Quantum cosmological gravitational waves?

Amaury Micheli and Patrick Peter *

Abstract General relativity and its cosmological solution predicts the existence of tensor modes of perturbations evolving on top of our Friedman-Lemaître-Robertson-Walker expanding Universe. Being gauge invariant and not necessarily coupled to other quantum sources, they can be seen as representing pure gravity. Unambiguously showing they are indeed to be quantised would thus provide an unquestionable proof of the quantum nature of gravitation. This review will present a summary of the various theoretical issues that could lead to this conclusion.

Keywords

Cosmological perturbation theory, tensor modes, gravitational waves, quantum cosmology, perturbative quantum gravity.

1 Introduction

Cosmology is a major player when it comes to quantum gravity effects. Indeed, on top of our Friedman-Lemaître-Robertson-Walker (FLRW) expanding Universe, one expects various modes of perturbations to be present, whose classical occurrence is believed to result from initial quantum vacuum fluctuations. In the usual linear
formalism [1, 2], using the FLRW underlying symmetry group (isotropy and homogeneity), they can be categorised into three components, namely scalars, vectors and tensors. At this order, upon which we focus attention below, these components decouple. In a different situation with a background endowed with other symmetries, perturbations can still be expanded in the relevant representations of the associated group; they also naturally decouple at linear order (see, e.g. Ref. [3] for Bianchi I).

Scalar modes, detected long ago in the cosmic microwave background, initiating large-scale structure formation, are distributed in a way that is compatible with quantum vacuum fluctuations in the very early times, often during a phase of inflation. This can be seen as requiring quantisation of gravity, and although many authors consider it does, others argue that gauge issues and coupling with matter render the conclusion not as clear as one would wish.

In an ever-expanding FLRW universe with dynamics driven by GR or any local theory of gravity, with no specific source in the matter fields to induce them, vector perturbations are expected to have decayed long ago so as to be mostly undetectable now [4]. One of the above hypothesis needs to be invalidated to potentially render them cosmologically relevant. Non local theories are expected to yield conclusions similar to local ones [5]. A contracting phase in the universe as implemented in bouncing models [6, 7] can lead to some increase of vector modes [8] which are however limited if produced by means of some coupling with scalar modes initially set to quantum vacuum fluctuations [9], leading to the conclusion that bouncing models are generally stable under vector perturbations. For fully quantum cosmological models however, the situation may not be as clear [10]. In any case, the question of their quantum origin would lead to similar doubts regarding the quantumness of gravity itself; they are conveniently ignored in most studies, and likewise in the present review.

Finally, one is left with the tensor modes, which are gauge invariant and with no obvious coupling to other quantum sources. General relativity (GR) applied to primordial cosmology shows their dynamics to be that of two time-dependent massive scalar fields; most models then demand they should be quantised and set in a vacuum state. The observation of their resulting properties in the absence of quantum anisotropic pressure, jointly with those of the scalar modes, could provide an unambiguous and thus indisputable hint that gravitation itself should acquire the status of a quantum theory.

2 Tensor modes in general relativistic cosmology

Before focusing on the quantum features expected from gravitational waves, let us briefly recap the underlying classical theory. The starting point of our discussion is the FLRW background universe, defined by its scale factor function $a(\eta)$ depending on the (conformal) time $\eta$ and spatial 3D metric $\gamma_{ij}$, with tensorial perturbations $h_{ij}$. In that case, ignoring both scalar and vector modes which are not the subject of this analysis, one sets the metric as
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\[
\begin{align*}
\text{d}x^2 &= g_{\mu\nu}\text{d}x^\mu\text{d}x^\nu = a^2(\eta) \left[ \text{d}\eta^2 + (\gamma_{ij} + h_{ij}) \text{d}x^i\text{d}x^j \right],
\end{align*}
\]

(1)

(we use units such that the velocity of light is \( c = 1 \) and with \( h_{ij} \) assumed transverse and traceless, i.e. \( D^i h_{ij} = 0 \) and \( h_i^i = \gamma_i^i h_{ij} = 0 \),

the 3D covariant derivative \( D^i \) being derived from the corresponding metric \( \gamma_{ij} \). Noting \( H = a'/a \) the conformal Hubble function and \( \mathcal{K} \) the spatial curvature associated with the background metric \( \gamma_{ij} \), the equation of motion for \( h_{ij} \) is found to be

\[
\begin{align*}
\ddot{h}_{ij} + 2H \dot{h}_{ij} + (2\mathcal{K} - \Delta) h_{ij} &= 8\pi G_N a^2 \pi_{ij},
\end{align*}
\]

(2)

where \( \Delta = \gamma_{ij} \partial_i \partial_j \), \( p \) is the background pressure and \( \pi_{ij} \) the anisotropic stress. For many of the known components of matter, it is vanishing (however, see e.g. [11, 12] and references therein), and we shall make the assumption that \( \pi_{ij} = 0 \) from now on.

In what follows, we set \( \mathcal{K} \to 0 \) and thus identify the background spatial metric \( \gamma_{ij} \to \delta_{ij} \) as the 3D curvature has been measured to be vanishingly small. Technically, considering a non-vanishing curvature merely amounts to changing the spectrum (and eigenfunctions) of the Laplace-Beltrami operator used below for the mode decomposition [13], so that the calculations and discussions presented below can be generalised in a straightforward way if applied to epochs in which the assumption \( \mathcal{K} = 0 \) may not be valid.

Let us thus first decompose the tensor perturbations in Fourier modes through

\[
\begin{align*}
h_{ij}(\mathbf{x}, \eta) &= \sqrt{\frac{32\pi G_N}{(2\pi)^3 a(\eta)}} \int \frac{d^3k}{a^3} w_{ij}(k, \eta) e^{ik \cdot x}.
\end{align*}
\]

(3)

with \( w^*_i(-k, \eta) = w_{ij}(k, \eta) \) to ensure \( h_{ij} \in \mathbb{R} \), so that, from Eq. (2), a given mode satisfies

\[
\begin{align*}
w_{ij}'' + \omega_k^2 w_{ij} &= 0,
\end{align*}
\]

(4)

where we defined the module \( k := \vert k \vert \geq 0 \) and the time-varying frequency

\[
\begin{align*}
\omega_k^2 &= k^2 - \frac{a''}{a}.
\end{align*}
\]

(5)

At this point, one notes that whenever the scale factor behaves as a power-law of the conformal time\(^5\) \( a(\eta) \propto \vert \eta \vert^\alpha \), then \( a''/a = \alpha(\alpha - 1)/\eta^{-2} = (\alpha - 1)\mathcal{H}^2/\alpha \). This in particular encompasses the cases of cosmological interest where a single fluid

\footnote{A prime denotes differentiation with respect to conformal time, e.g. \( a' := da/d\eta \).}

\footnote{In appropriate units for the comoving coordinates \( x^i \), it can be scaled to \( \mathcal{K} = 0, \pm 1 \). For most of the practical applications we shall deal with in this review, we shall consider the simplest, and inflation-motivated, flat case with \( \mathcal{K} = 0 \).}

\footnote{The numerical factor \( \sqrt{32\pi G_N} \) is included here for later convenience.}

\footnote{We write the absolute value of the conformal time in what follows, as it is negative in many situations, in particular during inflation.}
dominates the Friedmann dynamics, as well as the de Sitter inflationary expansion. The condition $k^2 \gg |a''/a|$ then becomes $kH^{-1} \approx k|\eta| \ll 1$, so that, in terms of the physical wavelength $\lambda \propto a/k$, one has $\lambda \ll H^{-1}$: such a mode, much smaller than the Hubble scale $H^{-1}$, is said to be sub-Hubble. Conversely, modes with $k^2 \ll |a''/a|$ are called super-Hubble.

Let us temporarily restrict attention to a sub-Hubble mode $k^2 \gg |a''/a|$. Eq. (4) then simplifies to $w'' + k^2 w = 0$, whose solution reads $w = \alpha_j \exp(\pm ik\eta)$. For a mode propagating in the $+x^3-$direction, this yields $h_{ij} = \alpha_j \exp[\pm ik(x^3 - \eta)]/a(\eta)$. The first constraint, namely $\partial^x h_{ij} = 0$, implies $k'\alpha_j = k\alpha_j = 0$, so that for $k \neq 0$, one is left with $\alpha_1$, $\alpha_2$ and $\alpha_2$ as the only non vanishing components (the symmetries of $w_{ij}$ are identical to those of $h_{ij}$). The second constraint, $h_i^i = 0$, translates into $\alpha_2 = -\alpha_1$, so the mode has only two independent degrees of freedom. The matrix $\alpha_j$ can be rewritten explicitly as

$$\alpha_j = \begin{pmatrix} \alpha_{11} & \alpha_{12} & 0 \\ \alpha_{12} & -\alpha_1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \alpha_1 + \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \alpha_2.$$

The matrices $P_j^+$ and $P_j^-$ represent the two polarisations of the gravitational wave, whose associated tensor perturbations read

$$h_{ij}(x, \eta) = h_x(t - z) P_j^+ + h_+(t - z) P_j^-,$$

with $\{t, x, y, z\} = \{a\eta, ax^1, ax^2, ax^3\}$ the physical coordinates.

Consider a test particle following the trajectory of affine parameter $\lambda$, i.e. $\lambda^\mu(\lambda)$, and initially at rest in the TT-frame where the metric has the form (1) with $h_{ij}$ given by (7), namely, assuming the scale factor $a$ to be constant during the passage of the wave,

$$\text{d}s^2 = -\text{d}t^2 + [1 + h_+(z - t)] \text{d}x^2 + [1 - h_+(z - t)] \text{d}y^2 + 2h_x(z - t)\text{d}x\text{d}y + \text{d}z^2.$$

From (8), one can evaluate the connections while the wave passes, and it turns out that $\Gamma^\eta_{\eta\eta} = 0$, so that the motion of a particle following a geodesic is unaltered as it moves with the reference frame; it appears at rest at all times. It is therefore not possible to detect a gravitational wave using a single particle.

