

**Decoherence and entropy of primordial fluctuations. I. Formalism and interpretation**

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(Received 15 May 2008; published 26 September 2008)

We propose an operational definition of the entropy of cosmological perturbations based on a truncation of the hierarchy of Green functions. The value of the entropy is unambiguous despite gauge invariance and the renormalization procedure. At the first level of truncation, the reduced density matrices are Gaussian and the entropy is the only intrinsic quantity. In this case, the quantum-to-classical transition concerns the entanglement of modes of opposite wave vectors, and the threshold of classicality is that of separability. The relations to other criteria of classicality are established. We explain why, during inflation, most of these criteria are not intrinsic. We complete our analysis by showing that all reduced density matrices can be written as statistical mixtures of minimal states, the squeezed properties of which are less constrained as the entropy increases. Pointer states therefore appear not to be relevant to the discussion. The entropy is calculated for various models in Paper II.

DOI: [10.1103/PhysRevD.78.065044](https://doi.org/10.1103/PhysRevD.78.065044)

PACS numbers: 03.70.+k, 04.62.+v

**I. INTRODUCTION**

The standard predictions of inflation are in noteworthy agreement with the recent observations [1]. Yet several aspects of inflation remain poorly understood. Among these is the so-called quantum-to-classical transition of cosmological perturbations.

In the inflationary scenario, primordial power spectra of gravitational waves and scalar perturbations result from the parametric amplification of vacuum fluctuations which begins once the modes exit the horizon. In the course of this unitary evolution, modes of opposite wave vector become more and more entangled. However, the primordial power spectra are impervious to this entanglement [2,3] because, for this expectation value, the relative contribution of the quantum correlations is inversely proportional to the amplification factor. Therefore, as far as (today) observational data are concerned, one can safely use a stochastic ensemble of growing modes in place of the pure entangled state predicted by the quantum treatment.

Yet, this distinction matters for other observables. In particular, the calculation of the entropy and that of back-reaction effects (like any kind of radiative corrections) must be addressed in the quantum settings. Although these aspects are related, in these papers we specifically consider the question of decoherence. We split the presentation into two papers, called I and II. In Paper II [4], we calculate the entropy in various models. In the present paper we focus on the formulation of the question. There is no way around this first step. Even though we have some notions of general features of decoherence, there is no universal description of it. It occurs in a variety of ways, depending

on whether the system is chaotic [5], fermionic [6], a two-level system [7], or dominated by tunneling events [8]. Decoherence must be analyzed case by case.

Let us therefore present the specific difficulties regarding cosmological perturbations. The first is of a technical nature. It is due to the fact that these perturbations are described by weakly interacting quantum fields propagating on a fixed background geometry. Renormalization is then a necessary step in the calculation of any observable (e.g. the power spectrum) beyond tree level. This technical operation is efficiently achieved at the level of Green functions. However, the customary approach to decoherence consists of defining the reduced density matrix as a solution of the so-called master equation [9]. The latter being an operator equation, it is not clear how the renormalization and ordering should be done (for non-Gaussian quantum field theories). One could proceed so that the values of a sufficient number of independent physical quantities coincide with the values calculated in a perturbative Lagrangian formalism. Assuming that this technical step could be done, the master equation would then be used to calculate other quantities, e.g. the entropy. This approach is, however, unnecessarily complicated, because all that is needed to define the reduced density matrix and to calculate the entropy are the renormalized Green functions. We therefore work from the onset with the latter.

The second difficulty concerns the physical nature of the environment. Indeed, since one is describing adiabatic perturbations, one cannot introduce “external” dynamical degrees of freedom that will act as an environment. (If one does so, and postulates that these have white noise, decoherence obtains by construction; see [10,11]. But it is based on a mechanism which might not be relevant in inflation, and it occurs at a rate which is unknown, because both the coupling strength and the statistical properties of the extra

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degrees of freedom are *ad hoc*.) In Paper II we therefore calculate the entropy in the context of physically motivated inflationary models.

Finally, let us point out that, in relation to the former difficulty, Green functions offer the possibility of defining well-defined and intrinsic coarse graining procedures, namely, by truncating at a given level, and in a self-consistent manner, the hierarchy of Green functions. In these papers, we shall study the first nontrivial level: we only retain the (dressed) two-point correlation function, and set to zero all higher order connected correlation functions. In the case of weak interactions (which is the case of gravitational interactions at energies below the Planck scale), this is a legitimate approximation. To conclude this presentation, let us note again that the master-equation approach seems inadequate in an inflationary context: it is neither clear how to properly define it without referring to renormalized quantities, nor how to actually trace over the “unobservable” degrees of freedom when reducing the density matrix.

The reduced density matrices defined by truncating the hierarchy at the first level are Gaussian and homogeneous density matrices (GHDM). These factorize in two-mode sectors characterized by opposite wave vectors ( $\mathbf{k}$ ,  $-\mathbf{k}$ ). The class of reduced density matrices being defined, we can turn to the calculation of the entropy and to the analysis of the quantum-to-classical transition. For the entropy, we argue that its value is unambiguous, despite infinities of quantum field theory and gauge invariance. We also prove that, during inflation, the entropy is the only intrinsic property of GHDM. Indeed, the values of the other quantities (e.g. the number of quanta) depend on the choice of the canonical variables which are not univocally defined because the frequency is not constant.

To address the question of the quantum-to-classical transition, we need to classify the reduced density matrices into “classical” and “quantum” states. The quantum properties of GHDM are linked to the entanglement of modes of opposite wave vectors. The quantum-to-classical transition thus occurs when this entanglement is lost (which happens when the state is neither pure nor thermalized, but at a sharp frontier in between). This gives an operational definition of classical states and of the time of decoherence for GHDM.

To apply this definition, one must first select creation and destruction operators. The latter are well defined only if the Hamiltonian is time independent. This criterion, as well as the other criteria discussed in Sec. VI, are therefore unambiguous during the radiation dominated era [3], but not during inflation. Yet, within a given representation, separability is a meaningful concept which yields to a physical picture of entanglement.

This physical interpretation is developed in Secs. VI and VII A. In particular, in Sec. VII A, we link decoherence to the possibility of writing GHDM as statistical mixtures of

minimal states (displaced squeezed states), the squeezing of which is less and less constrained as the entropy increases. In Sec. VII B, we argue that pointer states are not relevant to describe the decoherence of primordial fluctuations.

We have organized the paper as follows. Section II recapitulates the properties of the state of the linear perturbations. The coarse graining is defined in Sec. III, where the properties of the GHDM are also summarized. Classicality is then defined as separability, as explained in Sec. V. Sections III and V aim also at clarifying our previous work [3]. In Sec. IV, we identify the von Neumann entropy as the only intrinsic statistical property of these states. This establishes that it is unambiguous despite the redundancy of Einstein’s equations and the ambiguities from the perturbative renormalization of Green functions. In Sec. VI, the definition of separable states is compared to three alternative equivalent criteria of classicality, and to one nonequivalent criterion. Our concluding remarks in Sec. VII B concern the irrelevance of pointer states to the question of the quantum-to-classical transition.

## II. THE STATE OF LINEAR PERTURBATIONS

### A. Settings

In models with one inflaton field, the dynamics of linearized (scalar and tensor) perturbations is similar to the evolution of a massless scalar field  $\varphi$  in the background space-time [12]. The latter is a Friedmann-Robertson-Walker space-time with flat spatial section. The line element is

$$ds^2 = a^2(\eta)[-d\eta^2 + \delta_{ij}dx^i dx^j]. \quad (1)$$

The Hubble parameter  $H = d \ln a / dt$  is slowly evolving. This variation is governed by  $\epsilon$ , the first slow-roll parameter,  $\epsilon = -d \ln H / d \ln a$ . We consider scalar perturbations; the treatment of tensor perturbations proceeds along similar lines. In this case,  $\varphi$  designates the Mukhanov-Sasaki variable which is a linear combination of the inflaton perturbations of the gravitational potential. Its Hamiltonian is unique up to a boundary term which corresponds to a particular choice of canonical variables. We will come back to this important point in Sec. III C. If we choose the conjugate momentum of  $\varphi$  to be  $\pi = \partial_\eta \varphi$ , the Hamiltonian describing the evolution of linear perturbations is

$$H = \int d^3k H_{\mathbf{k}, -\mathbf{k}},$$

$$H_{\mathbf{k}, -\mathbf{k}} = |\pi_{\mathbf{k}}|^2 + \left(k^2 - \frac{\partial_\eta^2 z}{z}\right) |\varphi_{\mathbf{k}}|^2, \quad (2)$$

where  $\varphi_{\mathbf{k}}$  ( $= \varphi_{-\mathbf{k}}^*$ ) is the Fourier transform of the field amplitude, and  $\pi_{\mathbf{k}}$  its conjugate momentum. The time-dependent function  $z$  relates  $\varphi$  to  $\zeta$ , the scalar primordial curvature perturbation (defined on hypersurfaces orthogo-

nal to the comoving worldlines [12])

$$\varphi(t, \mathbf{x}) = z(t)\zeta(t, \mathbf{x}), \quad z(t) = \frac{a\sqrt{\epsilon}c_s}{4\pi G}. \quad (3)$$

In single field inflation, the sound velocity is  $c_s = 1$ .

