}^-$ or in terms of the corresponding out operators $\hat{c}^+$ and $\hat{c}^-$:

$$\begin{aligned} \hat{\varphi}(\mathbf{x},\eta) &= \int\frac{d^3k}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}^{\text{in}}(\eta)^*\hat{a}_{\mathbf{k}}^-+e^{-i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}^{\text{in}}(\eta)\hat{a}_{\mathbf{k}}^+] \\ &= \int\frac{d^3k}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}^{\text{out}}(\eta)^*\hat{c}_{\mathbf{k}}^-+e^{-i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}^{\text{out}}(\eta)\hat{c}_{\mathbf{k}}^+]\ , \end{aligned} \tag{42}$$

where $u_{\mathbf{k}}^{\text{in}}(\eta)$ and $u_{\mathbf{k}}^{\text{out}}(\eta)$ are the positive frequency mode functions in the in and out states, respectively. For the particular case under consideration, the operators $\hat{c}_{\mathbf{k}}^+$ and $\hat{c}_{\mathbf{k}}^-$ are related to $\hat{a}_{\mathbf{k}}^+$ and $\hat{a}_{\mathbf{k}}^-$ via a Bogoliubov transformation

$$\begin{aligned} c_{\mathbf{k}}^- &= a_{\mathbf{k}}^-\cosh r_k - a_{-\mathbf{k}}^- e^{2i\varphi_k}\sinh r_k\ , \\ c_{\mathbf{k}}^+ &= -a_{-\mathbf{k}}^+ e^{-2i\varphi_k}\sinh r_k + a_{\mathbf{k}}^+\cosh r_k\ . \end{aligned} \tag{43}$$

The real functions $r_k(\eta)$ and $\varphi_k(\eta)$ are called squeeze parameter and squeeze angle, respectively [21,22]. The initial state is taken to be the vacuum $|0\rangle_{\text{in}}$ defined by $\hat{a}_k^-|0\rangle_{\text{in}}=0$ for all $\mathbf{k}$.

The expectation value of the number of particles at late times in the $\mathbf{k}$ mode is

$$\langle n_{\mathbf{k}}\rangle=\langle 0_{\text{in}}|c_{\mathbf{k}}^+c_{\mathbf{k}}^-|0_{\text{in}}\rangle=\sinh^2 r_k\ . \tag{44}$$

Hence, for large values of the squeeze parameter r_k, we should expect that the quantum field $\hat{\varphi}$ can with good accuracy be described as a classical field φ_{cl}, since if $r_k\gg1$, the condition $\langle n_{\mathbf{k}}\rangle\gg1$ to be in the region of applicability of the classical limit is satisfied. In this limit, the correlation functions of the classical field φ_{cl} should coincide with the corresponding expectation values of the operator $\hat{\varphi}$, e.g.,

$$\begin{aligned} \langle\varphi_{\text{cl}}(\mathbf{x},\eta)\varphi_{\text{cl}}(\mathbf{y},\eta)\rangle &\simeq \langle 0_{\text{in}}|\hat{\varphi}(\mathbf{x},\eta)\hat{\varphi}(\mathbf{y},\eta)|0_{\text{in}}\rangle \\ &\equiv \langle\hat{\varphi}(\mathbf{x},\eta)\hat{\varphi}(\mathbf{y},\eta)\rangle\ . \end{aligned} \tag{45}$$

Hence, in the classical limit both of our formulas for the entropy should be applicable and give the same result. In the following we show that this is indeed true.

First of all, we need to calculate the correlation functions of $\hat{\varphi}$ in terms of the squeeze parameters. Taking into account that at late times (in the out state)

$$u_{\mathbf{k}}^{\text{out}}(\eta) \sim e^{i\omega_k \eta} , \quad \omega_k = \sqrt{k^2 + m_{\text{out}}^2} , \tag{46}$$

where m_{out} is the mass in the out phase and, using (43), we find the following expressions for the late time correlation functions [23]:

$$\begin{aligned}
&\langle \varphi(\mathbf{x},\eta)\varphi(\mathbf{y},\eta) \rangle \\
&\quad = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{1}{2\omega_k} \\
&\qquad \times (2\sinh^2 r_k + 1 - \sinh 2r_k \cos 2\delta_k) , \\
&\langle \pi(\mathbf{x},\eta)\pi(\mathbf{y},\eta) \rangle \\
&\quad = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{\omega_k}{2} \\
&\qquad \times (2\sinh^2 r_k + 1 + \sinh 2r_k \cos 2\delta_k) , \\
&\langle \varphi(\mathbf{x},\eta)\pi(\mathbf{y},\eta) \rangle \\
&\quad = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{i}{2} (1 - i\sinh 2r_k \sin 2\delta_k) ,
\end{aligned} \tag{47}$$