Writing the line element as $\text{d}s^2 = -\text{d}t^2 + \text{d}l^2$, we consider two particles located on the TT-$x$ axis (i.e. $y = z = 0$) with coordinates $x$ and $x + \Delta x$. Their proper distance is obtained from (8): the relation $\text{d}l = \sqrt{\Gamma^\lambda + \lambda_\lambda} \text{d}x \simeq \left[1 + \frac{1}{2} h_+(t)\right] \text{d}x$, can be integrated to yield $\Delta l_x = \left[1 + \frac{1}{2} h_+(t)\right] \Delta x$. Similarly, considering two particles lying along the $y$ axis, one obtains $\Delta l_y = \left[1 - \frac{1}{2} h_+(t)\right] \Delta y$, so that as the separation along one direction is elongated, the other is compressed, and vice versa. A similar calculation on particles set on the $y = \pm x$ lines permits to visualize the effect of the $h_x$ polarisation. Setting our test particles along a ring in the $(x, y)$ plane, such as shown
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Fig. 1 Effect of a gravitational wave mode $P^+$ or $P^\times$ as it passes through a ring of test particles, producing '+' or '×' shapes as time goes through a full period of the wave: starting with an initially circular ring at $t = 0$, its shape is modified and shown here for different values of time, namely $T/4$, $T/2$ and $3T/4$ for a period $T = 2\pi/k$.

in Fig. 1, one gets the + and × shapes as the wave propagates in the $z$–direction, hence the names of the polarisation modes.

For a general wave vector $k = kn$ in the arbitrary direction parametrised by the angles $\varphi$ and $\theta$ (see Fig. 2), namely $n = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$, one sets

$$w_{ij}(k, \eta) = \sum_{\lambda = +, \times} P^{(\lambda)}_{ij}(n) f_{\lambda}(k, \eta), \quad (9)$$

with $P^{(\lambda)}_{ij}(n)$ the polarisation tensors and $f_{\lambda}$ the associated functions solutions of the mode equation (4). Fig. 2 shows the vectors $e_a (a = 1, 2)$ generating the plane orthogonal to the direction of propagation. Defined through

$$e_1 = -\frac{1}{\sin \theta} \frac{\partial n}{\partial \varphi} = \left( \begin{array}{c} \sin \varphi \\ -\cos \varphi \\ 0 \end{array} \right) \quad \text{and} \quad e_2 = \frac{\partial n}{\partial \theta} = \left( \begin{array}{c} \cos \theta \cos \varphi \\ \cos \theta \sin \varphi \\ -\sin \theta \end{array} \right),$$

so that $n = e_1 \times e_2$, they satisfy $e_a \cdot e_b = \delta_{ab}$ and $n \cdot e_a = 0$. Demanding $h_{ij}$ to be transverse and traceless translates into

$$k^i P^{(\lambda)}_{ij} = 0, \quad \text{and} \quad P^{(\lambda)}_{ij} \delta^{ij} = 0, \quad (10)$$

and one can check that the choice

$$P^+_{ij} = \frac{1}{\sqrt{2}} \left[ (e_2)_i (e_2)_j - (e_1)_i (e_1)_j \right] \quad \text{and} \quad P^\times_{ij} = -\frac{1}{\sqrt{2}} \left[ (e_1)_i (e_2)_j + (e_2)_i (e_1)_j \right]$$

$$\begin{align*}
(11)
\end{align*}$$
satisfies all the constraints (10); they reduce to those appearing in (6) for $\mathbf{k} = k\mathbf{z}$ (choosing $\varphi \to 0$ or $\varphi \to \pi$ as it is then undetermined). One can check straightforwardly that the relations

\[ P_{ij}^+ (n) P_{ij}^+ (n) = P_{ij}^\times (n) P_{ij}^\times (n) = 1 \quad \text{and} \quad P_{ij}^+ (n) P_{ij}^\times (n) = 0 \quad (12) \]

hold.

Let us note at this point that the transformation $n \to -n$, which amounts to $(\theta, \varphi) \to (\pi - \theta, \varphi + \pi)$, implies $e_1 \to -e_1$ and $e_2 \to e_2$, so that

\[ P_{ij}^+ (-n) = P_{ij}^+ (n) \quad \text{and} \quad P_{ij}^\times (-n) = -P_{ij}^\times (n). \quad (13) \]

From (9) and the reality condition below (3), one then finds that

\[ f^+ (\mathbf{k}, \eta) = f^+ (\mathbf{k}, \eta) \quad \text{and} \quad f^\times (\mathbf{k}, \eta) = -f^\times (\mathbf{k}, \eta), \]

the extra minus sign in the cross-polarisation reflecting the fact that the gravitational wave transforms according to a spin-2 representation and not as a scalar. This sign is however inconvenient as it requires the functions $f_2$ to explicitly depend on the direction of propagation of the gravitational wave.

This issue is solved by considering another basis instead of the $+$ and $\times$ polarisations:
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\[ \epsilon_{ij}^{\pm} := \frac{1}{\sqrt{2}} \left( p_{ij}^{+} \pm ip_{ij}^{-} \right), \]  \hspace{1cm} (14)

resulting in the new expansion

\[ w_{ij}(k, \eta) = \sum_{\lambda=\pm} \epsilon_{ij}^{(\lambda)}(n) \mu_\lambda(k, \eta), \]  \hspace{1cm} (15)

where now one recovers the usual reality conditions in the form

\[ \mu_\pm(-k, \eta) = \mu_{\mp}(k, \eta), \]  \hspace{1cm} (16)

because \[ \left[ \epsilon_{ij}^{\pm}(-n) \right]^* = \epsilon_{ij}^{\mp}(n). \]

Note also that the orthogonality relations become

\[ \epsilon_i^{\pm}\epsilon_j^{\mp} = 1 \] and \[ \epsilon_i^{\pm}\epsilon_j^{\pm} = 0 \] and that the coefficients of the expansion are related via

\[ \mu_{\pm}(k, \eta) = \frac{1}{\sqrt{2}} \left[ f_+(k, \eta) \mp if_-(k, \eta) \right]. \]  \hspace{1cm} (17)

Performing a rotation in the plane orthogonal to \( n \) by an angle \( \alpha \) amounts to rotating \( e_a \) through

\[
\begin{align*}
e_1 & \rightarrow e_1 \cos \alpha - e_2 \sin \alpha \\
e_2 & \rightarrow e_1 \sin \alpha + e_2 \cos \alpha
\end{align*}
\]

and one can check explicitly that the new polarisations transform according to

\[ \epsilon_{ij}^{\pm} \rightarrow e^{\pm 2\alpha} \epsilon_{ij}^{\pm}, \]  \hspace{1cm} (18)

i.e. they transform as tensors with helicity \( \pm 2 \) and are, therefore referred to as the helicity basis. Gathering all the above, one finds that Eq. (15) permits to show that, in general, the modes \( \mu_+ \) and \( \mu_- \) both satisfy the same equation of motion, which is nothing but Eq. (4) with the replacement \( w_{ij} \rightarrow \mu_{\pm}. \)

This can be derived directly from Eq. (4) using the expansion on the helicity basis, or going back to the Einstein-Hilbert action and performing an expansion in powers of \( h_{ij} \)

\[ S_{EH} = \frac{1}{16\pi G_N} \int d^4x \sqrt{-g} R = \frac{1}{16\pi G_N} \int d^4x \sqrt{-\left[ g^{(0)} + g^{(2)} \right]} \left[ R^{(0)} + R^{(2)} \right] + \cdots, \]

where the dots represent higher-order terms and the determinant is expanded as the exponent of the trace of a logarithm \( g = \det \left( g_{\mu\nu} \right) = \det \left( g^{(0)}_{\mu\nu} \right) \det \left( \delta^{\mu}_{\nu} + h^{\mu}_{\nu} \right) = a^4 \left[ 1 - \frac{1}{2} h^{\mu}_{\nu} h^{\nu}_{\mu} + \mathcal{O} (h^3) \right] \) and the first term vanishes due to the traceless condition, while the contribution from \( R^{(1)} \) vanishes identically if we assume the background to satisfy the equation of motion. The resulting action at second-order reads

\[ \delta^{(2)} S_T = \frac{1}{64\pi G_N} \int a^2(\eta) \left[ \frac{\partial h^{i}_{j}}{\partial \eta} \frac{\partial h^{j}_{i}}{\partial \eta} - \left( \partial_{\eta} h^{i}_{j} \right) \partial_{\eta} h^{j}_{i} \right] d^4x. \]  \hspace{1cm} (19)
Plugging the expansion (3) and the definition (15) into the action (19), leads to

\[ \delta^{(2)} S_T = \int d\eta \sum_{\lambda = \pm} \frac{1}{2} \int d^3 k \left[ (\mu^*_\lambda - \mathcal{H} \mu^*_\lambda) (\mu'_\lambda - \mathcal{H} \mu_\lambda) - k^2 \mu^*_\lambda \mu_\lambda \right]. \]  

(20)

Upon integrating the \( \mathcal{H} (\mu^*_\lambda \mu'_\lambda)' \) by parts, and using Parseval theorem to revert to real space, we get

\[ \delta^{(2)} S_T = \int d\eta \sum_{\lambda = \pm} \frac{1}{2} \int d^3 x \sqrt{g} \left[ (\mu'_\lambda)^2 - \gamma^{ij} \partial_i \mu_\lambda \partial_j \mu_\lambda + \frac{a''}{a} \mu^2_\lambda \right], \]  

(21)

where we wrote \( \mu_\lambda = \mu_\lambda(x, \eta) \) the inverse Fourier transform of \( \mu_\lambda(k, \eta) \). This is the action for two independent scalar fields \( \mu_+ \) and \( \mu_- \), with identical time-varying masses. One can check that the Euler-Lagrange equation for (21) gives back (4) for both polarisations. The form (20) allows for straightforward quantisation of the gravitational field as a collection of parametric oscillators, which is the subject of the following section.

3 Quantisation and time development

3.1 Historical perspective

Parker, in Ref. [14], was the first to use the above separation of the gravitational wave field into two minimally coupled scalar fields as a simpler route to quantisation, although previous works on (quantum) fields in curved spacetime had already identified the crucial prediction of (vacuum) amplification powered by the expansion of the Universe, including for gravitational waves. Particle creation following a change in boundary conditions of a system was shown in Ref. [15], but creation powered by an expanding Universe was first demonstrated by Parker in his seminal articles [16, 17, 18]. However, it was argued that massless non-zero spin fields, including gravitational waves, had to be conformally coupled to gravity so that no particle creation could occur. The production of gravitons, particles associated with gravitational waves, was studied in anisotropic universes in [19] and hinted at in [20] but Grishchuk [21] was the first to lift the misunderstanding and to compute the ensuing gravitational wave amplification in an isotropic expanding universe. Despite the use of a classical treatment, the corresponding quantum particle pair creation was noted and the existence of a primordial gravitational wave background put forward. Several authors then attempted to compute the spectrum of this background based on spontaneous pair creation from the vacuum still using a classical treatment and different initial conditions and renormalisation procedures as, e.g. in Refs. [22, 23, 24]. Finally, in [24], graviton production due to an early de Sitter phase of expansion, not yet called inflation, was considered with the Bunch-Davies vacuum [25] providing the relevant initial conditions.
Although acknowledged as originating from vacuum fluctuation, the dynamics of primordial gravitational waves was first analysed classically as successive stages of parametric amplifications, either using a classical field and possibly fixing the initial conditions to match quantum vacuum fluctuations [21, 22, 24, 26, 27], or using mode functions [14, 28]. Another presentation, equivalent to the latter, consists in understanding the amplification of the waves as successive Bogoliubov transformations [29] where the initial state is chosen as the vacuum in an asymptotically Minkowski region. Finally, it was latter recognised [30], moving to the Schrödinger picture, that the evolution puts the gravitational waves in a squeezed state. A good parallel presentation of the classical and quantum descriptions can be found in [31].