We quantize each two-mode system  $(\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}})$  in the Schrödinger picture (SP) which is best adapted to describe the Gaussian states considered in the following sections. The field amplitude is decomposed at a given time  $\eta_{\text{in}}$  in terms of time-independent creation and annihilation operators

$$\begin{aligned} \varphi_{\mathbf{k}}(\eta_{\text{in}}) &= \frac{1}{\sqrt{2k}}(a_{\mathbf{k}}^{\text{in}} + a_{-\mathbf{k}}^{\text{in}\dagger}), \\ \pi_{\mathbf{k}}(\eta_{\text{in}}) &= -i\sqrt{\frac{k}{2}}(a_{\mathbf{k}}^{\text{in}} - a_{-\mathbf{k}}^{\text{in}\dagger}), \end{aligned} \quad (4a)$$

where  $a^{\text{in}}$  and  $a^{\text{in}\dagger}$  verify the commutation relations

$$[a_{\mathbf{k}}^{\text{in}}, a_{\mathbf{k}'}^{\text{in}\dagger}] = \delta^{(3)}(\mathbf{k} - \mathbf{k}'). \quad (5)$$

The free vacuum will be taken to be the Bunch-Davis (BD) vacuum, defined as the state which minimizes the Hamiltonian (2) in the asymptotic past,

$$a_{\mathbf{k}}^{\text{in}}|0 \text{ in}\rangle = 0, \quad \text{for } \eta_{\text{in}} \rightarrow -\infty. \quad (6)$$

Alternately, in the Heisenberg picture (HP), it corresponds to the state with only positive frequencies in the asymptotic past. In the decomposition of the field amplitude  $\varphi_{\mathbf{k}}(\eta) = a_{\mathbf{k}}^{\text{in}}\varphi_{\mathbf{k}}^{\text{in}}(\eta) + a_{-\mathbf{k}}^{\text{in}\dagger}\varphi_{\mathbf{k}}^{\text{in}*}(\eta)$ , the mode functions  $\varphi_{\mathbf{k}}^{\text{in}}$  verify

$$(i\partial_{\eta} - k)\varphi_{\mathbf{k}}^{\text{in}}|_{k\eta \rightarrow -\infty} = 0. \quad (7)$$

In a de Sitter background,  $a = -1/H\eta$ , they are given by

$$\varphi_{\mathbf{k}}^{\text{in}}(\eta) = \frac{1}{\sqrt{2k}}\left(1 - \frac{i}{k\eta}\right)e^{-ik\eta}. \quad (8)$$

As is well known, there are no linear scalar perturbations in a purely de Sitter background. The solution (8) merely serves the purpose of writing the modes in a closed form. In the slow-roll approximation, the scalar perturbation spectra in the long wavelength limit ( $k\eta \ll 1$ ) can be inferred from the above solutions by the substitution  $H \mapsto H_k/\sqrt{\epsilon_k}$  where the background quantities are evaluated at horizon crossing, i.e.  $k = a_k H_k$ .

The free evolution corresponding to the Hamiltonian (2) preserves the Gaussianity and the purity of the initial state (6). In addition, each two-mode sector can be analyzed independently since the state and the Hamiltonian split into a tensor product and a sum, respectively,

$$\begin{aligned} |\Psi_{\text{in}}(\eta)\rangle &= \bigotimes_{(1/2)\mathbf{k}'s} |\Psi_{\mathbf{k}, -\mathbf{k}}(\eta)\rangle, \\ |\Psi_{\mathbf{k}, -\mathbf{k}}(\eta)\rangle &= \mathcal{T} \exp\left(-\int_{-\infty}^{\eta} d\eta' H_{\mathbf{k}, -\mathbf{k}}(\eta')\right)|0 \text{ in}, (\mathbf{k}, -\mathbf{k})\rangle, \end{aligned} \quad (9)$$

where the tensor product is over half of the wave vectors since  $|\Psi_{\mathbf{k}, -\mathbf{k}}\rangle$  is a two-mode state.

## B. The covariance matrix

Because the pairs of modes are statistically independent in the state (9), we consider only one such pair and drop the index  $(\mathbf{k}, -\mathbf{k})$ . To use only one formalism throughout the paper, from now on we adopt the density matrix notation

$$\rho(\eta) = |\Psi\rangle\langle\Psi|. \quad (10)$$

Since  $\rho(\eta)$  is Gaussian, its statistical properties are summarized in the one- and two-times correlation functions. The former vanish identically by statistical homogeneity. Many of the second moments vanish as well, also because of statistical homogeneity, namely  $\text{Tr}(\rho\varphi_{\pm\mathbf{k}}^2) = \text{Tr}(\rho\pi_{\pm\mathbf{k}}^2) = \text{Tr}(\rho\varphi_{\mathbf{k}}\pi_{\mathbf{k}}) = \text{Tr}(\rho\varphi_{-\mathbf{k}}\pi_{-\mathbf{k}}) = 0$ . Finally, due to the relation  $\varphi_{\mathbf{k}}^{\dagger} = \varphi_{-\mathbf{k}}$  and similarly for  $\pi_{\mathbf{k}}$ , the remaining covariances can be conveniently condensed into a  $2 \times 2$  matrix (instead of  $4 \times 4$ ) that we shall also call the covariance matrix,

$$\begin{aligned} C &\equiv \frac{1}{2} \text{Tr}(\rho\{V, V^{\dagger}\}) = \begin{pmatrix} \mathcal{P}_{\varphi} & \mathcal{P}_{\varphi\pi} \\ \mathcal{P}_{\varphi\pi} & \mathcal{P}_{\pi} \end{pmatrix}, \\ V &= \begin{pmatrix} \sqrt{k}\varphi_{\mathbf{k}} \\ \pi_{-\mathbf{k}}/\sqrt{k} \end{pmatrix}, \end{aligned} \quad (11)$$

where the  $\mathcal{P}$ 's are functions of  $\eta$  and  $k$ . In the inflationary phase (approximated by a de Sitter evolution), they are given by

$$\mathcal{P}_{\varphi} = \frac{k}{2} \langle\{\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}}\}\rangle = k|\varphi_{\mathbf{k}}^{\text{in}}|^2 = \frac{1}{2}\left(1 + \frac{1}{x^2}\right), \quad (12a)$$

$$\mathcal{P}_{\pi} = \frac{1}{2k} \langle\{\pi_{\mathbf{k}}, \pi_{-\mathbf{k}}\}\rangle = k^{-1}|\partial_{\eta}\varphi_{\mathbf{k}}^{\text{in}}|^2 = \frac{1}{2}\left(1 - \frac{1}{x^2} + \frac{1}{x^4}\right), \quad (12b)$$

$$\mathcal{P}_{\varphi\pi} = \frac{1}{2} \langle\{\varphi_{\mathbf{k}}, \pi_{-\mathbf{k}}\}\rangle = 2 \text{Re}[\varphi_{\mathbf{k}}^{\text{in}*} \partial_{\eta}\varphi_{\mathbf{k}}^{\text{in}}] = -\frac{1}{2x^3}, \quad (12c)$$

where  $\{\cdot, \cdot\}$  is the anticommutator and we used the notation  $x = k\eta$ .

We introduce an additional representation of the state  $\rho$  which clearly displays the entanglement between modes of opposite wave vectors:

$$n \equiv \text{Tr}(\rho(\eta)a_{\mathbf{k}}^{\text{in}\dagger}a_{\mathbf{k}}^{\text{in}}), \quad (13a)$$

$$c \equiv \text{Tr}(\rho(\eta)a_{\mathbf{k}}^{\text{in}}a_{-\mathbf{k}}^{\text{in}}). \quad (13b)$$

$n$  is real while  $c$  is complex. The utility of this representation stems from the fact that  $n$  is simply related to the power spectrum while  $|c|$  measures the strength of the correlations between the two modes. These three real numbers provide an equivalent representation of the covariance matrix since inverting Eqs. (4) and inserting into (13) gives

$$\begin{aligned} n + \frac{1}{2} &= \frac{1}{2}(\mathcal{P}_\varphi + \mathcal{P}_\pi), & \text{Re}(c) &= \frac{1}{2}(\mathcal{P}_\varphi - \mathcal{P}_\pi), \\ \text{Im}(c) &= \mathcal{P}_{\varphi\pi}. \end{aligned} \quad (14)$$

As we shall see in Sec. III D, the determinant of  $C$  is related to  $S$ , the von Neumann entropy of the state. With (12), one finds that the  $x$  (time) dependence drops out and thus

$$\det(C) = \frac{1}{4} \iff |c|^2 = n(n+1) \iff S = 0. \quad (15)$$

The minimal value that  $\det(C)$  can take is  $1/4$ . When this lower bound is saturated, the state minimizes the Heisenberg uncertainty relations since  $\det(C) = \mathcal{P}_\varphi \mathcal{P}_\pi - \mathcal{P}_{\varphi\pi}^2 \geq 1/4$ .

The state of the linear perturbations is therefore characterized by a single function, the power spectrum  $\mathcal{P}_\varphi(k, \eta)$  (and an angle that plays no part in this paper). In realistic models, i.e. with interactions, the complete description of the system requires the full hierarchy of connected correlation functions. Such knowledge is out of reach, and in practice, one resorts to a coarse grained description. This gives a reduced state  $\rho_{\text{red}}$  characterized by a nonzero entropy. The choice of the correlations that are discarded must be done on physical grounds and in a way consistent with the dynamics. This is the subject of the next section.

### III. COARSE GRAINING AND REDUCED GAUSSIAN DENSITY MATRICES

In Sec. III A, we present an operational definition of reduced density matrices appropriate for interacting field theories. The advantages of this definition will be emphasized in Paper II through the analysis of explicit models. We apply it to cosmological perturbations in Sec. III C in the simplest case, the Gaussian approximation. The properties of the Gaussian states are summarized in Sec. III D.

#### A. Operational definition of coarse graining

The program begins with the specification of a finite set of ‘‘relevant’’ observables  $\{\hat{\mathcal{O}}_1, \dots, \hat{\mathcal{O}}_n\}$  (which can be functions of both time and space or momentum). This set defines our knowledge about the state and the dynamics (see Appendix A where this important aspect is emphasized) of the system. In general, the finite set  $\{\hat{\mathcal{O}}_1, \dots, \hat{\mathcal{O}}_n\}$  allows only for a partial reconstruction of this state. The reconstruction is performed in the following way. The *reduced* density matrix  $\rho_{\text{red}}(\bar{\mathcal{O}}_1, \dots, \bar{\mathcal{O}}_n)$  is defined by the constraints on the expectation values  $\bar{\mathcal{O}}_j$  of these observables,

$$\text{Tr}(\rho_{\text{red}}) = 1, \quad \text{Tr}[\rho_{\text{red}}(\bar{\mathcal{O}}_1, \dots, \bar{\mathcal{O}}_n)\hat{\mathcal{O}}_j] \equiv \bar{\mathcal{O}}_j. \quad (16)$$

There is of course an infinite number of density matrices verifying these constraints. However, to be consistent with our hypothesis that the  $\hat{\mathcal{O}}_j$  are the only observables accessible to us, we must choose the density matrix  $\rho_{\text{red}}$  which

maximizes the entropy given the constraints (16):

$$S[\rho_{\text{red}}] \geq S[\rho], \quad (17)$$

where

$$S[\rho] = -\text{Tr}(\rho \ln \rho). \quad (18)$$

The formal solution of this variational problem is [13]

$$\begin{aligned} \rho_{\text{red}} &= \frac{1}{Z_{\mathcal{O}}} \exp\left(-\sum_{j=1}^n \lambda_j \hat{\mathcal{O}}_j\right), \\ Z_{\mathcal{O}} &= \text{Tr}\left[\exp\left(-\sum_{j=1}^n \lambda_j \hat{\mathcal{O}}_j\right)\right]. \end{aligned} \quad (19)$$

[If these observables depend on space-time, one should read  $\int d^3x \lambda(t, \mathbf{x}) \hat{\mathcal{O}}_j(t, \mathbf{x})$ .] This is an out-of-equilibrium generalization of Gibbs canonical and grand canonical states which reduce to these distributions in equilibrium.