where the angle δ_k is

$$\delta_k(\eta) = \int d\eta [\omega_k(\eta) - \varphi_k] . \tag{48}$$

Hence, it follows immediately that

$$\begin{aligned}
&\int d^3z \langle \varphi(\mathbf{x})\varphi(\mathbf{z}) \rangle \langle \pi(\mathbf{z})\pi(\mathbf{y}) \rangle \\
&\quad = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{1}{4} [(2\sinh^2 r_k + 1)^2 \\
&\qquad - \sinh^2 2r_k \cos^2 2\delta_k]
\end{aligned} \tag{49}$$

and

$$\begin{aligned}
&\int d^3z \langle \varphi(\mathbf{x})\pi(\mathbf{z}) \rangle \langle \pi(\mathbf{z})\varphi(\mathbf{y}) \rangle \\
&\quad = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \frac{1}{4} [(2\sinh^2 r_k + 1)^2 \\
&\qquad - \sinh^2 2r_k \cos^2 2\delta_k] .
\end{aligned} \tag{50}$$

Taking into account (45) we can substitute (49) and (50) into (38) to determine the entropy of the field in the classical limit. The two terms (49) and (50) evidently cancel each other, giving vanishing entropy. But this is no surprise since we started in a pure state whose entropy must vanish and since the evolution of the system is unitary, thus preserving the entropy. The information about the final state is complete.

To associate entropy with the final state we must coarse grain the system, i.e., neglect some information. Typically, this will be information which is very sensitive to any kind of perturbation, either of the system or of the state. In our example, the phases δ_k will depend sensitively on a perturbation, whereas the amplitudes will not. (In the language of Sec. III, the amplitude is the principal quantum number and the phases are averaged over.) The coarse graining leads to decoherence, which is a necessary condition for the quantum to classical transition. Note that the decohering process picks out the preferred basis of coherent states in which large occupation numbers are the sign of classicality.

The nature of the decohering process (or in other words of perturbation mentioned above) is a subject of independent analysis. There are several mechanisms; which one is realized will depend on the particular system under investigation. Interactions with other fields (which can be viewed as an environment) will induce stochasticity of the phases. Weak self interactions of the scalar field may also induce large changes in phases. Approximating the state of the system (e.g., neglecting decaying modes in examples in which the mass is constant at early and late times but changes in between) will have the same effect.

Returning to our example, let us define the coarse grained entropy by at first averaging the two point correlation functions (47) over the phases δ_k and substituting the thus obtained "reduced" correlation functions into (38) to find the reduced operator $\mathcal{D}_{\text{red}}$ which will be

$$\mathcal{D}(\mathbf{x}-\mathbf{y}) = \int \frac{d^3k}{(2\pi)^3} \sinh^2 r_k (1 + \sinh^2 r_k) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} . \tag{51}$$

Then, according to (41), the classical field definition of entropy gives

$$s \cong \int d^3k \ln \sinh^2 r_k \tag{52}$$

in the classical limit $\sinh^2 r_k \gg 1$. Taking into account (44) we obtain

$$s \simeq \int d^3k \ln n_k \tag{53}$$

for $n_k \gg 1$, in agreement with the result for the entropy obtained in Sec. III [see (19)].

We conclude that in the cases in which both of our formulas for the entropy from Secs. III and IV are applicable, the results coincide as they should.

VI. COSMOLOGICAL PERTURBATIONS

Our goal is to apply the definition of nonequilibrium entropy developed in the previous sections to the gravitational field. Specifically, we will calculate the entropy of a stochastic background of gravitational waves and of linearized density perturbations. To set the stage, we briefly review the theory of linearized cosmological perturbations [24].

We consider linearized perturbations of metric and matter fields about a homogeneous and isotropic background cosmological model. There are three types of fluctuations, scalar, vector, and tensor perturbations, which are distinguished by their transformation properties under background space coordinate changes. Vector modes decay and are irrelevant for cosmology. Hence, we shall focus on scalar modes (density perturbations) which couple to density, pressure, and tensor modes (gravitational waves).

Although it may at a first glance seem that both density perturbations and gravitational waves are described by several independent fields, the analysis can in both cases be reduced to the theory of a single scalar field [15,16]; and hence the formalism developed in previous sections to determine the entropy of a nonequilibrium dynamical system becomes applicable.

A. Gravitational waves

Gravitational waves are linearized purely gravitational fluctuations about a homogeneous and isotropic background metric $g^{(0)}_{\mu\nu}$. For simplicity we will consider a spatially flat universe given by the invariant line element

$$ds^2=a^2(\eta)(d\eta^2-\delta_{ij}dx^i dx^j) , \tag{54}$$

η being conformal time and $a(\eta)$ denoting the scale factor. The metric perturbation $\delta g_{\mu\nu}=a^2 h_{\mu\nu}$ for gravitational waves is transverse and traceless and satisfies $h_{00}=h_{0i}=0$.