In this section, we first proceed to the canonical quantisation of the field in the Heisenberg picture following [14]. This is the standard approach; we refer to Refs. [32, 33, 34] for textbooks dealing with scalar fields or gravitational waves. We then review different formal approaches to the evolution of a quantised gravitational wave field on an FLRW background. We begin by using a description in terms of a Bogoliubov transformation, then make the connection with mode functions and finally move to the Schrödinger picture, introducing squeezing parameters and the phase-space representation of the state. We use these different approaches to discuss the mechanism of graviton creation in curved spacetime. This then leads to a discussion of how these particles back-reacts on the geometry. Finally, we use these analyses to compute the properties of primordial gravitational waves produced from the vacuum by the cosmological expansion and discuss their quantum origin.

### 3.2 Canonical quantisation and Bogoliubov transformation

Let us consider one of the two fields $\mu_\lambda$ in Eq. (21). It so happens that for the study of time evolution in terms of Bogoliubov transformations and squeezing, it is useful, and standard [30], to keep the total derivative that was dropped in the process of integration by part between eqs. (20) and (21). The Lagrangian thus obtained reads

$$L_\lambda = \frac{1}{2} \int d^3 x \left[ \left( \mu_\lambda' \right)^2 - 2 \mathcal{H} \mu_\lambda \mu_\lambda - \partial_i \mu_\lambda \partial^i \mu_\lambda + \mathcal{H}^2 \mu_\lambda^2 \right].$$

(22)

The canonically conjugate momentum to $\mu_\lambda$ is

$$\pi_\lambda (x, \eta) = \frac{\delta L_\lambda}{\delta \mu_\lambda'} = \mu_\lambda' - \mathcal{H} \mu_\lambda,$$

(23)

so the Hamiltonian reads

$$H_\lambda = \frac{1}{2} \int d^3 x \left[ \pi_\lambda^2 + \mathcal{H} (\pi_\lambda \mu_\lambda + \mu_\lambda \pi_\lambda) + \partial_i \mu_\lambda \partial^i \mu_\lambda \right],$$

(24)

---

Note that the exact same analyses on quantisation and time evolution can be repeated for scalar perturbations during inflation with the same type of equations [35].
the second term being written in a symmetric way, which is classically irrelevant but prepares for quantisation. We proceed to canonical quantisation by imposing equal-time canonical commutation relations (we now drop the \( \lambda \) subscripts)
\[
\hat{\mu}(x, \eta), \hat{\pi}(x', \eta) = i\hbar \delta(x - x'), \quad \tag{25a}
\]
\[
\hat{\mu}(x, \eta), \hat{\mu}(x', \eta) = \hat{\pi}(x, \eta), \hat{\pi}(x', \eta) = 0. \quad \tag{25b}
\]

Going to Fourier-space these relations are equivalent to
\[
\hat{\mu}_k(\eta), \hat{\pi}_{k'}(\eta) = i\hbar \delta(k + k'), \quad \tag{26a}
\]
\[
\hat{\mu}_k(\eta), \hat{\mu}_{k'}(\eta) = \hat{\pi}_k(\eta), \hat{\pi}_{k'}(\eta) = 0, \quad \tag{26b}
\]
and the Hamiltonian reads
\[
\hat{H} = \int_{\mathbb{R}^3} d^3k \hat{H}_{\pm k} = \int_{\mathbb{R}^3} d^3k \left[ \hat{\mathcal{H}}_{\pm k} + \mathcal{H}_{\pm k} \hat{\mu}_{\pm k} + \mathcal{H}_{\pm k} \hat{\mu}_{-k} + k^2 \hat{\mu}_k \hat{\mu}_{-k} \right], \quad \tag{27}
\]
where \( \hat{H}_{\pm k} \) is the Hamiltonian for the \( \pm k \) sector. Observe that, as required by homogeneity, only the modes \( \pm k \) are coupled and the coupling only depends on the norm \( k \), as required by isotropy. In order to expand \( \hat{H} \) into a sum of independent Hamiltonians \( \hat{H}_{\pm k} \) for the bi-modes \( \pm k \), we restrict the integration to be over the top-half half of the Fourier space, denoted by \( \mathbb{R}^3^+ \), e.g. by selecting only the vectors \( k \) with positive \( k_z \) component, and dropping the original global factor of a half.

Let us first analyse the evolution of one such pair of modes \( \pm k \) in a situation where the term in \( \mathcal{H} \) can be neglected with respect to the others, so that \( \hat{\mu} \) is just a free scalar field in Minkowski spacetime. With \( \mathcal{H} \to 0 \), the Hamiltonian \( \hat{H} \) is time-independent and we can introduce the usual creation/annihilation operators for a real scalar field
\[
\hat{\mu}_k(\eta) = \sqrt{\frac{\hbar}{2k}} \left[ \hat{a}_k(\eta) + \hat{a}^\dagger_{-k}(\eta) \right], \quad \tag{28a}
\]
\[
\hat{\pi}_k(\eta) = -i\sqrt{\frac{\hbar k}{2}} \left[ \hat{a}_k(\eta) - \hat{a}^\dagger_{-k}(\eta) \right]. \quad \tag{28b}
\]

The equal-time commutation relations assume the standard form
\[
\left[ \hat{a}_k, \hat{a}^\dagger_{k'} \right] = \delta(k - k') \quad \text{and} \quad \left[ \hat{a}_k, \hat{a}_k \right] = \left[ \hat{a}^\dagger_k, \hat{a}^\dagger_k \right] = 0. \quad \tag{29}
\]

The Hamiltonian \( \hat{H}_{\pm k} \) then separates into two harmonic oscillators of frequency \( k \)
\[
\hat{H}_{\pm k}^{(0)}(0) = \hbar k \left( \frac{1}{2} \hat{a}^\dagger_k \hat{a}_k + \frac{1}{2} \hat{a}^\dagger_{-k} \hat{a}_{-k} \right), \quad \tag{30}
\]
and the Heisenberg equations of motions
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\[ i\hbar \frac{d\hat{a}_k^{(\dagger)}}{d\eta} = \left[ \hat{a}_k^{(\dagger)}, \hat{H}_{\pm k} \right] \]

give \( \hat{a}_k(\eta) = \hat{a}_k(0)e^{-i\eta} \). Including the friction term proportional to the Hubble function \( \mathcal{H} \), the Hamiltonian now reads

\[ \hat{H}_{\pm k} = \hbar \left( \hat{a}_k^{\dagger} \hat{a}_k + \frac{1}{2} \right) + \hbar \left( \hat{a}_-^{\dagger} \hat{a}_- + \frac{1}{2} \right) - i\mathcal{H} \hbar \left( \hat{a}_k - \hat{a}_-^{\dagger} \right). \quad (31) \]

The additional term corresponds to an interaction with a time-dependent classical source, the expanding background, acting through \( \mathcal{H} \). It couples the \( \pm k \) modes by creating/destroying pairs of particles with opposite momentum; \( \hat{a}_k \) is paired with \( \hat{a}_-^{\dagger} \) and similarly for their hermitian conjugate. These terms are the only quadratic interactions terms that respect homogeneity. The Heisenberg equations of motions accordingly only mixes \( \hat{a}_k \) with \( \hat{a}_k^{\dagger} \)

\[ \frac{d}{d\eta} \left( \begin{array}{c} \hat{a}_k \\ \hat{a}_k^{\dagger} \end{array} \right) = \left( \begin{array}{c} -i\mathcal{H} \\ \mathcal{H}i \end{array} \right) \left( \begin{array}{c} \hat{a}_k \\ \hat{a}_k^{\dagger} \end{array} \right). \quad (32) \]

The operators at any further time \( \eta \) can then be expressed as a linear combination of operators at an earlier time \( \eta_{\text{in}} \)

\[ \left( \begin{array}{c} \hat{a}_k(\eta) \\ \hat{a}_k^{\dagger}(\eta) \end{array} \right) = \left( \begin{array}{cc} \alpha_k(\eta) & \beta_k(\eta) \\ \beta_k^{\ast}(\eta) & \alpha_k^{\ast}(\eta) \end{array} \right) \left( \begin{array}{c} \hat{a}_k(\eta_{\text{in}}) \\ \hat{a}_k^{\dagger}(\eta_{\text{in}}) \end{array} \right). \quad (33) \]

The system (32) is equivalent to

\[ \frac{d}{d\eta} \left( \begin{array}{c} \alpha_k \\ \beta_k^{\ast} \end{array} \right) = \left( \begin{array}{c} -i\mathcal{H} \\ \mathcal{H}i \end{array} \right) \left( \begin{array}{c} \alpha_k \\ \beta_k^{\ast} \end{array} \right), \quad (34) \]

with \( \alpha_k(\eta_{\text{in}}) = 1 \) and \( \beta_k(\eta_{\text{in}}) = 0 \) as initial conditions. One can check that Eq. (34) implies the quantity \( |\alpha_k|^2 - |\beta_k|^2 \) is conserved, while the commutation relations (29) impose

\[ |\alpha_k|^2 - |\beta_k|^2 = 1. \quad (35) \]

At any fixed \( \eta \), a transformation like (33) respecting the condition (35) is called a Bogoliubov transformation [36]. Notice that the equations of motion, and so the Bogoliubov coefficients, only depend on the norm \( k \). The evolution of the quantum field has thus been reduced to finding the coefficients of a time-dependent Bogoliubov transformation. A convenient way to analyse this situation is to introduce mode functions.
3.3 Mode functions