The  $\lambda_n$  are Lagrange multipliers. The constraints on the expectation values (16) are therefore written as

$$\bar{\mathcal{O}}_j = -\frac{\partial}{\partial \lambda_j} \ln Z_{\mathcal{O}}. \quad (20)$$

One then inverts this system of  $n$  equations to express the Lagrange multipliers in terms of the expectation values

$$\lambda_j = \lambda_j(\bar{\mathcal{O}}_1, \dots, \bar{\mathcal{O}}_n) \quad (21)$$

and substitutes in (19). The von Neumann entropy of the solution  $\rho_{\text{red}}$  is the Legendre transform of the logarithm of the partition function  $Z_{\mathcal{O}}$ ,

$$S[\rho_{\text{red}}] = \ln Z_{\mathcal{O}} + \sum_{j=1}^n \lambda_j \bar{\mathcal{O}}_j = S(\bar{\mathcal{O}}_1, \dots, \bar{\mathcal{O}}_n). \quad (22)$$

For quantum fields, one notices the close resemblance between  $\ln Z_{\mathcal{O}}$  and the generating functional of Green functions, and between  $S$  and the effective action.

Notice that the solution (19) is formal. Ambiguities stem from the noncommutativity of the operators  $\hat{\mathcal{O}}_j$ . As a result, (22) is strictly valid only when all the  $\hat{\mathcal{O}}_j$  commute [see also Eq. (A3) and the following comment]. In the following we will only consider Gaussian density matrices. The theory of their representation is well developed, and we shall rely on this body of work. In particular, the ordering ambiguities in (19) and (22) can be resolved. The correct formula of the entropy is given by Eqs. (26) and (27).

#### B. Application to quantum fields

For quantum fields, the above program transposes into the following. We start from the observation that the knowledge of the Green functions of a (self-)interacting field is equivalent to the knowledge of the state of that field. A coarse graining is therefore naturally defined by a truncation of the BBGKY (Bogolyubov, Born, Green,



Kirkwood, and Yvon) hierarchy of Green functions at a given rank  $N$ . As explained above, to be self-consistent, the hierarchy of Green functions must be closed.

This coarse graining is the field theoretic version of Boltzmann's *Ansatz*. In the latter,  $N$ -body interactions are neglected for  $N \geq 3$  and the object of physical interest is the one-particle correlation function. Beyond the Gaussian approximation, this coarse graining is formalized in terms of the so-called  $n$ -particle irreducible representations of the effective action [14].

### C. Coarse grained description of metric perturbations

Let us apply this program to the scalar perturbation  $\varphi$ . The lowest nontrivial order of truncation is at  $N = 2$ . The reduced density matrix is then defined by the anticommutator of  $\varphi$ . The corresponding reduced density matrices  $\rho_{\text{red}}$  which maximize  $S$  are Gaussian [15]. These states will be described in detail in the next sections. Here we wish to give a qualitative understanding of this coarse graining.

Each Fourier component of the anticommutator describes the effective evolution of the two-mode sector ( $\varphi_{\mathbf{k}}, \varphi_{-\mathbf{k}}$ ) and can be analyzed separately, as it was the case in the linearized treatment. The growth of entropy associated with the coarse graining in the present case can therefore be described by the set of Gaussian two-mode density matrices  $\rho_{\mathbf{k}, -\mathbf{k}}^{\text{red}}$ . Each of them characterizes the loss of entanglement between the two modes in the presence of interactions, which are self-interactions of gravity or (and) interactions of the metric perturbations with other fields (e.g. the fields of the standard model of particle physics or isocurvature perturbations in multi-inflaton field scenarios). The environmental degrees of freedom are thus either the collection of the modes  $\varphi_{\mathbf{k}' \neq \mathbf{k}}$ , or modes of other fields.

Returning to the formalism, for each two-mode,  $\rho_{\mathbf{k}, -\mathbf{k}}^{\text{red}}$  is defined by the anticommutator

$$G_a(\eta, \eta'; k) = \frac{1}{2} \int d^3x e^{i\mathbf{k}\cdot\mathbf{x}} \text{Tr}[\rho_{\text{tot}}(\eta_{\text{in}}) \times \{\varphi(\eta, \mathbf{x}), \varphi(\eta', \mathbf{0})\}], \quad (23)$$

where the in-state  $\rho_{\text{tot}}(\eta_{\text{in}})$  is the interacting vacuum of the total system. It replaces the Bunch-Davis vacuum of linearized modes.  $\varphi(\eta, \mathbf{x})$  is the Heisenberg operator of the nonlinear metric perturbations. In the SP, using (11),  $\rho_{\text{red}}(\eta)$  is the Gaussian density matrix possessing the following covariance matrix:

$$\begin{aligned} \mathcal{P}_\varphi &= G_a(\eta, \eta; k), & \mathcal{P}_{\varphi\pi} &= \partial_{\eta'} G_a(\eta, \eta'; k)|_{\eta=\eta'}, \\ \mathcal{P}_\pi &= \partial_\eta \partial_{\eta'} G_a(\eta, \eta'; k)|_{\eta=\eta'}. \end{aligned} \quad (24)$$

It will indeed be shown in [4] that in the Gaussian approximation it is always possible to make a canonical transformation  $(\varphi, \pi') \mapsto (\varphi, \pi = \partial_\eta \varphi)$ . As we recalled in Sec. IV, the entropy is invariant under canonical transformations. Throughout this paper we use this Gaussian approximation. Since the interactions do not spoil the

property of statistical homogeneity, the reduced states can be described in the same way as the pure state of the linear perturbations (Sec. II). Only the values of the covariance matrix element differ. These are now given by (24) in place of (12). We call these states GHDM.

### D. Entropy of $\rho_{\text{red}}$

To measure the strength of the correlations between  $\mathbf{k}$  and  $-\mathbf{k}$ , we introduce the parameter  $\delta$  defined by

$$|c|^2 \equiv n(n+1-\delta), \quad 0 \leq \delta \leq n+1. \quad (25)$$

The standard inflationary distribution of Sec. II is maximally coherent and corresponds to  $\delta = 0$ . The least coherent distribution corresponds to  $\delta = n+1$ . The entropy (17) is a strictly growing function of  $\delta$ . It is related to the determinant of the covariance matrix by

$$S = -\text{Tr}(\rho \ln \rho) = 2[(\bar{n}+1) \ln(\bar{n}+1) - \bar{n} \ln(\bar{n})], \quad (26)$$

where the parameter  $\bar{n}$  is defined by

$$(\bar{n} + \frac{1}{2})^2 \equiv \det(C) = \frac{1}{4} + n\delta. \quad (27)$$

The prefactor 2 in (26) accounts for the fact that  $\rho$  is the state of two modes. In the range  $\delta \gg 1/n$ ,  $n \gg 1$ , the expression (26) of the entropy simplifies,

$$\bar{n} \simeq \sqrt{n\delta}, \quad S = \ln(n\delta) + O(1). \quad (28)$$

These equations have a simple geometric interpretation that we will use in Secs. VI and VII A. The instantaneous eigenvectors of the covariance matrix are given by the rotated canonical variables

$$\begin{aligned} \Phi_{\mathbf{k}}(\eta) &= \cos\theta \sqrt{k} \varphi_{\mathbf{k}}^{\text{in}} + \sin\theta \frac{\pi_{\mathbf{k}}^{\text{in}}}{\sqrt{k}} \\ &= \frac{1}{\sqrt{2}} (\hat{a}_{\mathbf{k}}^{\text{in}} e^{-i\theta} + \hat{a}_{-\mathbf{k}}^{\text{in}\dagger} e^{+i\theta}), \\ \Pi_{\mathbf{k}}(\eta) &= -\sin\theta \sqrt{k} \varphi_{\mathbf{k}}^{\text{in}} + \cos\theta \frac{\pi_{\mathbf{k}}^{\text{in}}}{\sqrt{k}} \\ &= \frac{-i}{\sqrt{2}} (\hat{a}_{\mathbf{k}}^{\text{in}} e^{-i\theta} - \hat{a}_{-\mathbf{k}}^{\text{in}\dagger} e^{+i\theta}). \end{aligned} \quad (29)$$

The angle  $\theta = \theta(\eta) = \frac{1}{2} \arg(c(\eta))$  gives the orientation of the eigenbasis of the covariance matrix with respect to the (fixed) original variables  $\varphi_{\mathbf{k}}^{\text{in}}$  and  $\pi_{-\mathbf{k}}^{\text{in}}$ . The eigenvalues of the covariance matrix are the variances of  $\Phi$  and  $\Pi$ ,

$$\langle\langle \Phi_{\mathbf{k}}, \Phi_{\mathbf{k}}^\dagger \rangle\rangle = n + \frac{1}{2} + |c| = 2n + O(1, \delta), \quad (30a)$$

$$\langle\langle \Pi_{\mathbf{k}}, \Pi_{\mathbf{k}}^\dagger \rangle\rangle = n + \frac{1}{2} - |c| = \frac{\delta}{2} + O\left(\frac{1}{n}\right), \quad (30b)$$

and  $\langle\langle \Phi_{\mathbf{k}}, \Pi_{\mathbf{k}}^\dagger \rangle\rangle = 0$ . Hence, when  $\delta \gg 1/n$ , one has

$$\det(C) \simeq n\delta \simeq \mathcal{A} \Rightarrow S \simeq \ln \mathcal{A}, \quad (31)$$

where  $\mathcal{A}$  is the area under the  $1 - \sigma$  contour in phase space.