The action $S_{\rm gr}$ for gravitational waves can be obtained by expanding the Einstein action

$$S=-\frac{1}{6l^2}\int R\sqrt{-g}\, d^4x \ , \quad l^2=\frac{8\pi G}{3} \tag{55}$$

to second order in the perturbation variables, with the result

$$S_{\rm gr}=\frac{1}{24l^2}\int d^4x\, a^2(h_k^{i\prime}h_i^{k\prime}-h^i_{k,e}h^k_{i,e}) , \tag{56}$$

where the derivative with respect to η is denoted by a prime. Varying this action yields the following equation of motion for h^i_j:

$$h_j^{i\prime\prime}+2\frac{a'}{a}h_j^{i\prime}-\Delta h^i_j=0 . \tag{57}$$

In order to reduce the study of gravitational waves to the analysis of a single scalar field, we expand h^i_j in a Fourier series [15]:

$$h^i_j(\mathbf{x},\eta)=\int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}}G^i_j(\mathbf{k})a^{-1}u_k(\eta) , \tag{58}$$

where $G^i_j(\mathbf{k})$ is the polarization tensor of a gravitational wave with wave vector $\mathbf{k}$. The mode functions $u_k(\eta)$ can be used to define a scalar field φ,

$$\varphi(\mathbf{x},\eta)=\left[\frac{1}{12l^2}\right]^{1/2}\int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{k}\cdot\mathbf{x}}[G^i_j(\mathbf{k})G^j_i(\mathbf{k})]^{1/2}u_k(\eta) , \tag{59}$$

in terms of which the action (56) becomes

$$S_{\rm gr}=\frac{1}{2}\int d^4x\left[\varphi'^2-\varphi_{,i}\varphi_{,i}+\frac{a''}{a}\varphi^2\right] . \tag{60}$$

This action coincides with the action of a free scalar field with time-dependent mass $m\,(m^2=-a''/a)$ in flat spacetime.

Based on the above equivalence between the gravitational radiation field and the scalar field $\varphi(\mathbf{x},\eta)$, we can use the general definitions of entropy developed in Secs. III and IV to define the entropy in gravitational radiation. This will be done in Sec. VII.

B. Density perturbations

The theory of linearized density perturbations can also be reduced to the analysis of a single scalar field [25]. However, the reduction process is more complicated than in the case of gravitational waves.

Density perturbations are scalar-type metric fluctuations which couple to energy density and pressure. At first sight, the most general scalar type metric perturbation $\delta g_{\mu\nu}(\mathbf{x},\eta)$ can be expressed in terms of four free functions. However, two of these functions describe pure gauge modes [26], i.e., inhomogeneities which correspond to a change of the background space-time coordinates. The easiest and most physical way to avoid gauge artifacts is to adopt a manifestly gauge invariant formalism [26] (for a pedagogical introduction see Ref. [16], for a comprehensive review see Ref. [15]). In this approach, scalar-type metric perturbations are characterized by two functions which are, via the linearized Einstein equations, coupled to matter inhomogeneities. The two gauge-invariant functions $\Phi(\mathbf{x},\eta)$ and $\Psi(\mathbf{x},\eta)$ can easily be identified by transforming to longitudinal gauge (the system of coordinates in which $\delta g_{\mu\nu}$ is diagonal):

$$\delta g_{\mu\nu}=a^2\begin{bmatrix}2\Phi & 0\\ 0 & 2\Psi\delta_{ij}\end{bmatrix} . \tag{61}$$

For scalar matter and for an ideal gas, $\Phi=\Psi$ as a consequence of the $i\neq j$ Einstein equation (for these forms of matter $\delta T_{ij}\sim\delta_{ij}$).

At this point, the description of density perturbations has been reduced to prescribing a gauge-invariant combination v of matter perturbation and metric fluctuations in terms of which the action for perturbations can be expressed in the form [27]

$$S_v=\frac{1}{2}\int d^4x\left[v'^2-c_s^2 v_{,i}v_{,j}\delta^{ij}+\frac{z''}{z}v^2\right] , \tag{62}$$

where $c_s^2=1$ for scalar field matter and $c_s^2=p/\rho$ for ideal gas matter. The variable $z(\eta)$ is a combination of background-dependent factors. For a perfect fluid and for a scalar field as matter,

$$z=a\beta^{1/2}/\mathcal{H}c_s \ , \quad \beta=\mathcal{H}^2-\mathcal{H}' , \tag{63}$$

where $\mathcal{H}=a'/a$.

All gauge-invariant variables (such as Φ) can be expressed in terms of the variable v via the Einstein equations. For example, the metric potential Φ which characterizes the amplitude of metric perturbations in longitudinal gauge [see (61)] is expressed in terms of v in the following manner:

$$\Delta\Phi=-\left[\frac{3}{2}\right]^{1/2} l\frac{\beta}{\mathcal{H}c_s^2}\left[\frac{v}{z}\right]' \tag{64}$$

(valid for both scalar field and hydrodynamical matter).