Having observed that the dynamics only mixes $\hat{a}_k$ and $\hat{a}^\dagger_{-k}$, we have a basis on which to expand $\hat{\mu}$. Inserting (33) in the Fourier expansion of the field $\hat{\mu}$, we get

$$\hat{\mu}_k(\eta) = u_k(\eta) \hat{a}_k(\eta_m) + u_k^*(\eta) \hat{a}^\dagger_{-k}(\eta_m),$$  \hspace{1cm} (36a)

$$\hat{\pi}_k(\eta) = U_k(\eta) \hat{a}_k(\eta_m) + U_k^*(\eta) \hat{a}^\dagger_{-k}(\eta_m),$$  \hspace{1cm} (36b)

where $u_k$ and $U_k$ are defined by

$$u_k(\eta) = \frac{\alpha_k(\eta) + \beta_k^*(\eta)}{\sqrt{2k}},$$  \hspace{1cm} (37a)

$$U_k(\eta) = -i\sqrt{\frac{k}{2}}[\alpha_k(\eta) - \beta_k^*(\eta)].$$  \hspace{1cm} (37b)

Using these functions, we get the so-called mode expansion of the field $\hat{\mu}$

$$\hat{\mu}(x, \eta) = \int \frac{d^3k}{(2\pi)^{3/2}} \left[e^{ik\cdot x} u_k(\eta) \hat{a}_k(\eta_m) + e^{-ik\cdot x} u_k^*(\eta) \hat{a}^\dagger_{-k}(\eta_m)\right],$$  \hspace{1cm} (38)

and a similar expression for $\hat{\pi}$ with $U_k$ instead of $u_k$. It can be checked from (33) that $u_k$ simply obeys the same equation of motion (4) as the classical field $\mu_k(x, \eta)$; the momentum mode function $U_k$ is then determined by

$$u_k' = \mathcal{H} u_k + U_k.$$  \hspace{1cm} (39)

Finally, the conserved quantity $|\alpha_k|^2 - |\beta_k|^2$ maps to the Wronskian $W(u_k, u_k^*) = u_k^* u_k' - u_k u_k'^*$, which is a conserved quantity of (4), so the condition (35) translates in the normalisation

$$W(u_k, u_k^*) = -i.$$  \hspace{1cm} (40)

Any function $u_k$ solution of (4) which satisfies the normalisation condition of the Wronskian is called a mode function.

We now have a dictionary between the Bogoliubov and mode function presentations. Solving the system (34) with initial conditions $\alpha_k(\eta_m) = 1$ and $\beta_k(\eta_m) = 0$ is equivalent to solving (4) for $u_k$ with initial conditions $u_k(\eta_m) = 1/\sqrt{2k}$ and $u_k'(\eta_m) = -i\sqrt{k/2} + \mathcal{H} (\eta_m)$, $U_k$ being determined by Eq. (39). Using mode functions the quantum dynamics reduces to the classical one. This justifies the classical treatment used in works cited in introduction of this section; it is simply a consequence of working at linear order and we will encounter other manifestations of this fact when studying phase-space representation.
### 3.4 Squeezed states

The time evolution was described so far in the Heisenberg picture. We now show how to move to the Schrödinger picture and introduce the squeezing formalism. This formulation was initially proposed in Ref. [30] and we use conventions matching those of [37]. Without loss of generality, the Bogoliubov coefficients (33) can be parametrised using three real coefficients $r_k$, $\varphi_k$, and $\theta_k$ through

$$
\alpha_k(\eta) = e^{-i \theta_k(\eta)} \cosh[r_k(\eta)],
$$

$$
\beta_k(\eta) = -e^{i(\theta_k(\eta) + 2\varphi_k)} \sinh[r_k(\eta)],
$$

where $r_k$ and $\varphi_k$ are respectively called the squeezing parameter and angle, collectively referred to as the squeezing parameters. We define the 2-mode squeezing and the 2-mode rotation operators by

$$
\hat{S}(r_k, \varphi_k) = \exp \left[ \int_{R^3^+} d^3 k \left( r_k e^{-2i\varphi_k} \hat{a}_k \hat{a}_{-k} - r_k e^{2i\varphi_k} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \right) \right],
$$

$$
\hat{R}(\theta_k) = \exp \left[ -i \int_{R^3^+} d^3 k \theta_k \left( \hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} \right) \right],
$$

where the integrals are again, as in (27), performed over half the Fourier space and the creation and annihilation operators are understood to be evaluated at $\eta_m$. The operators $\hat{S}$ and $\hat{R}$ defined through (42) are unitary and one can check that

$$
\hat{a}_{\pm k}^{(\dagger)}(\eta) = \hat{R}^{\dagger}(\theta_k) \hat{S}^{\dagger}(r_k, \varphi_k) \hat{a}_{\pm k}^{(\dagger)}(\eta_m) \hat{S}(r_k, \varphi_k) \hat{R}(\theta_k),
$$

where the parameters are that of Eq. (41) and we have made their time dependence implicit for display convenience. The time evolution equation (33) is seen to correspond to the application of a rotation of parameter $\theta_k(\eta)$ followed by a squeezing of parameters $r_k(\eta)$ and $\varphi_k(\eta)$ on the operators.

Any operator $\hat{O}(\eta)$ in the Heisenberg picture can be written as a combination of $\hat{a}_{\pm k}^{(\dagger)}(\eta)$ so we have

$$
\langle \Psi(\eta_m)| \hat{O}(\eta) |\Psi(\eta_m) \rangle = \langle \Psi(\eta_m)| \hat{R}^{\dagger} \hat{S}^{\dagger} \hat{O}(\eta_m) \hat{S} \hat{R} |\Psi(\eta_m) \rangle,
$$

$$
= \langle \Psi(\eta)| \hat{O}(\eta_m)|\Psi(\eta) \rangle.
$$

where $|\Psi(\eta)\rangle = \hat{S} \hat{R} |\Psi(\eta_m)\rangle$ is the Schrödinger evolved state of the system. Choosing the waves to be initially in the vacuum of $\hat{a}_{\pm k}^{(\dagger)}(\eta_m)$ for all modes $k$ (we return to this point later) yields

$$
|\Psi(\eta)\rangle = \prod_{\pm k} \hat{S}(r_k, \varphi_k) \hat{R}(\theta_k) |0_k, 0_{-k} \rangle = \prod_{\pm k} |2MS, r_k, \varphi_k \rangle,
$$

where we have defined the 2-mode squeezed state (2MS) for the modes $\pm k$. 

\[ |2 MS, r_k, \phi_k \rangle = \hat{S}(r_k, \phi_k) |0_k, 0_{-k} \rangle = \frac{1}{\cosh(2r_k)} \sum_{n=0}^{+\infty} \left( -\tanh 2r_k e^{2\phi_k} \right)^n |n_k, n_{-k} \rangle. \] (46)

The last expression can be computed using a Baker-Campbell-Hausdorff formula on the squeezing operator, now restricted to a single \( \pm \mathbf{k} \) sector \[38\] and \( |n_k, n_{-k} \rangle \) is the state with \( n \) particles in the mode \( k \) and \( -k \). Note that the rotation angle \( \theta_k \) has dropped from (46) because the vacuum is invariant under the rotation operator and the product involved is over all directions.

Following \[39\], one can quickly derive the associated wavefunction of a single pair of modes by assuming that, at the initial time, the corresponding state is annihilated by both annihilation operators, i.e.,

\[ \hat{a}_{\pm k} \langle \eta_0 | 0_k, 0_{-k} \rangle = 0. \] (47)

Since \( \hat{S} \) is unitary (\( \hat{S}^\dagger \hat{S} = \mathbb{1} \)), this is also

\[
0 = \hat{S}(r_k, \phi_k) \hat{a}_{\pm k} \hat{S}^\dagger (r_k, \phi_k) \hat{S}(r_k, \phi_k) |0_k, 0_{-k} \rangle,
\]

\[
= \hat{S}(r_k, \phi_k) \hat{a}_{\pm k} \hat{S}^\dagger (r_k, \phi_k) |2 MS, r_k, \phi_k \rangle,
\] (48)

where the transformation on the left corresponds to the inverse of Eq. (43) for \( \theta_k = 0 \). Inverting the Bogoliubov transformation (33) and using (28), the relation (48) becomes

\[
\left[ \hat{\mu}_{\pm k} + \frac{i}{\hbar} \left( \frac{1 - i\gamma_2}{\gamma_1} \right)^{-1} \pi \hat{\pi}_{\pm k} \right] |2 MS, r_k, \phi_k \rangle = 0
\] (49)

where, anticipating the next section, we have introduced the matrix entries

\[ \gamma_1 = \cosh(2r_k) - \cos(2\phi_k) \sinh(2r_k), \] (50a)

\[ \gamma_2 = -\sin(2\phi_k) \sinh(2r_k). \] (50b)

Projecting Eq.(49) onto the \( \mu_{\pm k} \)-representation of the wavefunction\footnote{Formally, the wavefunction is the projection of the relevant state on the basis \( \{ \mu_{\pm k} \} \), i.e. \( \Psi(\mu_k, \mu_{-k}) = \langle \mu_{\pm k} | 2 MS, r_k, \phi_k \rangle \).} by setting \( \hat{\mu}_{\pm k} \rightarrow \mu_{\pm k} \) and \( \hat{\pi}_{\pm k} \rightarrow -i\hbar \partial / \partial \mu_{\pm k} \). The wavefunction solution of Eq. (49) reads

\[
\Psi(\mu_k, \mu_{-k}) = \sqrt{\frac{k}{\pi \hbar}} \exp \left( \frac{1 - i\gamma_2}{\gamma_1} \mu_{\pm k} \right),
\] (51)

which we normalised, using (16), to \( \int |\Psi|^2 d\mu_k d\mu_{-k} = 1 \).

When the squeezing parameters are those determined by Eqs. (41), this gives the wavefunction of any \( \pm k \) mode of the gravitational waves. One can also provide a description in terms of the squeezed state parameters only by recasting (33) into a set of differential equations involving only \( r_k, \phi_k \) and \( \theta_k \). One finds that the system
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\[
\begin{align*}
\frac{dr_k}{d\eta} &= -\mathcal{H} \cos (2\varphi_k), \\
\frac{d\varphi_k}{d\eta} &= -k + \mathcal{H} \coth (2r_k) \sin (2\varphi_k), \\
\frac{d\theta_k}{d\eta} &= k - \mathcal{H} \tanh (r_k) \sin (2\varphi_k),
\end{align*}
\]

(52a), (52b), (52c)

should indeed hold. Note that the equations describing the time evolution of the squeezing parameters \( r_k \) and \( \varphi_k \), namely (52a) and (52b), are independent of \( \theta_k \). These equations are however rarely solved directly, as it is easier to first solve Eq. (4) for the mode function, then deduce the Bogoliubov coefficients by inverting (37) and finally, using (41), obtain the expression of the squeezing parameters. The virtue of the squeezing formalism is rather to give a clear phase space representation of the system’s evolution. Such representation can be obtained using the Wigner quasi-probability distribution [40] to which we now turn.