#### IV. THE INTRINSIC PROPERTIES OF GHDM

The von Neumann entropy  $S = -\text{Tr}(\rho \ln(\rho))$  is manifestly an intrinsic property of the state. We show that for GHDM it is the only intrinsic property. Important consequences are then derived.

##### A. Entropy as the unique intrinsic property

To illustrate the question, let us first consider the following situation. In place of the Mukhanov-Sasaki variable, one could choose instead to work directly with the curvature perturbation  $\zeta$ . The quadratic part of the Lagrangian is

$$S_\zeta = \frac{1}{8\pi G} \int dt d^3x \epsilon(t) [a^3 (\dot{\zeta})^2 - a(\nabla\zeta)^2], \quad (32)$$

where  $\dot{\zeta} = \partial_t \zeta = a^{-1} \partial_\eta \zeta$ . The conjugate momentum of the curvature perturbation is

$$\pi_\zeta(t) = \frac{a^3 \epsilon}{4\pi G} \dot{\zeta}(t). \quad (33)$$

Assuming the slow-roll condition  $\epsilon \simeq \text{cte}$  and  $\dot{\epsilon}/H\epsilon \simeq \text{cte}$ , the modes with positive frequency in the asymptotic past are

$$\zeta_k(\eta) = \zeta_k^0 (1 + ik\eta) e^{-ik\eta}, \quad |\zeta_k^0|^2 = \frac{4\pi G}{\epsilon_k} \frac{H_k^2}{2k^3}. \quad (34)$$

From this solution and (33), one obtains the following expressions for the covariance matrix at tree level:

$$\mathcal{P}_\zeta \equiv \frac{1}{2} \langle \{\zeta_{\mathbf{k}}(\tau), \zeta_{-\mathbf{k}}(\tau)\} \rangle = |\zeta_k^0|^2 (1 + x^2), \quad (35a)$$

$$\mathcal{P}_{\zeta\pi} \equiv \frac{1}{2} \langle \{\zeta_{\mathbf{k}}(\tau), \pi_{-\mathbf{k}}(\tau)\} \rangle = -\frac{a^3 \epsilon}{4\pi G} H x^2 |\zeta_k^0|^2, \quad (35b)$$

$$\mathcal{P}_\pi \equiv \frac{1}{2} \langle \{\pi_{\mathbf{k}}(\tau), \pi_{-\mathbf{k}}(\tau)\} \rangle = \left( \frac{a^3 \epsilon}{4\pi G} \right)^2 H^2 x^4 |\zeta_k^0|^2. \quad (35c)$$

Despite the differences with the variances (12), one checks that  $\det(C) = 1/4$ . The determinant of the covariance matrix, and hence the entropy, are invariant under the linear canonical transformation  $(\varphi, \pi) \mapsto (\zeta, \pi_\zeta)$ .

More generally, the entropy does not depend on the choice of canonical variables. Indeed, canonical transformations are linear symplectic transformations of the covariance matrix. The intrinsic properties of  $\rho_{\text{red}}$  are therefore the symplectic invariants [of the group  $\text{Sp}(4, \mathbf{R})$  for a system of two modes]. The symplectic invariants of  $4 \times 4$  covariance matrices are known [16]. When the constraint of statistical homogeneity is added, these invariants degenerate into a single quantity, namely, the determinant of  $C$ . In other words,  $\det(C)$  is the unique intrinsic property of the effective Gaussian state  $\rho_{\text{red}}$  of the cosmological perturbations. ‘‘Unique’’ here is employed in the sense of an equivalence class: any quantity which can be expressed in terms of  $\det(C)$  only, e.g. the entropy, characterizes the same quantity. It is interesting to notice that this uniqueness rests on statistical homogeneity.

We now apply this result to prove that the entropy is well defined despite the redundancy of Einstein’s equations and the arbitrariness in the definition of the perturbatively renormalized Green functions.

##### B. Entropy and gauge invariance

The entropy of metric perturbations is independent of the choice of gauge. The reason is that, in a change of coordinates  $x^\mu \mapsto x^\mu + \xi^\mu$ , the Lagrangian (of Einstein-Hilbert plus the inflaton) changes by a total derivative. It can therefore be seen as a canonical transformation. That the entropy is a gauge invariant quantity can also be seen independently from the fact that we quantize gauge invariant variables like the Mukhanov-Sasaki variable or the comoving curvature perturbations.

##### C. Entropy and renormalization

To show the independence of the entropy of the renormalization scheme, we proceed in three steps. We consider first renormalizable field theories in Minkowski space, then generalize to nonrenormalizable theories in Minkowski space, and finally to nonrenormalizable theories on a curved background. In what follows we are only considering the entropy per two-mode.

For renormalizable theories in Minkowski space, we have to examine two potential sources of ambiguities, the parameters of the Lagrangian and the wave function renormalization. First consider the parameters. They are local terms in the effective action, and therefore appear as local terms in the equation of the propagator. It can be checked (see Paper II) that they are not responsible for the change of entropy.

In a renormalizable theory, after renormalization of the bare parameters, the renormalized Green’s functions are numerically equal to the bare ones, up to a multiplication factor given by the wave function renormalization constant ( $s$ ) to the appropriate power. The field strength renormalization is also a canonical transformation, and therefore leaves the entropy unchanged. The quadratic part of the bare Hamiltonian is, in general,

$$H = \frac{1}{2} \int d^3x \left( Z_\pi \frac{\pi^2}{\kappa^2 \epsilon a^3} + Z_\zeta \kappa^2 \epsilon a (\nabla\zeta)^2 \right), \quad (36)$$

where  $Z_\pi$  and  $Z_\zeta$  renormalize the operators  $\langle \pi(x)\pi(y) \rangle$  and  $\langle \zeta(x)\zeta(y) \rangle$ . The commutation relation  $[\zeta(t, \mathbf{x}), \pi(t, \mathbf{y})] = i\delta^{(3)}(\mathbf{x} - \mathbf{y})$  implies

$$Z_\pi = \frac{1}{Z_\zeta}. \quad (37)$$

The renormalization of the wave function therefore leaves  $\det(C)$  unchanged since the two products  $\langle \zeta_{\mathbf{k}}(t)\zeta_{-\mathbf{k}}(t) \rangle \times \langle \pi_{\mathbf{k}}(t)\pi_{-\mathbf{k}}(t) \rangle$  and  $\langle \{\zeta_{\mathbf{k}}(t), \pi_{-\mathbf{k}}(t)\} \rangle^2$  involve the same number of  $\zeta$  and  $\pi$ .

The situation is a little different in a nonrenormalizable theory (still in Minkowski space) because the cancellation of divergences at the order  $L$  of the loop expansion requires counterterms with higher derivatives. However, at order  $L$ , these counterterms are local and therefore do not change the entropy. In other words, the nonlocal parts of the effective action [e.g. in Fourier space terms like  $\ln(-k^2/\mu^2)$  or  $\sqrt{-k^2/\mu^2}$ ] responsible for the growth of entropy are precisely those predicted by the quantum theory [17]. Irrelevant operators containing more than two derivatives require some care, since the equation of the two-point function is then higher than second order and can no longer be solved from the knowledge of the covariance matrix at an initial time. These higher derivative terms are generally discarded in a self-consistent perturbative treatment, because the extra solutions of the propagation equation are not analytic in the limit  $\hbar \rightarrow 0$  [18]. In this self-consistent perturbative sense, these counterterms do not introduce ambiguities to the definition of the entropy.

Transposition to a curved background should not alter these conclusions because the previous considerations about the canonical structure, the distinction between local and nonlocal corrections and their distinct contributions to the entropy, and the role of higher derivative operators, still hold on a curved background. However, we have not verified explicitly for the models of Paper II that the counterterms do not introduce ambiguities in a self-consistent perturbative treatment. We leave this analysis for future work.

## V. SEPARABLE DENSITY MATRICES AS CLASSICAL STATES

To interpret the value of the entropy induced by a given coarse graining, we need a classification of the corresponding reduced states. In the class of two-mode density matrices there exists an operational definition of classical states. After recalling the definition of separability, we explain why it cannot be applied unambiguously to cosmological perturbations during the inflationary era.

### A. Definition and characterization of separable states

The state (9) is entangled, i.e. it violates some Bell inequalities [19]. We recall that this entanglement refers to the correlations between the modes of opposite wave vectors. The definition of classicality called separability is a statement on the nature of these correlations. Explicitly, separable states do not violate *any* Bell inequality based on pairs of observables, each of them acting only in one sector, i.e. on  $\mathbf{k}$  or on  $-\mathbf{k}$ . These states can therefore be represented as a convex sum of tensor products of density matrices [20],

$$\rho_{\text{sep}} = \sum_l p_l \rho_{\mathbf{k}}^{(l)} \otimes \rho_{-\mathbf{k}}^{(l)}, \quad p_l \geq 0. \quad (38)$$

Unlike entangled states, these can be prepared with local classical operations (in the sense that one can prepare the states  $\rho_{\mathbf{k}}^{(l)}$  and  $\rho_{-\mathbf{k}}^{(l)}$  without making the modes  $\mathbf{k}$  and  $-\mathbf{k}$  interact), and by using a random generator (characterized by the probabilities  $p_l$ ). Although physically transparent, this definition (38) is of little practical use because of the difficulty of proving or disproving the existence of the set of  $\rho^{(l)}$  and  $p_l$ . Fortunately, for Gaussian states, a criterion of separability is known [21]. For the GHDM, it is expressed as the following inequality on the parameter  $\delta$  [3]:

$$\rho_{\text{red}} \text{ separable} \iff \delta = 1. \quad (39)$$

In brief, GHDM fall into two disjoint classes, separable states ( $\delta \geq 1$ ) which are operationally indistinguishable from stochastic ensembles, and entangled states ( $\delta < 1$ ) characterized by a departure of the anticommutator from classical correlations. This is the definition of a classical GHDM that we adopt.

Finally, at the threshold of separability, the entropy is equal to one-half of the entropy of the thermal state with the same value of  $n$  (for  $n \gg 1$ ), see Eq. (28),

$$S(n, \delta = 1) = \frac{1}{2} S_{\text{max}}(n) \simeq \ln(n). \quad (40)$$

## B. Discussion

From (14), we see that the values of  $n$  and  $c$ , and therefore that of  $\delta$  as well, depend on the choice of canonical variables. As explained in Sec. IV, only the combination

$$\det(C) = (n + \frac{1}{2})^2 - |c|^2 \quad (41)$$

does not. This poses a fundamental limitation to the applicability of the criterion of separability to systems with a time-dependent Hamiltonian, and therefore to the cosmological perturbations during inflation; see (2).