In conclusion, we have been able to reduce the action for scalar metric perturbations to that of a free scalar field with mass $m^2=-z''/z$. However, in contrast with the case of gravitational perturbations, the spatial gradient term has a prefactor c_s^2. In the radiation-dominated period of the evolution of the Universe this term implies that density perturbations propagate with the speed of sound $c_s=1/\sqrt{3}$. In the matter-dominated period, $c_s=0$. This has important consequences for our ability to define the notion of "particle number" of a given field configuration for different equations state.

VII. ENTROPY OF COSMOLOGICAL PERTURBATIONS

In the previous section we demonstrated that the action for both gravitational waves and for density perturbations can be reduced to the action of a free scalar field. Hence the formalism of Secs. III and IV can be used to define the nonequilibrium entropy of the gravitational field.

In order to use the quantum definition of entropy of Sec. III we need a well-defined notion of particles. For gravitational waves described by the action (60) and in the special case when $a''=0$ (which is realized in the radiation dominated period when $a(\eta)\sim\eta$) the mass term in (60) vanishes, and hence the notion of particles is well defined and the particle number remains constant. In contrast, during an inflationary period $a(\eta)=-1/(H\eta)$, and this leads to a negative time-dependent effective square mass $m^2=-a''/a$ in (60) which is

$$m^2=-2/\eta^2 \ . \tag{65}$$

Because of this time dependent mass, there will be in this case particle production and corresponding increase in entropy. Focusing on modes with comoving wave number k, the time dependent mass induces an effective potential

$$V_{\mathrm{eff},k}(\varphi)=\frac{1}{2}\left[k^2-\frac{2}{\eta^2}\right]\varphi^2 \ . \tag{66}$$

Hence, the increase in particle number is significant on scales which satisfy

$$k<-\sqrt{2}/\eta=\sqrt{2}Ha \ , \tag{67}$$

which (up to a factor of $\sqrt{2}$) is exactly the condition for the wavelength $k^{-1}a$ to be larger than the Hubble radius H^{-1}. Similarly, in the matter dominated period when $a(\eta)\sim\eta^2$ there is a nonvanishing effective potential. In terms of η the potential takes precisely the form (65). Hence, (66) and (67) also apply in this case.

In the following, we shall evaluate the entropy for the spectrum of gravitational waves produced in an inflationary universe. From the previous discussion, we see that the magnitude of the entropy is generated by "parametric amplification" [28] of the number of gravitons in each mode which occurs during inflation on scales larger than the Hubble radius. On scales which enter the Hubble radius after t_{eq}, the time of equal matter and radiation, an additional amplification takes place during the matter dominated epoch. However, we emphasize that although the magnitude of the "potential" entropy is set by the inflationary phase, in order to get any nonvanishing entropy there needs to be a loss of correlations due to some coarse graining (see Sec. V).

The precise nature of the decohering process for gravitational waves and density perturbations is a separate topic of investigation. For some ideas on how decoherence arises we refer the reader to Ref. [29]. However, decoherence may not be complete. In particular, in Ref. [30] it is pointed out that phase correlations between $\mathbf{k}$ and $-\mathbf{k}$ modes are preserved for wavelengths which are comparable to the Hubble radius. As long as modes with different $|\mathbf{k}|$ decohere, the computations described below are unchanged.

The situation for density perturbations is similar. During the period of radiation domination, it follows from (63) that $z''=0$. Hence, as in the case of gravitational waves, the notion of particles is well defined, the particle number is time independent, and hence the entropy per mode remains constant. During inflation, it follows from (63) that $z''/z\simeq a''/a=2/\eta^2$, and that, therefore, as for gravitational waves, particle creation for modes with wavelengths larger than the sound horizon H^{-1} occurs, which leads to an increase in the occupation number of each mode. The analysis of density perturbations is more complex in the matter-dominated period since $c_s^2=0$. Hence no occupation number can be defined. In this case we must use the classical framework of Sec. IV in order to define the entropy.

In the following, we will first calculate the entropy per mode of gravitational waves and density perturbations which were produced during inflation in a cosmological model in which the Universe is radiation dominated at late times and argue that the result for the more realistic case is the same.

A. Gravitational radiation

To estimate the entropy of gravitational radiation produced during inflation, it is convenient to express the expectation value $\langle n_{\mathbf{k}}\rangle$ of the number operator in each mode $\mathbf{k}$ (or, correspondingly, the squeeze parameter r_k) in terms of the spectral density of the two-point correlation function of the metric h^i_j. Since this spectrum $|\delta^h(k)|$ was calculated in the particular models of interest to us in Ref. [31], we can then use these results to estimate the entropy via formulas (52) or (53) (the result will be the same since on the scales of interest $n_k\gg 1$).

We can only justify the appearance of entropy for perturbations on scales smaller than the Hubble radius, since the mode functions do not oscillate on larger scales. Hence, when calculating the entropy in gravitational radiation at some late time, we will only consider scales smaller than the Hubble radius at that time.