3.5 Wigner function

Consider a system described by a density matrix \( \hat{\rho} \) and represented by \( n \)-pairs of canonically conjugate hermitian operators \( \hat{X} = \{(\hat{q}_i, \hat{p}_i)\}_{i\in[1,n]} \) of the same dimension. The Wigner function is a function of \( 2n \) phase space variables \( X = \{(q_i, p_i)\}_{i\in[1,n]} \) defined by

\[
W(X) = \frac{1}{(2\pi \hbar)^n} \int d^n\bar{x} e^{-i\frac{\bar{x} \cdot \hat{p}}{\bar{\hbar}}} \left\langle \hat{O} \left| \hat{q} + \frac{\bar{x}}{2} \right| \hat{q} - \frac{\bar{x}}{2} \right\rangle,
\]

(53)

where the states entering the averaging are product eigenstates of \( \hat{q}_i \). The right hand side of (53) is the Weyl transform of \( \hat{\rho}_k / (2\pi)^n \). This transform maps any observable \( \hat{O} \), which is a function of operators in \( \hat{X} \), to a function \( \hat{O}(X) \) of the associated classical variables \( X \). A crucial property is that the expectation value of any such observable \( \hat{O} \) can be computed by treating the Wigner function as a probability measure for the Weyl transform

\[
\left\langle \hat{O} \right\rangle = \mathbb{E} \left[ \hat{O}(X) \right] = \int W(X) \hat{O}(X) \mathcal{D}X,
\]

(54)

where the integral is over all the relevant variables in \( X \) and we denoted \( \mathbb{E} \) the stochastic average with respect to the Wigner function. Equation (54) then allows to compute averages using the Wigner function as any classical phase-space probability distribution. Finally, the von-Neumann equation of motion for the density matrix can be mapped into an equation of motion for the Wigner function, namely [41]

\[
i\hbar W(X) = H(\hat{q}, \hat{p}) \ast W - W \ast H(\hat{q}, \hat{p}),
\]

(55)
where the non-commutative $\ast$-product is defined by

$$f(\vec{q}, \vec{p}) \ast g(\vec{q}, \vec{p}) = f\left(\vec{q} + \frac{i\hbar}{2} \partial_{\vec{q}}, \vec{p} - \frac{i\hbar}{2} \partial_{\vec{p}}\right) g(\vec{q}, \vec{p}),$$ \hspace{1cm} (56a)

$$= f(\vec{q}, \vec{p}) g\left(\vec{q} - \frac{i\hbar}{2} \partial_{\vec{q}}, \vec{p} + \frac{i\hbar}{2} \partial_{\vec{p}}\right).$$ \hspace{1cm} (56b)

The Wigner function therefore furnishes a complete representation of the state of the system and its evolution in phase space.

Two remarks are in order here. First, in general, the Wigner function is not everywhere positive making it only a quasi-probability distribution. It can be shown that, for pure states, it is everywhere positive only when it takes the form [42]

$$W(X) = \frac{1}{(\pi\hbar)^n \sqrt{\det \gamma}} \exp\left(-\frac{X^T \gamma^{-1} X}{\hbar}\right),$$ \hspace{1cm} (57)

which is completely determined by $\gamma$, the covariance matrix, defined by

$$\gamma_{ab} = \langle \hat{X}_a \hat{X}_b + \hat{X}_b \hat{X}_a \rangle.$$ \hspace{1cm} (58)

Such states are called Gaussian states and are widely used in quantum optics, see [43] for a review. Second, for evolution under a quadratic Hamiltonian $H(\hat{X})$, the dynamics (55) simply reduces to the classical Liouville equation $^8$

$$W(X) = \{H(X), W(X)\},$$ \hspace{1cm} (59)

the curly brackets denoting the usual classical Poisson brackets.

Equation (59) can be solved by the method of characteristics i.e. by evolving the initial distribution along the classical trajectories given by $H$. This is another manifestation of the fact that, at quadratic order, the quantum dynamics reduces to the classical one. In addition, this implies that an initially Gaussian state will remain Gaussian under a quadratic Hamiltonian and that its evolution is thus summarised in that of its covariance matrix $\gamma$.

Both of the above discussed simplifications apply to cosmological perturbations at linear order, to which we return by considering a pair of modes $\pm k$. These two degrees of freedom represented by the four operators $\hat{\mu}_{\pm k}$ and $\hat{\pi}_{\pm k}$. These four operators are not hermitian and related to one another by hermitian conjugation. We can however build two such pairs of operators by taking the real and imaginary parts of $\hat{\mu}_{\pm k}$ and $\hat{\pi}_{\pm k}$ (up to a factor of $\sqrt{2}$, introduced for further convenience), namely

\footnote{For a detailed derivation in the special case of cosmological perturbations see Appendix H of [37].}
One can straightforwardly check that those are indeed Hermitian and canonically conjugate i.e. \([\hat{\mu}_k^s, \hat{\pi}_k^s] = i\delta(k - k')\delta_{s,s'}\) and \([\hat{\mu}_k^s, \hat{\mu}_k^{s'}] = [\hat{\pi}_k^s, \hat{\pi}_k^{s'}] = 0\) where \(s = \text{R, I}\). We arrange them in the vector \(\hat{X}_{\text{R/I}} = (k^{1/2}\hat{\mu}_{\pm k, \text{R}}, k^{-1/2}\hat{\pi}_{\text{R}}, k^{1/2}\hat{\mu}_{\pm k, \text{I}}, k^{-1/2}\hat{\pi}_{\text{I}})^\dagger\), where we have introduced factors of \(k\) to give the same dimension to all entries in the vector, whose associate vector of classical variables is denoted \(X_{\text{R/I}}\). The Wigner function with respect to these variables is defined by

\[
W_{\pm k}(X_{\pm k}) = \frac{1}{(2\pi\hbar)^2} \int e^{-\frac{i}{\hbar} (\sigma_k^x x + \sigma_k^y y)} \left( \mu_k^R + \frac{x}{2}\mu_k^I + \frac{y}{2}\rho_k^I \right) \mu_k^R - \frac{x}{2}\mu_k^I - \frac{y}{2}) \, dx\, dy.
\]

In terms of the variables (60), the Hamiltonian \(\hat{H}_{\pm k}\) separates into two equal Hamiltonian over the \(\text{R/I}\) sectors that thus evolve independently

\[
\hat{H} = \frac{\hbar}{2} \int_{\mathbb{R}^3} d^3 k \sum_{s = \text{R,I}} [(\sigma_k^x)^2 + 2\mathcal{H} (\mu_k^s\pi_k^s + \pi_k^s\mu_k^s) + k^2 (\mu_k^s)^2] = \int_{\mathbb{R}^3} d^3 k \sum_{s = \text{R,I}} \hat{H}_k^s.
\]

Similarly, the wavefunction (51) factorises into a product of two wavefunctions over each sector \(\Psi(\mu_k, \mu_{-k}) = \Psi(\mu_k^s)\Psi(\mu_k^s)\) with

\[
\Psi(\mu_k^s) = \left(\frac{k}{\pi\hbar n_1}\right)^{1/4} e^{-\frac{k}{2\hbar} \frac{1 - m^2}{m_1} (\mu_k^s)^2},
\]

and the covariance matrix is block diagonal in the \(\text{R/I}\) partition \(\gamma = \gamma^\text{R} \oplus \gamma^\text{I}\). These separations are in fact imposed by the homogeneity of the state that requires \(\langle \hat{a}_k^\dagger \hat{a}_k^\dagger \rangle = \langle \hat{a}_k^2 \rangle = 0\), which can be recast in the vanishing of all \(\text{R/I}\) cross terms [44]. Eq. (63) is nothing else than the wavefunction of a one-mode squeezed state of parameter \(\gamma_k, \phi_k\) [45]. Going from the \(\pm k\) operators to the \(\text{R/I}\) operators allows to view a 2-mode squeezed state as a product of two 1-mode squeezed states \(^9\). Such transformations are studied in details in [46].

Since the wavefunction (63) is Gaussian, then so is the associated Wigner function \(W^s\); vacua and squeezed states are indeed Gaussian states. Note that their gaussianity is preserved by the evolution because \(\hat{H}_k^s\) is quadratic. The Wigner function (61) also factorises into \(W_{\pm k} = W^R (\hat{\mu}_k^R, \hat{\pi}_k^R) W^I (\hat{\mu}_k^I, \hat{\pi}_k^I)\). Both sectors have identical covariance matrix, namely

\(^9\text{This fact can be directly seen by factorizing the 2-mode squeezing operator } \hat{S}(\gamma_k, \phi_k) \text{ into two 1-mode squeezing operators for the } \text{R/I} \text{ creation/annihilation operators defined via (28) where } \pm k \text{ operators are replaced by } \text{R/I} \text{ operators.}\)
expressed in terms of the squeezing parameters

Using (65) and the parametrisation (41), the covariance matrix can be conveniently

treated. Using (65) and the parametrisation (41), the covariance matrix can be conveniently

evened.

We can compute its contour levels. Owing to gaussianity, those are ellipses whose pa-


tion of the original $\hat{S}^\mu_k$ and $\hat{S}^\nu_k$ operators (one can also check that $\langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle = 0$).

Using (65) and the parametrisation (41), the covariance matrix can be conveniently

evened.

where we expressed the entries of the covariance matrix in terms of two-point func-


tion of the original $\hat{S}^\mu_k$ and $\hat{S}^\nu_k$ operators (one can also check that $\langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle = 0$).

Using (65) and the parametrisation (41), the covariance matrix can be conveniently

evened.

\[ \langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle = \langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle = \langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle, \]

\[ \gamma_1 = 2k \langle (\hat{\mu}_k^\nu)^2 \rangle = 2k \langle (\hat{\mu}_k^\mu)^2 \rangle = k \langle \{ \hat{\mu}_k^\nu, \hat{\mu}_k^\mu \} \rangle, \] (65a)

\[ \gamma_2 = \gamma_1 = \langle \hat{\mu}_k^\nu \hat{\mu}_k^\mu + \hat{\mu}_k^\mu \hat{\mu}_k^\nu \rangle = \langle \hat{\mu}_k^\nu \hat{\mu}_k^\mu + \hat{\mu}_k^\mu \hat{\mu}_k^\nu \rangle = \langle \hat{\mu}_k^\nu \hat{\mu}_k^\mu + \hat{\mu}_k^\mu \hat{\mu}_k^\nu \rangle, \] (65b)

\[ \gamma_2 = 2k \langle (\hat{\nu}_k^\nu)^2 \rangle = 2k \langle (\hat{\nu}_k^\mu)^2 \rangle = \frac{1}{k} \langle \{ \hat{\nu}_k^\nu, \hat{\nu}_k^\mu \} \rangle, \] (65c)

where we expressed the entries of the covariance matrix in terms of two-point func-


tion of the original $\hat{S}^\mu_k$ and $\hat{S}^\nu_k$ operators (one can also check that $\langle \hat{S}^\nu_k \hat{S}^\mu_k + \hat{S}^\mu_k \hat{S}^\nu_k \rangle = 0$).