For instance, in place of the variables  $(\varphi_{\mathbf{k}}, \pi_{-\mathbf{k}} = \partial_{\eta} \varphi_{\mathbf{k}})$  and the Hamiltonian (2), one could choose to work with the variables  $\varphi_{\mathbf{k}}$  and  $\tilde{\pi}_{-\mathbf{k}} = \partial_{\eta} \varphi_{\mathbf{k}} - (z'/z)\varphi_{\mathbf{k}}$ , as done, for instance, in [2]. In this case the corresponding Hamiltonian is

$$H_{\mathbf{k}, -\mathbf{k}} = |\tilde{\pi}_{-\mathbf{k}}|^2 + k^2 |\varphi_{\mathbf{k}}|^2 + \frac{\partial_{\eta} z}{z} (\tilde{\pi}_{-\mathbf{k}} \varphi_{\mathbf{k}} + \tilde{\pi}_{\mathbf{k}} \varphi_{-\mathbf{k}}). \quad (42)$$

We leave it to the reader to verify that in the Bunch-Davis vacuum the functional dependence of the variances is different from Eq. (14) while  $\det(C) = 1/4$ . However, the canonical transformation from these two sets of variables mixes modes of opposite wave vectors; i.e. it belongs to  $\text{Sp}(4)$  but not to its subgroup  $\text{Sp}(2) \times \text{Sp}(2)$ . The property of  $(\mathbf{k}, -\mathbf{k})$  separability is therefore not stable under such canonical transformations.

As a result, the threshold of separability (40) depends, during inflation, on the choice of canonical variables. The inequality  $\delta \geq 1$  is in fact an inequality on the eigenvalues

of the so-called partial transpose of the density matrix [21]. Namely, the lowest eigenvalue should be larger than the variance in the vacuum state. Hence, for any choice of the creation and annihilation operators  $(a_{(i)}, a_{(i)}^\dagger)$ , it yields  $\delta_{(i)} \geq 1$ . Therefore a separable state in the  $i$  representation can be entangled in other representations related to it by a Bogoliubov transformation mixing the modes  $\mathbf{k}$  and  $-\mathbf{k}$ .

In this we find another illustration of the well-known fact that when the frequency varies, one loses some of the useful characterizations of quantum states. Remember that in time-dependent backgrounds there is no intrinsic definition of the occupation number, even though the expectation value of the stress tensor stays well defined. Here, even though the entropy is well defined, the criterion of classicality is not clearly defined as long as the frequency significantly varies (to be more precise, outside the validity domain of the WKB approximation.) Since there is no clear notion of particle as pair creation (or mode amplification) proceeds, there is no clear distinction between quantum and classical states, as illustrated by the criterion of separability.

On the contrary, during the radiation dominated era, this ambiguity disappears since the mode frequency of the Mukhanov-Sasaki variable is constant (because  $z = \text{cte}$ ) [12]. Then, defining classical states as the separable ones presents several advantages. First, since it relies on the possibility of violating Bell inequalities, it is an operational definition. Second, the separation between quantum and classical states is sharp. This contradicts the common belief that the quantum-to-classical transition is fuzzy. Being sharp, “the time of decoherence” is also precisely defined. Starting from an entangled state, this transition occurs at the time when  $\delta$  crosses 1.

## VI. OTHER CRITERIA OF CLASSICALITY

We show the equivalence between separability and three other classicality criteria. The latter suffer from the same ambiguities during inflation as the one of separability. They must therefore be compared to each other in the same representation, e.g. that defined in Sec. II. We conclude by discussing a class of inequivalent criteria which do not suffer from the above ambiguity but which are based on another arbitrary choice.

### A. Criteria equivalent to separability

#### 1. The broadness of the Wigner representation

A first alternative criterion was introduced in [22] for one-mode systems, generalized in [23] to two-mode systems, and applied to cosmological perturbations in [11]. It rests on the observation that, in many respects, the Wigner representation behaves like a probability density over phase space, except for the fact that it can have a finer structure than  $\hbar$  and, in particular, can take negative values in small regions.

We recall that the Wigner function can be defined by [for a system with canonical variables  $(q, p)$ ]

$$W_\rho(q, p) \equiv \int \frac{d\Delta}{2\pi} e^{ip\Delta} \rho\left(q - \frac{\Delta}{2}, q + \frac{\Delta}{2}\right). \quad (43)$$

For Gaussian states,  $W_\rho$  is Gaussian and its covariance matrix is  $C$  of Eq. (11). Although it is positive everywhere, we see from Eq. (30b) that when  $\delta < 1$ , the variance of the subfluctuant variable  $\Pi$  is smaller than the variance in the vacuum. The criterion of classicality therefore consists of asking that the Wigner representation does not contain features that are smaller than those of the Wigner function in the vacuum state (this definition includes the case of negative values). For GHDM, we therefore expect that this is the case when

$$\langle \Pi \Pi^\dagger \rangle \geq \frac{1}{2}, \quad (44)$$

i.e.  $\delta \geq 1 + O(1/n)$ , which is equivalent to the criterion (39) for large  $n$ .

This requirement is made more precise by asking that the Wigner representation of  $\rho_{\text{red}}$  is broad enough to be the Husimi (or  $Q$ ) representation of some normalizable density matrix  $\rho'$ . Indeed, the Wigner representation of a state  $\rho'$  is mapped onto its  $Q$  representation by a convolution with a Gaussian function of covariance matrix  $\frac{1}{2}$ , i.e.

$$Q_{\rho'}(q, p) = \int \frac{dq' dp'}{2\pi} e^{-(q-q')^2 - (p-p')^2} W_{\rho'}(q', p'), \quad (45)$$

which explains why the Husimi representation  $Q_{\rho'}$  of  $\rho'$  is a broader function than its Wigner representation  $W_{\rho'}$ . Moreover, the Husimi representation  $Q_{\rho'}$  of any density matrix is positive because  $Q_{\rho'}(q, p)$  is the expectation value of  $\rho'$  in the coherent state  $|(q + ip)/\sqrt{2}\rangle$ . We show in Appendix B that the GHDM  $\rho$  verifying this condition are

$$\delta \geq \delta_Q = 1 + \frac{1}{4n} = \delta_{\text{sep}} + \frac{1}{4n}, \quad (46)$$

as anticipated from the heuristic argument in the previous paragraph. It is larger than the condition of separability, but only slightly, and the two criteria are equivalent in the limit  $n \gg 1$  relevant for cosmological perturbations.

#### 2. $P$ representability

A second alternative definition of classicality is the requirement that  $\rho_{\text{red}}$  admits a  $P$  representation as defined by Glauber [3,24]. It means that the states can be written as a statistical mixture of coherent states,

$$\begin{aligned} \rho_{P\text{-repr}} \equiv & \int \frac{d^2v}{\pi} \frac{d^2w}{\pi} P(v, w) |v, \mathbf{k}\rangle \langle v, \mathbf{k}| \\ & \otimes |w, -\mathbf{k}\rangle \langle w, -\mathbf{k}|, \end{aligned} \quad (47)$$

where  $P(v, w)$  is a normalizable Gaussian distribution. A  $P$ -representable state is obviously separable. In general,



the converse is not true, but it turns out that for GHDM  $P$  representability and separability are equivalent. Hence a GHDM is  $P$  representable if, and only if,

$$\delta \geq 1 = \delta_{\text{sep}}. \quad (48)$$

To avoid any misunderstanding, we emphasize that this condition does not mean that coherent states are “the pointer states.” These have only been used as a resolution of the identity. We shall return to this point in the next section.

### 3. Decay of off-diagonal matrix elements

A third alternative condition of classical two-mode states is provided by the decay of interference terms of macroscopically distinct states, sometimes referred to as Schrödinger cat states. Since this decay is asymptotic, this criterion is less precise than the other three criteria. However, it is qualitatively equivalent to them in the following sense. We refer to Appendix D in [3] for details. The off-diagonal matrix elements of the density matrix of the pure state (6) in, say, the basis of coherent states are correlated over a range  $\propto n$ . Using the coherent states as representative of semiclassical configurations of the field at a given time, the squeezed state is a linear superposition of macroscopically distinct semiclassical configurations. As for the entropy, see (40), the correlation length between off-diagonal matrix elements is very sensitive to the value of  $\delta$  in the range  $[0,1]$  where it decreases monotonously from  $O(n)$  to  $O(1)$  as  $\delta$  increases. For  $\delta \geq 1$ , the correlation length depends very slowly on  $\delta$  and stays  $O(1)$ . Hence the decay of the correlation length also distinguishes classical Gaussian states as those with  $\delta \geq 1$ .

### 4. Adding one quantum incoherently

There is a simple physical interpretation of the criterion  $\delta \geq 1$ . Such a density matrix is obtained from the pure state by adding incoherently one *quantum* on average [24]. One obtains

$$n \mapsto n' = n + \frac{1}{2}, \quad |c\rangle \mapsto |c'\rangle = |c\rangle = \sqrt{n(n+1)}. \quad (49)$$

We have split evenly the contribution of the quantum between each mode in order to preserve statistical homogeneity. One obtains that the corresponding value of  $\delta$  defined by  $|c'|^2 = n'(n'+1-\delta)$  is

$$\delta = 1 + \frac{1}{2n} + O\left(\frac{1}{n^2}\right), \quad (50)$$

in agreement with the other criteria when  $n \gg 1$ . As an interesting side remark, remembering Eq. (40), the fact that the entropy gain associated with this addition of one quantum is large clearly establishes the fragile character of the quantum entanglement.

## B. Inequivalent criteria

Let us now discuss a criterion [11,25] which is not equivalent to the above four criteria. Instead of adding incoherently one quantum, one can consider the entropy gain associated with the loss of one *bit* of information. Then, whatever the system is, the change of entropy is  $S = \ln(2)$ . Applying this criterion to the standard inflationary distribution, the value of the parameter  $\delta$  is

$$\delta_{\text{one bit}} \simeq \frac{0.4}{n}. \quad (51)$$

The statistical properties of the corresponding density matrix are essentially the same as those of the original pure state.<sup>1</sup> For instance, Bell inequalities are still violated, and the correlation length between off-diagonal matrix elements is still  $O(n)$ .