Combining (58) and (59) with the standard mode expansion of the quantum operator $\hat{\varphi}$ associated with φ, we obtain the following result for the operator $\hat{h}^i_j$:

$$\hat{h}^i_j(\mathbf{x},\eta)=(6l^2)^{1/2}a^{-1}\int \frac{d^3k}{(2\pi)^{3/2}}k^{-1/2}\frac{G^i_j(\mathbf{k})}{[G^m_n(\mathbf{k})G^n_m(\mathbf{k})]^{1/2}}[e^{-i\mathbf{k}\cdot\mathbf{x}}u^{\rm out}_{\mathbf{k}}(\eta)^* c^-_{\mathbf{k}}+e^{i\mathbf{k}\cdot\mathbf{x}}u^{\rm out}_{\mathbf{k}}(\eta)c^+_{\mathbf{k}}]\ , \qquad (68)$$

where $c^+_{\mathbf{k}}$ and $c^-_{\mathbf{k}}$ are creation and annihilation operators, respectively, of particles with comoving wave vector $\mathbf{k}$ at some late time and $u^{\rm out}_{\mathbf{k}}(\eta)\simeq e^{ik\eta}$ for perturbations on scales smaller than the Hubble radius ($k\eta\gg 1$).

The spectrum $\delta_h(\mathbf{k})$ of gravitational radiation is defined in terms of the two-point function of $\hat{h}^i_j$ by

$$\langle 0_{\rm in}|\hat{h}^i_j(\mathbf{x},\eta)\hat{h}^j_i(\mathbf{x}+\mathbf{r},\eta)|0_{\rm in}\rangle=\int_0^\infty \frac{dk}{k}\frac{\sin(kr)}{kr}|\delta_h(k)|^2 \qquad (69)$$

with $r=(\mathbf{r})$ and $k=|\mathbf{k}|$ and where $|0_{\rm in}\rangle$ is the initial vacuum state defined by $a^-_{\mathbf{k}}|0_{\rm in}\rangle=0$. On the other hand, this two-point function can be evaluated in terms of occupation numbers using (68):

$$\langle 0|\hat{h}^i_j(\mathbf{x},\eta)\hat{h}^j_i(\mathbf{x}+\mathbf{r},\eta)|0\rangle =\frac{6l^2}{2\pi}a^{-2}\int_0^\infty\frac{dk}{k}\frac{\sin kr}{kr}k^2(2\langle n_k\rangle+1)\ , \qquad (70)$$

where we took into account that $\langle 0_{\rm in}|\hat{c}^+_k\hat{c}^-_k|0_{\rm in}\rangle=\langle n_k\rangle$. Comparing (69) and (70) yields

$$2\langle n_k\rangle+1=\frac{2\pi}{6l^2}\frac{|\delta_h(k)|^2}{(k/a)^2}\ . \qquad (71)$$

Equation (71) can be applied to calculate the entropy of gravitational radiation in any cosmological model. Given the spectrum $\delta_h(k)$, the occupation numbers $\langle n_k\rangle$ are determined for each mode by (71), and the entropy per mode follows from (53).

To be specific, we evaluate the entropy in an inflationary universe. The spectrum of gravitational radiation originating in quantum fluctuations during the phase of exponential expansion has been calculated many times [31] (for an explicit derivation using the notation of this paper see Ref. [15]). The result is

$$\delta_h(k)=\frac{lH}{\sqrt{2}\pi}\begin{cases}(t_0k)^{-2}\ , & t_0^{-1}<k<t_0^{-1}z_{\rm eq}^{1/2}\ ,\\ (t_0k)^{-1}z_{\rm eq}^{-1/2}\ , & z_{\rm eq}^{1/2}t_0^{-1}<k<t_0^{-1}z_{\rm eq}^{-1/4}(t_0/t_R)^{-1/2}\ ,\end{cases} \qquad (72)$$

where t_0 is the present time and t_R corresponds to the end of inflation. $z_{\rm eq}$ is the redshift at the time of equal matter and radiation. The top line corresponds to scales which enter the Hubble radius after $t_{\rm eq}$, the bottom to those which enter during the period of radiation domination. Hence, from Eq. (71)

$$2\langle n_k\rangle+1=\frac{H^2}{6\pi k^2}\begin{cases}(t_0k)^{-4}\ , & t_0^{-1}<k<t_0^{-1}z_{\rm eq}^{1/2}\\ (t_0k)^{-2}z_{\rm eq}^{-1}\ , & z_{\rm eq}^{1/2}t_0^{-1}<k<t_0^{-1}z_{\rm eq}^{-1/4}(t_0/t_R)^{1/2}\ ,\end{cases} \qquad (73)$$

H being the Hubble expansion rate during the period of inflation.