Using (65) and the parametrisation (41), the covariance matrix can be conveniently

evened.

where the expressions for $\gamma_1$ and $\gamma_2$ correspond to those defined earlier when com-

puting the wavefunction. Finally in order to visualize this probability distribution,
we compute its contour levels. Owing to gaussianity, those are ellipses whose pa-

rameters can be computed through diagonalizing the quadratic form appearing in the
argument of the exponential in Eq. (57). It is readily done by performing a rotation
in phase space $X^S = R(\phi_k)X^S$ so that the covariance matrix of $X^S$ reads

\[ (\tilde{\gamma})^{-1} = \begin{pmatrix} e^{2r_k} & 0 \\ 0 & e^{-2r_k} \end{pmatrix}. \] (67)

Some contour levels of $W^S$ are plotted in Fig. 3; they provide a geometrical rep-

resentation of the state of the tensor perturbations in phase space and illustrate the
meaning of the squeezing parameters: the ellipse representing the $\sqrt{2} - \sigma$ contour has
semi-minor and semi-major axes of length $A_k = \sqrt{\hbar} e^{r_k}$ and $B_k = \sqrt{\hbar} e^{-r_k}$, which are
tilted by the angle $\phi_k$ in phase space. The fluctuations of the operator in the direc-
tion of the semi-major axis are exponentially amplified with respect to the vacuum;
this is called a super-fluctuant mode. On the other hand, the fluctuations of the oper-
ator related to the semi-major axis are exponentially suppressed, thus defining a
sub-fluctuant mode.

The presence of amplification and suppression is a manifestation of the existence
of a growing and a decaying solution in Eq. (4) [45]. Their complementary can be
traced back to the purity of the state which, for a Gaussian state, can be computed
directly in terms of the covariance matrix via [45]

\[ \rho_k = tr(\hat{\rho}^2) = \frac{1}{\sqrt{\text{det} (\gamma)}} = \frac{1}{\gamma_1 \gamma_2 - \gamma_1^2} = \frac{\hbar^2}{A_k^2 B_k^2} = \frac{\hbar^2 \pi^2}{S_k^2}, \] (68)
where $S_k$ is the area of the $\sqrt{2} \sigma$ contour defined by the points where the argument of the exponential in Eq (57) is unity. Since the purity of the state is preserved under Hamiltonian evolution, so is $S_k$. Therefore, the amplification in a given direction has to be balanced out with squeezing in another. Conversely, if the fluctuations in one direction are reduced, they increase in another. For any quantum state, $p_k \leq 1$ and so the area is minimal for a pure state $p_k = 1$, like the one we consider here, where $S_k = \pi \hbar$; this is a geometrical translation of the Heisenberg uncertainty principle forbidding to localise the system too precisely. Note that in general, due to the rotation $\phi_k$, the product uncertainty of the original pair $\left(\hat{\mu}_k, \hat{\pi}_k\right)$ does not saturate the inequality anymore.

![Fig. 3](image_url) $\sqrt{2} \sigma$ contour level of the Wigner function $W$ for $\phi_k = \pi/4$, $r_k = 1$ (green ellipse) and the vacuum state $r_k = 0$ (pink circle). This figure is adapted from [46].

In addition to granting an elegant geometrical representation of the state, the presentation in terms of 2-mode squeezed states is often used in the literature to discuss the quantumness of primordial gravitational waves and scalar perturbations alike. These aspects are discussed in Sec. 4.

### 3.6 Particle production

Having laid out the formalisms to follow the evolution of gravitational waves in cosmology, we want to give more physical insights into the evolution and show
that, under certain conditions, it can be understood as a process of particle creation. Bogoliubov transformations and mode functions are the appropriate way to describe this process in curved spacetime. We start by analysing their relation to particle content.

Consider two pairs of operators \((\hat{a}, \hat{a}^\dagger)\) and \((\hat{b}, \hat{b}^\dagger)\) related by a constant Bogoliubov transformation

\[
\hat{b} = \alpha \hat{a} + \beta \hat{a}^\dagger,
\]

with \((\alpha, \beta) \in \mathbb{C}^2\) such that \(|\alpha|^2 - |\beta|^2 = 1\). We define two vacua: \(|0\rangle_a\) with respect to the \(\hat{a}\) operators and \(|0\rangle_b\) with respect to the \(\hat{b}\) operators. The crucial observation is that these vacua do not coincide. The number of \(b\)-particles in the \(a\)-vacuum is always non-vanishing when the Bogoliubov transformation is non-trivial

\[
_a \langle 0 | \hat{b}^\dagger \hat{b} | 0 \rangle_a = |\beta|^2 > 0.
\]

The analysis carries over to the study of \(\pm k\) modes. Equation (46) shows that the vacuum of the operators \(\hat{a}_{\pm k}(\eta)\) is filled with particles associated to \(\hat{a}_{\pm k}(\eta)\) in Minkowski spacetime \((a' = 0)\), this form is uniquely selected (up to a phase) by requiring that the Hamiltonian is diagonal and that the vacuum thus defined is invariant under the Poincaré group so that it is shared by all inertial observers, or, equivalently, the vacuum is the ground state of the Hamiltonian [34]. In this situation there is a preferred set of operators selected by physical symmetries, which subsequently define preferred notions of vacuum and particle.

The procedure described above breaks down in an expanding Universe, \(a' \neq 0\), as the Poincaré group is no longer a symmetry of spacetime, \(\tilde{\omega}_k^2\) [see Eq. (27)] is time-dependent and can even become negative so that the existence of an energy minimum is not guaranteed anymore. We are left with no physically preferred vacuum in which no inertial detector would record the presence of particles. In this context, the choice of \(\hat{a}_{\pm k}(\eta)\) to perform the expansion (38) appears arbitrary.

A choice of operators in fact corresponds to a choice of mode functions, the latter being more convenient to work with. Consider the operators \(\hat{b}_{1, k}\) related to \(\hat{a}_{\pm k}(\eta)\) by the following time-independent Bogoliubov transformation

\[
\hat{b}_k = \rho_k \hat{a}_k(\eta) + \chi_k \hat{a}^\dagger_{-k}(\eta),
\]

with \((\rho_k, \chi_k) \in \mathbb{C}^2\) such that \(|\rho_k|^2 - |\chi_k|^2 = 1\). Inverting this transformation and inserting in (38), we get

\[
\hat{\mu}(x, \eta) = \int \frac{d^3 k}{(2\pi)^{3/2}} \left[ e^{i k \cdot x} v_k(\eta) \hat{b}_k + e^{-i k \cdot x} v_k^*(\eta) \hat{b}^\dagger_k \right],
\]

where
can be checked to be a mode function, i.e. a solution of (4) with a Wronskian normalised to $W(v_k, v_k^*) = (|\rho_k|^2 - |\chi_k|^2) W(u_k, u_k^*) = -i$. A similar expansion is found for $\hat{\pi}$, with $v_k$ replaced by new functions $V_k$ defined as the $U_k$s through the replacement $u_k \rightarrow v_k$.

We then have an alternative expansion of $\hat{\mu}$ and $\hat{\pi}$ over another set of mode functions and operators. The meaning of the operators in the expansion is set once the associated mode functions are fixed\(^\text{10}\), and a choice of mode functions corresponds to a choice of initial conditions for the solutions of (4). The normalisation of the Wronskian fixes one condition, and one is left to choose. For instance, the Minkowski operators (28) are associated to the mode function

$$u_k^{(M)}(\eta) = \frac{e^{-ik\eta}}{\sqrt{2k}},$$

(73)

corresponding to the initial conditions

$$u_k(\eta_0) = e^{-ik\eta_0} \quad \text{and} \quad u_k'(\eta_0) = ik\eta_0 e^{-ik\eta_0}.$$

(74)

For non-vanishing $\mathcal{H}$, $u_k^{(M)}$ is no longer a solution of (4). Yet, when analysing the evolution of the two helicities of the gravitational field in this context, we have used the associated operators (28). Their time-dependence then does not simply factorise in the running phase of $u_k^{(M)}$ and we have to deal with a continuous change of reference operators parametrised by a time-dependent Bogoliubov transformation. These operators correspond at any time $\eta$ to what would be the Minkowskian definition of particle and vacuum if the modulation were to stop at this instant. Alternatively, we can work with the operators defined at some fixed time $\eta_0$, as we did in Eq. (36), in which case the time-dependence is that of a mode function satisfying Eq. (4) which differs from that of $u_k^{(M)}$. As just discussed, when the background is time-dependent neither of these two sets of operators can be favoured to discuss the particle content of the field.

There are some situations where one can unambiguously define particles and their properties. One such case\(^\text{17}\) is that of a spacetime which is asymptotically Minkowski at both very early and very late times, i.e. one for which the scale factor varies in-between two asymptotic constant values

$$a(\eta) \xrightarrow{\eta \rightarrow -\infty} a_{\text{in}} \quad \text{and} \quad a(\eta) \xrightarrow{\eta \rightarrow +\infty} a_{\text{out}}.$$

We can therefore define asymptotically Minkowski “in” and “out” mode functions $u_k^{(\text{in/out})}$ and associated operators $\hat{a}_k^{(\text{in/out})}$ by requiring as initial condition that they match the Minkowski solution

\(^{10}\) This can be seen by expressing $\hat{b}_k$ in terms of the mode function and the fields $\hat{b}_k = -i \left[ V_k^* \hat{\mu}(k, \eta) - v_k^* \hat{\pi}(k, \eta) \right]$.\n
These mode functions are both solutions of (4) for any time $\eta$ and are therefore related by a *time-independent* Bogoliubov transformation
\[ u_k^{(\text{in})} \rightarrow \frac{\sqrt{2}k}{e^{-ik\eta}} \eta \rightarrow -\infty \]
and
\[ u_k^{(\text{out})} \rightarrow \frac{\sqrt{2}k}{e^{-ik\eta}} \eta \rightarrow +\infty . \]

These mode functions are both solutions of (4) for any time $\eta$ and are therefore related by a *time-independent* Bogoliubov transformation
\[ u_k^{(\text{in})} = \rho_k u_k^{(\text{out})} + \chi_k u_k^*^{(\text{out})} , \]
and, via (71), so are $\hat{a}_k^{(\text{in/out})}$, and it is straightforward to evaluate the number of particles produced by the non-trivial evolution of the background. We assume that the field is initially (in the “in” region) in the vacuum defined by the “in” operators where there exists a preferred notion of vacuum; we denote $|0\rangle_{\text{in}}$ this “in” vacuum.