## C. Summary

In conclusion, we have found that the various criteria of decoherence fall into two distinct classes. On the one hand, classical states with respect to the statistics of the anti-commutator  $\hat{O} = \{\varphi_{\mathbf{k}}(t), \varphi_{-\mathbf{k}}(t')\}$  are the separable states with  $\delta \geq 1$ . This criterion is ambiguous during inflation because it rests on a choice of canonical variables  $\varphi_{\mathbf{k}}, \pi_{\mathbf{k}}$ . On the other hand, a lower bound on the entropy  $S \geq \ln(N)$  is intrinsic, as only the value of the entropy is involved. However, we could not identify any operator(s) to which this criterion might refer. The value of  $N$  is therefore not dictated by any physical property of the state. (It might be provided by the resolution of observational data, but this would confirm that it does not characterize the state of the system.)

## VII. DECOHERENCE AND STATISTICAL MIXTURES

The two classes of criteria presented above seem *a priori* rather different, as the first class is based on the quantum properties of the system, whereas the second class is based on a lower bound for the entropy. In this section, we show

<sup>1</sup>It was noticed in [25] that adding one quantum yields to  $S = S_{\text{max}}/2$ , but no physical interpretation was mentioned. In this early work, the authors do not, however, refer to the criteria of Sec. VI A and prefer instead the criterion  $S = \ln(2)$ , referring to [26] for an experimental situation where decoherence is effective for such values. This reference is misleading. Indeed, the experimental observation of decoherence reported there concerns a system of a two-level atom in a cavity interacting with the electromagnetic field in a coherent state (the environment). One finds that the interferences are blurred when one photon is exchanged. Since the Hilbert space of the atom has two dimensions, the exchange of one photon between the system and the environment is equivalent to the exchange of one bit. In inflationary cosmology, since  $n \simeq 10^{100}$ , this correspondence is lost.

that these two criteria can be incorporated into a single treatment.

### A. A picture of decoherence

First we need to write two-mode density matrices as a tensor product of two one-mode density matrices. Indeed, recall that entangled states cannot be represented in the form (47). Instead, all GHDM can be decomposed as

$$\rho_{\mathbf{k}, -\mathbf{k}}(\delta) = \rho_1(\delta) \otimes \rho_2(\delta), \quad (52)$$

where 1 and 2 refer to a separation of the Hilbert space into two sectors defined by the variables

$$\varphi_{1,2} \equiv \frac{\varphi_{\mathbf{k}} \pm i\varphi_{-\mathbf{k}}}{\sqrt{2}}. \quad (53)$$

Because of homogeneity, the matrices  $\rho_1$  and  $\rho_2$  are characterized by the same covariance matrix  $C$ , which, moreover, coincides with that of  $\rho$ . Explicitly, one has

$$\begin{aligned} C_1 = C_2 &= \begin{pmatrix} \langle \varphi_1^2 \rangle & \frac{1}{2} \langle \{\varphi_1, \pi_1\} \rangle \\ \frac{1}{2} \langle \{\varphi_1, \pi_1\} \rangle & \langle \pi_1^2 \rangle \end{pmatrix} \\ &= \begin{pmatrix} \mathcal{P}_\varphi & \mathcal{P}_{\varphi\pi} \\ \mathcal{P}_{\varphi\pi} & \mathcal{P}_\pi \end{pmatrix} = C. \end{aligned} \quad (54)$$

In this way, the properties of the state of cosmological perturbations have been encoded into two fictitious one-mode systems. The entanglement ( $\delta < 1$ ) between modes of opposite wave vectors  $\mathbf{k}$  and  $-\mathbf{k}$  reflects into the existence of two subfluctuant variables  $\Pi_{1,2}$  as in Eq. (30b).

The question we address concerns the use of minimal Gaussian states  $|(v, \xi)\rangle$  of  $\varphi_{1,2}$ , i.e. squeezed coherent states, to represent the states  $\rho_{1,2}(\delta)$  as statistical mixtures in the following sense:

$$\rho_1(\delta) = \int \frac{d^2v}{\pi} P_\xi(v; \delta) |(v, \xi)\rangle \langle (v, \xi)|, \quad (55)$$

that is, by summing only over the complex displacement  $v$ . The basis of states we use therefore have a common orientation and elongation which is fixed by the squeezing parameter

$$\xi = r e^{2i\theta_c}. \quad (56)$$

Using the  $1\sigma$  contour in phase space, the state  $|(v, \xi)\rangle$  is represented by an ellipse of unit area, centered around  $(\bar{\varphi}_1 \propto \text{Re}(v), \bar{\pi}_1 \propto \text{Im}(v))$ , with a long axis (the superfluctuant direction)  $\langle \phi \phi^\dagger \rangle \propto e^{2r}$  making an angle  $\theta_c$  w.r.t. the horizontal  $\varphi_1$  axis. The latter is chosen for simplicity along the superfluctuant mode of  $\rho_1$  defined in Eq. (30a). Hence in this ‘‘frame’’  $\theta_c$  is the relative angle between the big axis of  $\rho_1$  and the big axis of  $|(v, \xi)\rangle$ ; see Eq. (C12).

As shown in Appendix C, the states  $\rho_{1,2}(\delta)$  can be represented as in (55) for any value of  $\delta$ . More interestingly, the choice of the basis vector, which is parametrized by  $\xi$ , is more limited when  $\delta < 1$ , in that the range of

allowed values of  $\theta_c$  belongs to a bounded interval which shrinks to zero as  $\delta \rightarrow 0$ . That is to say, the pure state ( $\delta = 0$ ) admits only one representation, itself. As  $\delta$  increases from zero, the allowed range of  $\theta_c$  increases but is necessarily strictly smaller than  $\pi/2$ . One can say that  $\rho_1$  ‘‘polarizes’’ the pavement (55) along its superfluctuant mode. In addition, the range of  $r$  also increases and the distribution  $P_\xi(v)$  becomes broader, which means that a growing number of families of minimal states can be used to represent  $\rho_1(\delta)$ . For any  $\delta < 1$ , one must have  $r > 0$ ; i.e. the states  $|(v, \xi)\rangle$  are necessarily squeezed (and as we saw, they tend to align with the big axis of  $\rho_1$ ). When the threshold of separability is approached, i.e.  $\delta \rightarrow 1^-$ , the lower bound of  $r$  decreases to zero. In this limit one can represent  $\rho_1(\delta \geq 1)$  with coherent states. Notice also that as  $\delta$  increases, the distribution  $\mathcal{P}_\xi(v; \delta)$  becomes broader (in  $v$ ) and, at the threshold of separability, does not have any structure finer than a unit cell of phase space. In this we recover what was observed in Sec. VIA 1.

The fact that  $\rho_1$  polarizes phase space is easy to understand *a contrario*. Indeed, consider the minimal states which are squeezed in the direction perpendicular to that of  $\rho_1$ , i.e.  $\theta_c = \pi/2$ . The corresponding spread in the subfluctuant variable  $\Pi$  of (29) is large. A statistical mixture of these states is necessarily spread out in the  $\Pi$  direction, i.e.  $\langle \Pi \Pi^\dagger \rangle > 1/2$ , that is  $\delta > 1$  [see (30)] and therefore  $S > S_{\max}/2$ .

Let us formulate these results the other way around in terms of  $\delta_\xi$  (or  $S_\xi$ ), the amount of decoherence (or entropy) needed for the state to be written in the  $\xi$  basis as in Eq. (55). According to what we just said, the further  $|(v, \xi)\rangle$  departs from  $\rho_1$ , the larger is  $\delta_\xi$  (and  $S_\xi$ ). For well-aligned  $|(v, \xi)\rangle$ , i.e. for  $\theta_c = 0$ ,  $\forall |\xi| = r \neq 0$ , we have  $\delta_\xi < \delta_{\text{sep}}$ , the minimal amount of decoherence to reach the separability threshold.

Hence, given a certain decoherence rate, these considerations translate into the time of decoherence  $t_\xi$ , i.e. the time  $t_\xi$  after which *any* initial state  $\rho_1(t_0)$  has evolved, as decoherence proceeds (as  $\delta$  increases), into the statistical mixture (55) for that value of  $\xi$ . When using again well-aligned  $|(v, \xi)\rangle$ , this defines  $t_{\text{sep}}$  as the maximal  $t_\xi$ . It is also the first time that the representation (47) is allowed.

### B. Ambiguity in choosing pointer states

Pointer states are meant to bridge the gap between the quantum and classical descriptions of a system [27,28]. The defining property of pointer states is their robustness over a given lapse of time  $t_{\text{p.s.}}$  which makes them the quantum counterparts of points in the phase space of classical mechanics. That is, once the system has been prepared into a given initial state and placed into contact with a given environment, pointer states are the states the least perturbed by the environment over  $t_{\text{p.s.}}$ . One generally obtains radically different pointer states whether  $t_{\text{p.s.}}$  is

much smaller or comparable to the dynamical time scales of the open dynamics (the proper frequency of the system or the characteristic time of dissipation).

To make the choice of  $t_{p.s.}$  less arbitrary, one often adds the requirement that any initial state of the system evolves, over a time  $t_D$ , into a density matrix which cannot be operationally distinguished from a statistical mixture of the pointer states. Since the evolution of both the pointer states and  $\rho$  are governed by the same dynamics, consistency requires that the times  $t_{p.s.}$  and  $t_D$  be commensurable.

As we saw at the end of Sec. VII A, choosing a family of pointer states [i.e. a pair  $(r, \theta_c)$ ] is arbitrary since it amounts to a choice of  $\delta_\xi$ , or to a choice of a lower bound  $S \geq \ln(N_\xi)$  which we recall is not dictated by physical considerations. The corresponding time of decoherence  $t_D = t_\xi$  is therefore arbitrary. But there is a more fundamental obstruction to the identification of a pointer basis during inflation; namely, pointer states refer to a choice of canonical variables, which is arbitrary when the Hamiltonian depends explicitly on time (compare, for instance, narrow wave packets in  $\varphi$  or  $\zeta$ ).