Choosing $H=10^{13}$ GeV, a value for which fluctuations from inflation have the right order of magnitude to seed galaxies [32], and comparing the entropy s_k per mode on galactic scales $k^{-1}\sim 10$ Mpc, we conclude from (73) that

$$s_k\sim 100\ln 10\ . \qquad (74)$$

Formula (74) can also be interpreted as giving the entropy in a volume $V=k^{-3}$ of gravitational waves with wave number of the order k. This quantity can be compared with the statistical fluctuations of the entropy of the cosmic microwave background (CMB). These fluctuations $\Delta s_{\rm CMB}(k)$ scale as

$$\Delta s_{\rm CMB}(k)\sim(k\lambda_\gamma)^{3/2}\ , \qquad (75)$$

where λ_γ is the characteristic wavelength of the CMB. Hence, for large k^{-1} (such as the scales mentioned above), the entropy in gravitational waves exceeds that in the statistical fluctuations of the CMB. This reflects the result that on cosmological distance scales the fluctuations produced by inflation are much larger than the Poisson noise in the background fields.

However, the total entropy density for the gravitational background is smaller than that of the CMB for which

$$S_{\rm CMB}\simeq(4\pi/3)T_0^3\ . \qquad (76)$$

From (53) it follows that the entropy density in gravitational radiation is

$$S_{\rm gr}\simeq(4\pi/3)k_c^3\ , \qquad (77)$$

where k_c is determined by

$$n(k_c)\simeq 1\ . \qquad (78)$$

From (73) it follows that

$$k_c\sim t_0^{-1}z_{\rm eq}^{-1/4}(t_0/t_R)^{1/2} \qquad (79)$$

and hence

$$S_{\rm GW}\sim(H/m_{\rm Pl})^{3/2}T_0^3\ . \qquad (80)$$

Comparing (77) and (80) we see that the total entropy density in gravitational waves is suppressed compared to the entropy of the CMB by a factor $(H/m_{\rm Pl})^{3/2}$. Nevertheless, as seen above, on large length scales, gravitational radiation dominates over the fluctuations of the entropy of the CMB.

B. Density perturbations

The approach for calculating the entropy of density perturbations follows what was done above for gravitational waves. The starting point is the expansion of the operator $\hat{\varphi}$ associated with the scalar field v of (62) (which contains all the information about density perturbations) in terms of late time creation and annihilation operators c_k^+ and c_k^-, respectively:

$$\hat{\varphi}(\mathbf{x},\eta)=\frac{1}{\sqrt{2}}\int\frac{d^3k}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{x}}v_k^{\rm out}(\eta)c_k^- +e^{-\mathbf{k}\cdot\mathbf{x}}v_k^{\rm out}(\eta)c_k^+] . \quad (81)$$

To simplify the consideration and to justify the notion of entropy, we will estimate the entropy on scales smaller than the Hubble radius at late times, assuming that in this late time interval the Universe is radiation dominated. In this case, the notion of particles is unambiguous since the mode functions $v_k(\eta)$ take the form

$$v_k(\eta)=(1/\sqrt{\omega})e^{i\omega\eta} \quad (82)$$

with $\omega=c_s k=k/\sqrt{3}$.

Using the relation (64) between the gauge-invariant relativistic potential Φ and the scalar field v valid when $c_s^2\neq 0$ we obtain [15]

$$\hat{\Phi}(\mathbf{x},\eta)=\left[\frac{3}{4}\right]^{1/2} l\frac{\beta^{1/2}}{a}\times\int\frac{d^3k}{(2\pi)^{3/2}}[e^{i\mathbf{k}\cdot\mathbf{x}}u_k^*(\eta)c_k^- +e^{-i\mathbf{k}\cdot\mathbf{x}}u_k(\eta)c_k^+] \quad (83)$$

with

$$u_k=\frac{z}{k^2c_s}\left[\frac{v_k}{z}\right]' . \quad (84)$$

As was done previously in the case of gravitational waves, the next step is to derive the relation between the spectrum $\delta_\Phi(k)$ of density perturbations

$$\langle 0_{\rm in}|\hat{\Phi}(0,\eta)\hat{\Phi}(\mathbf{r},\eta)|0_{\rm in}\rangle=\int_0^\infty\frac{dk}{k}\frac{\sin kr}{kr}|\delta_\Phi(k)|^2 \quad (85)$$

and the occupation number $\langle n_k\rangle$ defined with respect to the creation and annihilation operators introduced in (81). Using (83) it follows that

$$\langle 0_{\rm in}|\hat{\Phi}(0,\eta)\hat{\Phi}(\mathbf{r},\eta)|0_{\rm in}\rangle =\frac{3}{4}l^2\frac{\beta}{a^2}\int\frac{d^3k}{(2\pi)^3}(2\langle n_k\rangle+1)u_k^*u_k e^{i\mathbf{k}\cdot\mathbf{r}} . \quad (86)$$