In order to read the particle content at the end of evolution (in the “out” region) we need to use the “out” operators that define the Minkowski notion of particle there. The number of particles in the “out” region is given by
\[ n_{\text{out}}^{\pm} = \langle 0 | \hat{a}_k^{\dagger (\text{out})} \hat{a}_k^{(\text{out})} | 0 \rangle_{\text{in}} = |\chi_k|^2 . \]

This number is strictly positive and the same in the modes $\pm k$; this is the well-known phenomenon of pair production out of the vacuum, here powered by the background expansion. To evaluate the extent of this production quantitatively we have to compute the mode equation for both “in” and “out” conditions and match them. This computation can, for example, be done exactly in a 2d model where the scale factor evolves as a hyperbolic tangent between its asymptotic values [47].

Let us make the connection in this idealised case with the time-dependent Bogoliubov coefficients solving the dynamics of (33). First, note that the operators (28) coincide with those defined with respect to a mode function $u_k$ at times $\eta_0$ where it satisfies the Minkowski conditions (74). This can be checked directly upon inserting (28) in the expression of the operator in terms of the mode function and the fields at time $\eta_0$. This applies in both the “in” and “out” regions
\[ \hat{a}_{\pm k} (\eta) \rightarrow \hat{a}_{\pm k}^{(\text{in})} , \]
\[ \hat{a}_{\pm k} (\eta) \rightarrow \hat{a}_{\pm k}^{(\text{out})} . \]

The time-independent Bogoliubov coefficients between the “in” and the “out” states, therefore, correspond to the late time limit of the time-dependent Bogoliubov coefficients of Eq. (34)
\[ \rho_k = \alpha_k (\eta \rightarrow +\infty) \quad \text{and} \quad \chi_k = \beta_k (\eta \rightarrow +\infty) , \]
where the associated number of particles $\langle \hat{a}_{\pm k}^{\dagger (\eta)} \hat{a}_{\pm k}(\eta) \rangle$ and correlations are now meaningful. While it is not *a priori* the case at any intermediate times, since the scale factor is varying, we discuss in Sec. 3.8.2 how it is often possible to identify “in” and “out” regions for certain ranges of modes $k$ in the cosmological evolution.
Quantum cosmological gravitational waves?

Anticipating these considerations, we conclude by making a connection with Sec. 3.4 and studying the particle content of a 2-mode squeezed state. Those can also be fully characterised by the following three non-vanishing expectation values (two of them being equal)

\[ n_k = \langle \hat{a}_k^{\dagger} \hat{a}_k \rangle = \left( \frac{\gamma_{11} + \gamma_{22} - 2}{4} \right) = \sinh^2 (r_k), \quad (78a) \]

\[ c_k = \langle \hat{a}_k \hat{a}_{-k} \rangle = \left( \frac{\gamma_{11} - \gamma_{22}}{4} + i \frac{\gamma_{12}}{2} \right) = -\frac{1}{2} \sinh (2r_k) e^{2i\phi_k}. \quad (78b) \]

These expressions are obtained by inverting Eq. (28) and making use of Eqs. (65) and (66). The first expectation value \( n_k \) gives the number of particles in the modes \( k \) and \( -k \), which must be identical because of isotropy, while \( c_k \) encodes the 2-mode coherence of the pairs. Imposing the purity to be less than unity, \( p_k = \gamma_{11} \gamma_{22} - \gamma_{12}^2 \leq 1 \), yields the following bound on the magnitude of this coherence:

\[ |c_k| \leq \sqrt{n_k (n_k + 1)}. \quad (79) \]

For a pure state like that of the gravitons, the bound is saturated \( |c_k| = \sqrt{n_k (n_k + 1)} \), while for a thermal state \( c_k = 0 \). In this sense, the modes are uncorrelated in the thermal state and maximally correlated in a 2-mode squeezed state; they are even entangled [44]. We come back to this important point in Sec. 4.

3.7 Anomaly-induced semiclassical theory

The concept of particle associated with a quantum field is a global one in the sense that it is defined through modes; somehow, it can be understood, as described above, as the effect of geometry on matter, even when “matter” consists of tensor-like perturbations of the gravitational field itself. When coupled to classical GR in a semiclassical way, the quantum nature of gravitational waves, just like any other particle, may also manifest itself in another way, namely in the back reaction of their quantum fields on geometry; (see, e.g., the historical papers by M. J. Duff [48, 49, 50] who proposed it for the first time, and Refs. [51, 52] as well as the more recent Ref [53]). This approach is, therefore, the opposite of the above, making extensive use of the stress-energy tensor \( T_{\mu\nu}(x) \), which is a local quantity.

In this section, for the sake of notational simplicity, we set \( \hbar \to 1 \) as all the effects are quantum by nature.

3.7.1 Gravity with quantum fields

When quantum fields are described in a geometric background, it is customary to write the corresponding Einstein’s equations in the semiclassical form
so that geometry is now sourced by the renormalised stress-energy tensor \( \langle T_{\mu\nu} \rangle_{\text{ren}} \).

As the classical Einstein equations are derived from a variation of the vacuum Einstein-Hilbert term (possibly including a cosmological constant contribution),

\[
S_{\text{EHA}} = \frac{1}{16\pi G_N} \int d^4 x \sqrt{-g} (R + 2\Lambda),
\]

the stress-energy tensor being derived from the classical matter action \( S_m \) through

\[
T_{\mu\nu}^{\text{class}} = -\frac{2}{\sqrt{-g}} \frac{\delta S_m}{\delta g^{\mu\nu}},
\]

one can recover the semiclassical case (80) by similarly defining an effective action \( \Gamma[g_{\mu\nu}] \) such that

\[
\langle T_{\mu\nu} \rangle = -\frac{2}{\sqrt{-g}} \frac{\delta \Gamma}{\delta g^{\mu\nu}}.
\]

It can be shown that for a set of matter fields denoted generically by \( \phi \), and which can include scalar, gauge and fermion fields, whose dynamics is driven by the action \( S[\phi; g_{\mu\nu}] \), one finds

\[
e^{i\Gamma[g_{\mu\nu}]} = \int D\phi e^{iS[\phi; g_{\mu\nu}]},
\]

and the expectation value in (83) is then understandable in terms of "in" and "out" vacuum states:

\[
\frac{2}{\sqrt{-g}} \frac{\delta \Gamma}{\delta g^{\mu\nu}} = \frac{\langle 0|T_{\mu\nu}|0 \rangle_{\text{in}}}{\langle 0|0 \rangle_{\text{in}}},
\]

thereby automatically providing the required normalisation.

In order to integrate explicitly (85) and obtain the relevant effective action, one needs to know the matter content and its corresponding action. Compared to their flat space counterparts, fermionic and vectorial contributions are merely obtained by the minimal coupling, namely making the replacements \( \partial \rightarrow \nabla \) and using the metric \( g_{\mu\nu} \) to integrate. The scalar field case can also include an extra term, not present in the flat Minkowski situation, and one gets

\[
S_{\phi} = -\frac{1}{2} \int d^4 x \sqrt{-g} \left[ (\partial \phi)^2 + \xi_{ij} \phi^i \phi^j R \right],
\]

where we considered a set of scalars \( \{\phi^i\} = \phi \); a possible extra potential term \( V(\phi) \) can be added to this action. Eq. (86) involves a set of new dimensionless numbers \( \{\xi_{ij}\} \) which are called non-minimal parameters. For a single scalar field, this reduces to a single parameter; its special value \( \xi = \frac{1}{6} \) yields conformal invariance.

\[11\] We do not consider the Gibbons–Hawking–York boundary term in these discussions; it can be set to zero by assuming a compact manifold.
It turns out that the action derived from this procedure contains ultraviolet divergences that thus need to be renormalised. These lead to contributions that are purely geometrical, involving only scalars made out of the Riemann tensor $R_{\mu\nu\alpha\beta}(x)$ and its contractions. This is understandable as short wavelengths are only sensitive to local features of spacetime. Regularising and renormalising forces to introduce counterterms involving higher-order derivatives, and one is naturally led to the conclusion that in order to obtain a renormalisable theory of quantum matter on a classical curved spacetime, one must demand a geometrical framework that goes beyond general relativity.

Applying the procedure described above, the relevant vacuum classical action

$$S_{\text{vac}} = S_{\text{EH}} + S_{\text{HD}}$$

is found to include the usual Einstein-Hilbert term (81) in which both $G_N$ and $\Lambda$ are renormalised quantities, but another contribution, containing higher derivatives (HD) terms, needs be included, namely

$$S_{\text{HD}} = \int d^4x \sqrt{-g} \left( a_1 C^2 + a_2 E + a_3 \Box R + a_4 R^2 \right),$$

where

$$C^2 = R_{\mu\nu\alpha\beta}^2 - 2R_{\alpha\beta}^2 + \frac{1}{3}R^2$$

is the square of the Weyl tensor and

$$E = R_{\mu\nu\alpha\beta}^2 - 4R_{\alpha\beta}^2 + R^2$$

represents the Gauss-Bonnet topological term. The action (87) has been shown [54] to lead to a renormalisable (albeit containing unphysical ghosts or having non-unitarity issues) theory of quantum gravity. Details can be found in particular in [55] in the present volume. The parameter $a_3$ is irrelevant for the equations of motion since $\Box R$ is a surface term, while the $R^2$ term is at the origin of the most serious inflation model proposed by Starobinsky [56].