In brief, on the one hand, during inflation the question of finding “the” pointer states is not well defined. On the other hand, during the radiation dominated era the criterion of separability offers an unambiguous definition of classical states based on the statistical properties of the state. From these two facts we conclude that the concept of pointer states does not seem useful to analyze the decoherence of cosmological perturbations.

## VIII. SUMMARY

By truncating the hierarchy of Green functions, we first show how to get a reduced density matrix for the adiabatic perturbations, in a self-consistent manner, and from the interacting properties of the system itself, i.e. without introducing some *ad hoc* environmental degrees of freedom.

When truncating the hierarchy at the first nontrivial level, statistical homogeneity still implies that the density matrix factorizes into sectors of opposite wave vectors. Hence the reduced density matrix of each sector is determined by three moments related to the anticommutator function; see (24). This also implies that decoherence here describes the loss of the entanglement of these two modes. The level of decoherence is characterized by one real parameter in each sector, the parameter  $\delta$  introduced in (25).

We then show that the entropy  $S$  contained in each reduced two-mode density matrix is a well-defined quantity which monotonously grows with  $\delta$ . The important conclusion is that  $S$  is the only intrinsic quantity of these reduced density matrices, that is, the only quantity whose value does not depend on the choice of a pair of canonical variables.

After the entropy, we studied the quantum-to-classical transition. We show that the criterion of separability agrees with three other criteria, namely, the broadness of the Wigner function, the  $P$  representability, and the neglect of off-diagonal elements of the density matrix. During inflation, these four concepts are ill defined, because, contrary to the entropy, they require us to have selected some creation and destruction operators, which is ambiguous since the frequency significantly varies when modes are amplified.

We compare the above four criteria which give a large entropy at the threshold of classicality, see (40), to another class of criteria which give much smaller entropies, see (51), and explain why they differ so much. In the last section, we present a unified treatment of the reduced density matrices in which both types of criteria can be found. We show that each reduced density matrix can be written as statistical mixtures of minimal states which possess a well-defined range of the squeezing parameter  $\xi$  of Eq. (56). The details are given in Appendix C.

This analysis clearly shows that there is no intrinsic definition of a threshold of decoherence (or a critical entropy) at which the quantum-to-classical transition would occur during inflation. We also argue that the pointer states are of no help in providing such a definition.

In the next paper, we calculate the entropy for two dynamical models. It appears that no significant entropy is gained during single field inflation, so that the quantum-to-classical transition should occur during the adiabatic era. On the contrary, it is very efficient in multifield scenarios.

## ACKNOWLEDGMENTS

The work of D. C. is supported by the Alfried Krupp von Bohlen und Halbach Foundation.

## APPENDIX A: WHY BOTHER ABOUT THE COVARIANCE MATRIX ?

In this appendix, we emphasize the role of the dynamics and the canonical structure in defining reduced states and their associated entropy.

One may object to our analysis of the two-point function at different times on the grounds that one can only measure the values of this correlation function on our past light cone or on the last scattering surface. This objection can be answered as follows. The outcomes of a measurement are analyzed through the grid of a particular dynamical model. There are, in general, more dynamical variables necessary to write a consistent model than one can actually measure. The state of the system, either the exact state or a partial reconstruction of it, depends on both the outcome of the measurement (for instance, the values of the power spectrum and bispectrum) and the correlation functions.

As an example, we keep only the power spectrum and show that this assumption is untenable as it amounts to

ignoring the canonical structure of the theory. As a result, the von Neumann entropy of the reconstructed state is not well defined. Indeed, following the algorithm of Sec. III A, we write the *Ansatz* for the density matrix,

$$\rho_\zeta = \frac{1}{Z_\zeta} \exp\left(-\lambda \frac{k^3}{2\pi^2} \hat{\zeta}^2\right) = \int d\zeta P(\zeta) |\zeta\rangle\langle\zeta|, \quad (\text{A1})$$

$$Z_\zeta = \sqrt{\frac{\pi}{\lambda}},$$

where  $\lambda$  is a Lagrange multiplier ensuring that the power spectrum of  $\zeta$  has the measured value  $P_\zeta$ , i.e.  $\mathcal{P}_\zeta(q) = \text{Tr}(\rho_\zeta \hat{\zeta}_q \hat{\zeta}_{-q}^2) = 1/2\lambda$ . The distribution  $P(\zeta)$  is therefore

$$P(\zeta) = \frac{1}{\sqrt{2\pi\mathcal{P}_\zeta}} \exp\left(-\frac{k^3}{2\pi^2} \frac{\zeta^2}{2\mathcal{P}_\zeta}\right), \quad (\text{A2})$$

and the von Neumann entropy is then found to be

$$S = \ln Z_\zeta + \lambda \mathcal{P}_\zeta = \frac{1}{2} \ln(2\pi\mathcal{P}_\zeta) + \frac{1}{2}. \quad (\text{A3})$$

The constant  $1/2$  is universal and corresponds in this scheme to the entropy of the vacuum. For  $\mathcal{P}_\zeta \sim 10^{-10}$ , the entropy (A3) is negative. To cure these pathologies, we must add some physical input, i.e. enlarge the set of observables to include the variances  $\mathcal{P}_\pi$  and  $\mathcal{P}_{\zeta\pi}$ .

Another way to see the necessity of considering  $C$  rather than  $\mathcal{P}_\zeta$  alone is the following. Note that even though the state (A1) is Gaussian, we cannot calculate its von Neumann entropy from the formulas (11), (26), and (27). The latter are only valid for a state reconstructed from the anticommutator function. If one insists on doing so, one finds  $\mathcal{P}_\pi = \infty$  (since  $\rho_\zeta$  is diagonal in the field-amplitude basis), so that the entropy is infinite. The state  $\rho_\zeta$  must therefore be regularized first, by giving a finite width to  $\langle\pi^2\rangle$ . This operation is arbitrary without additional physical input about the dynamics.

## APPENDIX B: EQUIVALENCE OF THE CRITERIA OF SEPARABILITY AND OF BROADNESS OF THE WIGNER FUNCTION

Let us consider a Gaussian density matrix  $\rho$  of a bipartite system and let  $C$  be its covariance matrix. We adopt a different parametrization than in the text, following [21],

$$C = \text{Tr}(\rho\{A, A^\dagger\}) = \begin{pmatrix} n + \frac{1}{2} & 0 & 0 & c \\ 0 & n + \frac{1}{2} & c^* & 0 \\ 0 & c & n + \frac{1}{2} & 0 \\ c^* & 0 & 0 & n + \frac{1}{2} \end{pmatrix},$$

$$A = \begin{pmatrix} a_{\mathbf{k}} \\ a_{\mathbf{k}}^\dagger \\ a_{-\mathbf{k}} \\ a_{-\mathbf{k}}^\dagger \end{pmatrix}. \quad (\text{B1})$$

The positivity of the density matrix and the noncommutativity of the creation and annihilation operators puts a constraint on  $C$ , namely,

$$C + \frac{E}{2} \geq 0, \quad E = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (\text{B2})$$

This is the general form of the Heisenberg uncertainty relation for the second moments. Indeed, this condition puts a lower bound on the lowest eigenvalue of  $C$ , which, in the case of homogeneous states, reads  $n + 1/2 - \sqrt{|c|^2 + 1/4} \geq 0$ . The latter can be recast as the Heisenberg uncertainty relation,

$$\langle a_{\mathbf{k}} a_{\mathbf{k}}^\dagger \rangle \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \geq |\langle a_{\mathbf{k}} a_{\mathbf{k}} \rangle|^2. \quad (\text{B3})$$

A necessary and sufficient condition for the separability of a GHDM<sup>2</sup> is

$$\rho \text{ separable} \iff \Lambda C \Lambda + \frac{E}{2} \geq 0,$$

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad (\text{B4})$$

which gives  $n - |c| \geq 0$ , or  $\delta \geq 1$  using (25).

A different criterion than separability is used in [22]. With this condition, the Wigner representation of  $\rho$  must be broad enough to also be the  $Q$  representation of a density matrix  $\rho^l$ . We specialize to Gaussian states. To obtain the corresponding condition on the Wigner function, one simply notices that the convolution of the Wigner representation of a state  $\rho$  with a Gaussian of covariance matrix  $1/2$  yields the  $Q$  representation of that state,

$$W_\rho(V) = \frac{1}{\sqrt{\det C}} \exp\left(-\frac{1}{2} V^\dagger C^{-1} V\right) \mapsto$$

$$Q_\rho(V) = \frac{1}{\sqrt{\det C_Q}} \exp\left(-\frac{1}{2} V^\dagger C_Q^{-1} V\right),$$

$$\text{with } C \mapsto C_Q = C + \frac{1}{2}, \quad (\text{B5})$$

where  $V^\dagger = (\varphi, \pi^\dagger, \varphi^\dagger, \pi)$ . Hence the condition (B2) on  $C$  can be written as a similar condition for the covariances  $C_Q$  of the  $Q$  representation,

<sup>2</sup>We recall that a necessary condition for  $\rho$  to be a separable density matrix is that its partial transpose is a *bona fide* density matrix [29]. The partial transpose  $\rho_{\text{pt}}$  is, by definition, obtained from  $\rho$  by a transposition in one sector only, say  $-\mathbf{k}$ . In any basis  $|n, \mathbf{k}\rangle |m, -\mathbf{k}\rangle$ , this is written as  $\langle n, \mathbf{k} | \langle m, -\mathbf{k} | \rho_{\text{pt}} | m', -\mathbf{k}\rangle | n', \mathbf{k}\rangle = \langle n, \mathbf{k} | \langle m', -\mathbf{k} | \rho | m, -\mathbf{k}\rangle | n', \mathbf{k}\rangle$ . In Eq. (B4) this operation is implemented by the matrix  $\Lambda$ . Gaussian states are separable when this condition is satisfied [21].



$$C + \frac{1}{2}(E - 1) \geq 0. \quad (\text{B6})$$

In consequence, a necessary condition for the Wigner representation  $W_\rho$  of a state  $\rho$  to also be the  $Q$  representation  $Q_{\rho'}$  of a state  $\rho'$  is that the covariance matrix  $C$  of  $\rho$  verifies  $C + \frac{1}{2}(E - 1) \geq 0$ . For Gaussian states, this condition is also sufficient. Specializing now to the case of GHDM, we arrive at the conclusion

$$n^2 - 1/4 \geq |c|^2 \iff \delta \geq 1 + \frac{1}{4n}. \quad (\text{B7})$$

This is slightly more constraining than the separability condition  $n \geq |c|$ , but the difference between the two is not relevant when  $n \gg 1$ .