Making use of (82) and (84), and evaluating z during the period of radiation domination, we obtain

$$\langle 0_{\rm in}|\hat{\Phi}(0,\eta)\hat{\Phi}(\mathbf{r},\eta)|0_{\rm in}\rangle=\frac{9\sqrt{3}}{(2\pi)^2}l^2\eta^{-4}a^{-2}\int_0^\infty dk\, k^{-1}\frac{\sin kr}{kr}(2\langle n_k\rangle+1)k^{-2}\left[1+\frac{(k\eta)^2}{3}\right] . \quad (87)$$

Comparing (85) and (87) yields

$$2\langle n_k\rangle+1=\frac{(2\pi)^2}{9\sqrt{3}}(k\eta)^2(a\eta)^2 l^{-2}\left[1+\frac{(k\eta)^2}{3}\right]^{-1}\times|\delta_\Phi(k)|^2 , \quad (88)$$

which expresses the occupation numbers in terms of the spectrum of the relativistic potential for density perturbations.

The entropy for density perturbations can now be determined by combining (88) and (53). To be specific, we evaluate the entropy per mode in a model of chaotic inflation [33] with potential

$$V(\varphi)=\tfrac{1}{2}m^2\varphi^2 . \quad (89)$$

In this case, the spectrum of density perturbations immediately after inflation on scales which are larger than the Hubble radius is given by [15]

$$|\delta_k^\Phi|\simeq\frac{\sqrt{2}}{3\pi}lm\ln\left[\frac{\lambda}{\lambda_\gamma}\right] , \quad (90)$$

where λ_γ is the characteristic wavelength of the CMB. To obtain the late time spectrum, the decay of the amplitude of Φ on scales inside the Hubble radius must be taken into account. Assuming that the Universe is radiation dominated after inflation we obtain [15]

$$|\delta_k^\Phi|\simeq\frac{\sqrt{2}}{3\pi}lm\ln\left[\frac{\lambda}{\lambda_\gamma}\right]\left[\frac{\lambda}{t_0}\right]^2 \quad (91)$$

for $k\eta>1$ at time t_0.

Inserting (91) into (88) yields the following result for $k\eta\gg 1$:

$$2\langle n_k\rangle+1\sim(mt_0)^2\ln^2\left[\frac{\lambda}{\lambda_\gamma}\right]\left[\frac{\lambda}{t_0}\right]^4 . \quad (92)$$

Up to the logarithmic factor, this result agrees with the corresponding result (73) for gravitational waves.

For $m\sim 10^{13}$ GeV (the upper bound on m from constraints on the anisotropy of the CMB) we hence obtain the same entropy density per mode:

$$s_k\sim 100\ln 10 . \quad (93)$$

We conclude that the entropy per mode of density perturbations on large scales ($\lambda\gg\lambda_\gamma$), in particular, on scales of galaxies, clusters and large-scale structure, exceeds the statistical fluctuations of the entropy of the CMB. This supports the important role of the entropy of the gravitational field in the galaxy formation process.

The quantum approach of calculating the entropy of density perturbations breaks down during the matter dominated era. However, based on the considerations of Sec. V, it is easy to extend the analysis.

As discussed in Sec. IV, the classical definition (41) can easily be applied during the epoch of matter domination. The results obtained above will not change significantly. However, there are some interesting questions concerning coarse graining and time dependence of the entropy in a matter dominated universe which we shall consider elsewhere.

Formulas (71) and (88) can be used to calculate the entropy of gravitational waves and density perturbations in any cosmological model in which the spectra $\delta_h(k)$ and $\delta_\Phi(k)$ are known. In particular, the entropy of the gravitational field in topological defect models of structure formation [14] can easily be determined.

VIII. CONCLUSIONS

We have presented two general definitions of nonequilibrium entropy and applied them to calculate the entropy in gravitational perturbations and to give a measure of the entropy of linear density fluctuations and gravitational waves in a Friedmann universe.

Our first definition of entropy is based on the microcanonical ensemble and is applicable to systems with well-defined occupation numbers. The origin of the entropy is coarse graining: ignoring correlations in the form of information about quantum numbers other than the principal quantum number which is usually taken to be the energy.

The second definition of entropy applies to any stochastic classical field and expresses the entropy in terms of two-point correlation functions. The physical origin of entropy in this case is also due to coarse graining. We have shown that the entropy of scalar fields in an expanding universe satisfies the second law of thermodynamics. Any increase in entropy during Hamiltonian evolution is a consequence of coarse graining.

We have used the gauge-invariant theory of cosmological perturbations to give a consistent and unified definition of entropy of cosmological perturbations. On scales of galaxies and larger, this entropy is larger than the statistical fluctuations in the entropy of CMB photons on these scales. Hence, this entropy is important for structure formation in the Universe. However, the total entropy in density perturbations and in gravitational waves is smaller than the total entropy of the CMB.

It is our hope that the methods presented here can be used in many different situations. In particular, they might allow a definition of entropy of density perturbations beyond linear theory.