### APPENDIX C: REPRESENTATIONS OF PARTIALLY DECOHERED DISTRIBUTIONS

In this appendix we show that all partially decohered Gaussian distributions can be written as statistical mixtures of minimal states which belong to a certain family. As decoherence increases, the ranges of the parameters characterizing this family become larger. As the threshold of separability, the angle between the superfluctuant modes of the minimal states and that of the distribution becomes unrestricted.

The statistical homogeneity allows a formal reduction of the problem. One can decompose the field amplitude  $\phi_{\mathbf{q}}$  into its ‘‘real’’ and ‘‘imaginary’’ parts  $\phi_{\mathbf{q}} = (\phi_1 + i\phi_2)/\sqrt{2}$ , such that

$$a_1 = \frac{1}{\sqrt{2}}(a_{\mathbf{k}} + a_{-\mathbf{k}}), \quad a_2 = \frac{-i}{\sqrt{2}}(a_{\mathbf{k}} - a_{-\mathbf{k}}). \quad (\text{C1})$$

With this decomposition of the Hilbert space, GHD factorize

$$\rho_{\mathbf{k}, -\mathbf{k}} = \rho_1 \otimes \rho_2, \quad (\text{C2})$$

where  $\rho_1 = \rho_2$ . In addition, the parameters of (13) are given by

$$n = \text{Tr}(\rho_1 a_1^\dagger a_1), \quad c = \text{Tr}(\rho_1 a_1^2). \quad (\text{C3})$$

Similarly, for two-mode coherent states  $|v, \mathbf{k}\rangle \otimes |w, -\mathbf{k}\rangle = |v_1\rangle \otimes |v_2\rangle$  where  $v = (v_1 + iv_2)/\sqrt{2}$  and  $w = (v_1 - iv_2)/\sqrt{2}$ .

Let us consider a Gaussian density matrix  $\rho$  of a single mode, characterized by a value of  $0 \leq \delta \leq n + 1$ . We ask whether there exists a family of minimal Gaussian states  $|(v, \xi)\rangle$  and a Gaussian distribution  $P_\xi(v)$  such that

$$\hat{\rho}_\delta = \int \frac{d^2v}{\pi} P_\xi(v) |(v, \xi)\rangle \langle (v, \xi)|. \quad (\text{C4})$$

The minimal Gaussian states are chosen to be the displaced squeezed states

$$|(v, \xi)\rangle = D(v)S(\xi)|0\rangle, \quad (\text{C5})$$

where  $D(v) = e^{(va^\dagger - v^*a)}$  is the displacement operator and

$$S(\xi) = e^{(r/2)(e^{i\theta}a^{\dagger 2} - e^{-i\theta}a^2)} \quad (\text{C6})$$

the squeezing operator. The distribution  $P_\xi(v)$  is centered and is therefore defined by its covariance matrix  $C_\xi$ ,

$$P_\xi(v) = (\det C_\xi)^{-1/2} \exp\left\{-\frac{1}{2}X^\dagger C_\xi^{-1}X\right\}, \quad (\text{C7})$$

$$X = \begin{pmatrix} v \\ v^* \end{pmatrix}, \quad C_\xi = \begin{pmatrix} n_\xi & c_\xi \\ c_\xi^* & n_\xi \end{pmatrix}.$$

The moments of the state  $\rho$  defined in Eq. (13) are obtained from the ones of the distribution  $P_\xi$  by the definition (C3),

$$\begin{aligned} n &= \int \frac{d^2v}{\pi} P_\xi(v) \langle (v, \xi) | a^\dagger a | (v, \xi) \rangle \\ &= \int \frac{d^2v}{\pi} P_\xi(v) (|v|^2 + |\beta|^2), \\ c &= \int \frac{d^2v}{\pi} P_\xi(v) \langle (v, \xi) | a^2 | (v, \xi) \rangle \\ &= \int \frac{d^2v}{\pi} P_\xi(v) (v^2 + \alpha\beta). \end{aligned} \quad (\text{C8})$$

Here,  $\alpha$  and  $\beta$  are the Bogoliubov coefficients associated with the squeezed state  $|\xi\rangle$  by

$$\alpha = \text{ch}(r), \quad \beta = e^{-i2\theta_c} \text{sh}(r), \quad \xi = r e^{i\theta_c}. \quad (\text{C9})$$

Hence, the momenta of the distribution  $P_\xi$  are

$$n = n_\xi + |\beta|^2, \quad c = c_\xi + \alpha\beta. \quad (\text{C10})$$

The only constraints on  $n_\xi$  and  $c_\xi$  arise from the fact that the right-hand side of (C4) must be positive and normalizable in order to be a density matrix. These conditions are, respectively,

$$\rho \geq 0 \iff P_\xi \geq 0,$$

$$\text{Tr}(\rho) = 1 \iff \int \frac{d^2v}{\pi} P_\xi(v) = 1 \iff \det(C_\xi) \geq 0. \quad (\text{C11})$$

We write

$$\xi = r e^{i(2\theta_c + \arg(c))}, \quad (\text{C12})$$

where  $\theta_c$  is the angle made by the squeezed coherent states with the superfluctuant mode (the eigenvector of  $C$  with the largest eigenvalue). We now look for the range of values of  $x = e^{2r}$  and  $\theta_c$  allowed by the constraint on the determinant (C11), that is,

$$R(x) = Ax^2 + 2Bx + C \leq 0, \quad (\text{C13a})$$

$$A = n + \frac{1}{2} - |c| \cos(2\theta_c), \quad B = -(n\delta + \frac{1}{2}),$$

$$C = n + \frac{1}{2} + |c| \cos(2\theta_c). \quad (\text{C13b})$$

Since  $A > 0$ , the inequality (C13a) can only be satisfied if

the discriminant  $\zeta = B^2 - AC$  is positive. Since the coefficients  $A$ ,  $B$ , and  $C$  depend only on  $\theta_c$  and  $\delta$ , this gives an implicit constraint equation for  $\theta_c(\delta)$ ,

$$\zeta(\theta_c, \delta) = (n\delta)^2 - |c|^2 \sin^2(2\theta_c) \geq 0 \iff \sin^2(2\theta_c) \leq g(\delta) \equiv \frac{(n\delta)^2}{n(n+1-\delta)}. \quad (\text{C14})$$

The function  $g(\delta)$  is strictly growing over the interval  $0 \leq \delta \leq n+1$  and takes the special values  $g(0) = 0$  and  $g(1) = 1$ . We distinguish the following two cases:

- (1) If  $\delta \geq 1$  (the corresponding two-state is separable), all the values of  $\theta_c$  are allowed and the squeezed coherent states in (C4) can have an arbitrary orientation.
- (2) If  $0 \leq \delta < 1$ , the angle  $\theta$  can only vary into the interval  $[-\theta_M, +\theta_M]$  where the angular opening is defined by

$$\sin^2(2\theta_M) \equiv \frac{(n\delta)^2}{n(n+1-\delta)}. \quad (\text{C15})$$

The value  $\theta_M = \pi/2$  corresponds to  $\delta = 1$ . The interval  $[-\theta_M, +\theta_M]$  shrinks to zero as  $\delta$  decreases. In the limit  $\delta = 0$  (that is, for the pure squeezed state), the squeezed coherent states  $|(v, \xi)\rangle$  must be aligned with the superfluctuant mode of  $\rho_1$ .

We now specialize to the case  $0 \leq \delta \leq 1$  and we look for the range of allowed values of  $x$  for a given  $\delta$  and  $\theta$ . We first note that

$$1 \leq x \leq x_M \equiv 2[n + \frac{1}{2} + \sqrt{n(n+1)}]. \quad (\text{C16})$$

The lower bound comes from  $r = |\xi| \geq 0$ , and the upper bound from the requirement that the eigenvalues of  $C_\xi$  (which are expectation values) are positive, that is,  $n_\xi \geq |\beta|^2 = \text{sh}^2(r)$ . For the values of  $\theta_c$  such that the discriminant  $\zeta \geq 0$ ,  $R(x)$  of Eq. (C13a) is negative for  $x$  in the interval  $[x_-, x_+]$ , where the roots of the quadratic form are

$$x_\pm(\theta, \delta) = \frac{1}{A(\theta)} \left\{ \frac{1}{2} + n\delta \pm [(n\delta)^2 - |c|^2 \sin^2(2\theta)]^{1/2} \right\}. \quad (\text{C17})$$

For a given value of  $\delta$ , the length of the interval is a strictly decreasing function of  $\theta_c$ : the smaller the deviation between the superfluctuant directions of  $|(v, \xi)\rangle$  and  $\rho$ , the smaller the allowed range of  $x$ . Indeed, the smallest root decreases from  $x_-(0; \delta) = 2[n + 1/2 + |c|(\delta)]/(1 + 4n\delta) \geq x_M$  to  $x_-(\theta_M; \delta) = (1 + 2n\delta)/2A(\theta_M)$ , while the largest root decreases from  $x_+(0; \delta) = 4[n + 1/2 + |c|(\delta)] > x_M$  to  $x_+(\theta_M; \delta) = x_-(\theta_M; \delta) < x_M$ .

The common value of the roots at  $\theta_M$  means that, for this angle, there is a unique value of the squeezing parameter. Not surprisingly, for  $\delta = 1$ , this common value is 1, i.e.  $r = 0$ , and the fact that  $\theta$  can take any value corresponds to the isotropy of the coherent states.

To study the limit  $\delta \rightarrow 0$ , please notice that we can set  $\theta = 0$  and that  $x_+(0, \delta)$  is larger than  $x_M$  for  $\delta \ll 1$ . This means that  $x$  belongs to the interval  $[x_-(\theta), x_M]$  which shrinks to  $x_M$  since  $x_-(0; \delta)$  approaches  $x_M$  from below. In the limit of a pure state ( $\delta = 0$ ), there is a unique representation of the form (C4), the state itself [that is, the distribution of Eq. (C4) is  $P_\xi = \delta_{\text{Dirac}}^{(2)}(v_1)$ ].

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