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APPENDIX: CALCULATION OF THE DETERMINANT OF $\mathcal{D}(x-y)\approx\mathcal{D}^{xy}$

The determinant of the operator $\mathcal{D}(\mathbf{x}-\mathbf{y})\approx\mathcal{D}^{xy}$ arising in (38) can be calculated using the ζ-function method [34]. More generally, consider an operator $\mathcal{D}^{xy}$ with a discrete set of positive real eigenvalues a_i and eigenfunctions

$$f^{(i)}(\mathbf{x})\approx f_x^{(i)} \; ,$$
$$\mathcal{D}^{xy}f_y^{(i)}=\int d^3y\, \mathcal{D}(\mathbf{x}-\mathbf{y})f^{(i)}(\mathbf{y})=a_i\delta^{xy}f_y^{(i)} \; . \tag{A1}$$

This set of operators includes any operator with positive spectral density:

$$\mathcal{D}(\mathbf{k})=\int d^3z\, e^{-i\mathbf{k}\cdot\mathbf{z}}\mathcal{D}(\mathbf{z}) \; , \tag{A2}$$

which has support in a finite volume V, i.e., $\mathcal{D}(\mathbf{z})=0$ if $\mathbf{z}\notin V$.

The ζ function associated with such an operator is

$$\zeta_{\mathcal{D}}(s)=\sum_i \frac{1}{a_i^s} \; , \tag{A3}$$

where the sum extends over all nonzero eigenvalues. It follows that

$$\zeta'_{\mathcal{D}}(0)=\left.\frac{d\zeta_{\mathcal{D}}(s)}{ds}\right|_{x=0}=-\sum_i \ln a_i e^{-sa_i}|_{s=0}$$
$$=-\ln\left[\prod_i a_i\right] \tag{A4}$$

and hence

$$\det\mathcal{D}=\prod_i a_i=e^{-\zeta'_{\mathcal{D}}(0)} \; . \tag{A5}$$

Thus, the calculation of the determinant of $\mathcal{D}$ has been reduced to the evaluation of $\zeta'_{\mathcal{D}}(0)$.

Let us now introduce the heat kernel $G(\mathbf{x},\mathbf{y},\tau)$ associated with $\mathcal{D}$:

$$G(\mathbf{x},\mathbf{y},\tau)=\sum_i e^{-a_i\tau}f_x^{(i)}f_y^{(i)*} \; , \tag{A6}$$

which in the case under consideration depends only on $\mathbf{x}-\mathbf{y}$ and τ and satisfies the equation

$$\int \mathcal{D}(\mathbf{x}-\mathbf{z})G(\mathbf{z}-\mathbf{y})d^3\mathbf{z}=-\frac{\partial G(\mathbf{x}-\mathbf{y},\tau)}{\partial\tau} \tag{A7}$$

with the boundary condition

$$G(\mathbf{x}-\mathbf{y},0)=\delta(\mathbf{x}-\mathbf{y}) \; , \tag{A8}$$

a consequence of the completeness of the set of eigenfunctions. It is easy to check by explicit integration that

$$\zeta_{\mathcal{D}}(s)=\frac{1}{\Gamma(s)}\int_0^\infty d\tau\,\tau^{s-1}\int d^3\mathbf{x}\,G(\mathbf{x},\mathbf{x},\tau)\ . \qquad \text{(A9)}$$

Thus, in order to compute $\det\mathcal{D}$ we need to solve Eq. (A7) for $G(\mathbf{x},\mathbf{y},\tau)$ given the boundary condition (A8). It is convenient to work in Fourier space where Eq. (A7) takes the form

$$\mathcal{D}(\mathbf{k})G(\mathbf{k},\tau)=-\frac{\partial}{\partial\tau}(G(\mathbf{k},\tau)) \qquad \text{(A10)}$$

with the boundary condition

$$G(\mathbf{k},0)=1\ , \qquad \text{(A11)}$$

where

$$G(\mathbf{k},\tau)=\int G(\mathbf{z},\tau)e^{i\mathbf{k}\cdot\mathbf{z}}d^3z\ . \qquad \text{(A12)}$$

As a result we obtain the following solution of (A7):

$$G(\mathbf{x}-\mathbf{y},\tau)=\int d^3\mathbf{k}\,e^{\mathcal{D}(\mathbf{k})\tau}e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}\ . \qquad \text{(A13)}$$

Substituting (A13) into (A9) one finds

$$\zeta_{\mathcal{D}}(s)=V\int d^3\mathbf{k}\,e^{-s\ln\mathcal{D}(\mathbf{k})} \qquad \text{(A14)}$$

and, correspondingly,

$$\det\mathcal{D}=\exp\left[V\int \ln\mathcal{D}(\mathbf{k})d^3\mathbf{k}\right]\ , \qquad \text{(A15)}$$

where V is the volume of the support of $\mathcal{D}$.

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