### 3.7.2 Conformal anomalies

Let us consider a conformally invariant theory, i.e. for which the transformations

$$g_{\mu\nu} \rightarrow \bar{g}_{\mu\nu} = \Omega^2(x) g_{\mu\nu} \quad \text{and} \quad \phi \rightarrow \phi / \Omega(x)$$

(vector fields being left unchanged and spinors transforming with $\Omega^{-3/2}$) leaves the action $S$ unchanged. From this requirement, one finds that the trace of the energy-momentum tensor [51]

$$T^\mu_\mu[\bar{g}_{\alpha\beta}(x)] = -\frac{\Omega(x)}{\sqrt{-g(x)}} \frac{\delta S[\bar{g}_{\mu\nu}]}{\delta \bar{\Omega}(x)} \bigg|_{\Omega \rightarrow 1},$$

(90)
should vanish if (89) is a symmetry of $S$. This implies that the scalar fields are massless and $\xi \to \frac{1}{6}$. The identity (90) is true at the classical level, and indeed the conserved Noether current in this case reads

$$\left(2g_{\mu\nu} \frac{\delta}{\delta g_{\mu\nu}} + \sum_i k_i \phi_i \frac{\delta}{\delta \phi_i} \right) S[g_{\alpha\beta}(x), \phi(x)] = 0,$$  \hspace{1cm} (91)

in which the weights $k_i$ correspond to the various fields involved, with $k_s = -1$ for scalar fields, $k_f = -3/2$ for the fermions and $k_v = 0$ for the gauge fields.

At the quantum level, however, the trace $\langle T^\mu_\mu \rangle$ is no longer vanishing, as explicitly calculating it with the given matter content (scalar, vector and spinor fields) yields a renormalised expectation value [51]

$$\langle T^\mu_\mu \rangle = - (\omega C^2 + bE + c\Box R),$$  \hspace{1cm} (92)

where the $\beta$–functions $\omega$, $b$ and $c$ depend on the numbers of real scalar degrees of freedom $N_0$, four-component spinor fermions $N_{1/2}$ and vector fields $N_1$ in the underlying particle physics model. In practice, they are found to be

$$\left(\begin{array}{c}
\omega \\
b \\
c
\end{array}\right) = \frac{1}{360(4\pi)^2} \left(\begin{array}{c}
3N_0 + 18N_{1/2} + 36N_1 \\
-N_0 - 11N_{1/2} - 62N_1 \\
2N_0 + 12N_{1/2} - 36N_1
\end{array}\right).$$  \hspace{1cm} (93)

In the standard model (SM) of particle physics, where the SU(3)×SU(2)×U(1) is broken to SU(3)×U(1) through a Higgs doublet, the relevant numbers are $N_0^{\text{SM}} = 4$, $N_{1/2}^{\text{SM}} = 12$ (eight gluons, the intermediate $W^\pm$ and $Z^0$ and the photon) and $N_1^{\text{SM}} = 24$ (leptons and quarks, assuming a massive neutrino), one finds

$$\omega^{\text{SM}} = \frac{73}{480\pi^2}, \quad b^{\text{SM}} = -\frac{253}{1440\pi^2} \quad \text{and} \quad c^{\text{SM}} = -\frac{17}{720\pi^2}.$$  

Note that although $b$ is negative definite, the sign of $c$ depends on the exact matter content; measuring this sign somehow, e.g. through that of the primordial gravitational wave spectrum, could be an indirect way of getting information about the physics that should apply at high energies such as the grand unification (if any) scale. Note for instance that in the case of the minimal supersymmetric extension of the standard model (MSSM), the number of vector modes is unchanged ($N_{1/2}^{\text{MSSM}} = 12$), while the number of fermions is increased to $N_1^{\text{MSSM}} = 32$ and the proliferation of new scalar modes then yields $N_0^{\text{MSSM}} = 104$, leading to $c^{\text{MSSM}} = 1/(36\pi^2) > 0$.

Integrating the trace of (83) using (92) is a non-trivial task that has been achieved in Refs. [57, 58]. Ref. [59] suggested to rewrite the action in terms of two auxiliary scalar fields $\sigma$ and $\rho$ (see also [60] for an independent but equivalent formulation) which happens to be particularly useful for the gravitation wave discussion. It reads
\[ \Gamma = S_c[g_{\mu\nu}] + \int d^4x \sqrt{-g} \left( \frac{1}{2} \sigma \Delta_4 \sigma - \frac{1}{2} \rho \Delta_4 \rho + \ell_1 C^2 \rho \right) \]
\[ + \int d^4x \sqrt{-g} \left( \sigma \left[ k_1 C^2 + k_2 \left( E - \frac{2}{3} \Box R \right) \right] - \frac{1}{12} k_3 R^2 \right) , \tag{94} \]

where the integration constant \( S_c[g_{\mu\nu}] \) is conformally invariant, the covariant conformal fourth-order operator is (see Refs. [57, 58])
\[ \Delta_4 = \Box^2 + 2 R^\mu\nu \nabla_\mu \nabla_\nu - \frac{2}{3} R \Box + \frac{1}{3} R^\mu \nabla_\mu \]
and the coefficients are given in terms of those of (92) through
\[ k_1 = -\frac{\omega}{2 \sqrt{|b|}}, \quad k_2 = \frac{\sqrt{|b|}}{2}, \quad k_3 = c + \frac{2}{3} b \quad \text{and} \quad \ell_1 = \frac{\omega}{2 \sqrt{|b|}} \tag{95} \]
(recall \( b < 0 \)). This effective action stemming from the conformal anomaly (the Noether current is not conserved at the quantum level) should be added to the vacuum term \( S_{\text{vac}} \) of Eq. (87).

### 3.7.3 Anomaly-induced cosmology and gravitational waves

Let us apply the above discussion to the specific case of a cosmological framework which is our main subject, first by considering a background FLRW (conformally flat) solution and its tensorial perturbations.

The FLRW metric can be written as a conformal transformation of the Minkowski metric \( \eta_{\mu\nu} \) by setting \( g_{\mu\nu} = a^2(\eta) \eta_{\mu\nu} \). In this very simple case, variations of (94) with respect to the auxiliary fields \( \sigma \) and \( \rho \) yields
\[ \left( \partial_t^2 - \nabla^2 \right) \left( \sigma + 8 \pi \sqrt{|b|} \ln a \right) = 0 \quad \text{and} \quad \left( \partial_t^2 - \nabla^2 \right) \rho = 0, \tag{96} \]
with solutions
\[ \sigma = \sigma_h - 8 \pi \sqrt{|b|} \ln a \quad \text{and} \quad \rho = \rho_h, \tag{97} \]
in which \( \sigma_h \) and \( \rho_h \) are solutions of the homogeneous equation, \( \left( \partial_t^2 - \nabla^2 \right) f_h = 0 \); they can be set to zero in the cosmological context. In this case, one finds the relation
\[ \frac{d^n \sigma}{dr^n} = -8 \pi \sqrt{|b|} \frac{d^{n-1} H}{dr^{n-1}} \]
where \( H = \dot{a}/a \).

The above solution (97) with the FLRW metric can now be inserted into the full theory containing both (94) and the original vacuum (87). It leads to the modified Friedmann equation
in which we defined the Planck mass $M_p^2 = 8\pi G_N$. As could have been anticipated, this solution depends on $b$ and $c$, but neither on $\omega$ and $a_1$ since the Weyl tensor is conformally invariant, nor on $a_2$ and $a_3$ (surface terms), and we have set $a_4 \to 0$ to ensure the original theory is conformally invariant.

Inflationary solutions for (98) can be found in Refs. [56, 61, 62, 63, 64]. A simple case consists of a de Sitter solution $a \propto \exp(Ht)$ with $H$ constant, which transforms (98) into a quadratic algebraic equation for $H$ whose solutions

$$H^2 = \frac{M_p^2}{2|b|} \left( 1 \pm \sqrt{1 + \frac{4|b|\Lambda}{3M_p^2}} \right) \to \begin{cases} H_{\text{inf}}^2 = M_p^2/|b| & (+) \vspace{1em} \\ H_{\Lambda}^2 = 2\Lambda/3 & (-) \end{cases}$$

produce the two relevant extreme cases of present-day cosmological constant domination and initial inflation, with $H_{\text{inf}} \gg H_{\Lambda}$.

Tensor perturbations of the kind (1) in this context are slightly different from those of ordinary GR discussed in the previous sections. In particular, the mode equation (4) is now replaced by the slightly more involved fourth order equation (see Ref. [65] for details)
\[
\left(2f_1 + \frac{f_2}{2}\right) \ddot{h} + \left[3H(4f_1 + f_2) + 4f_1 + f_2\right] \ddot{h} + \left[3H^2 \left(6f_1 + \frac{f_2}{2} - 4f_3\right) + H \left(16 \dot{f}_1 + \frac{9}{2} \dot{f}_2\right) + 6H(f_1 - f_3) - \frac{16\pi^2}{3}|b| (H^2 - H)\right] \dot{h}
- (4f_1 + f_2) \frac{\nabla^2 \dot{h}}{a^2}
+ \left[2H(2\dot{f}_1 - 3\dot{f}_3) - \frac{21}{2} H \dot{H} (f_2 + 4f_3) - \frac{3}{2} \dot{H} (f_2 + 4f_3) + 3H^2 \left(4\dot{f}_1 + \frac{1}{2} \dot{f}_2 - 4\dot{f}_3\right) - 9H^3(f_2 + 4f_3) + H \left(4\dot{f}_1 + \frac{3}{2} \dot{f}_2 + \frac{3M_p^2}{4}\right)\right]
+ \frac{16\pi^2}{3} |b| (H + HH - 3H^3) \dot{h} - [H(4f_1 + f_2) + 4\dot{f}_1 + \dot{f}_2] \frac{\nabla^2 \dot{h}}{a^2}
+ \left[\frac{16\pi^2}{3} |b| (2\dot{H} + 12HH + 9H^2 - 6H^2H - 15H^4) + \frac{M_p^2}{2} (2\dot{H} + 3H^2) - 4H\dot{H} (8\dot{f}_1 + 9\dot{f}_2 + 30\dot{f}_3) - 8\ddot{H} (\dot{f}_1 + \dot{f}_2 + 3\dot{f}_3) - H^2 (4\ddot{f}_1 + 6\ddot{f}_2 + 24\ddot{f}_3)
- 4H (\dot{f}_1 + \dot{f}_2 + 3\dot{f}_3) - H^3 (8\dot{f}_1 + 12\dot{f}_2 + 48\dot{f}_3)
- (36\dot{H}H^2 + 18H^2 + 24HH + 4\ddot{H}) (f_1 + f_2 + 3f_3)\right] h
+ \left[2 \left(2H^2 + H\right) (f_1 + f_2 + 3f_3) + \frac{1}{2} H (4\dot{f}_1 + \dot{f}_2) + \frac{M_p^2}{2} - \frac{1}{2} f_2\right]
- \frac{16\pi^2}{3} |b| (H + 5H^2) \frac{\nabla^2 \dot{h}}{a^2} + \left(2f_1 + \frac{1}{2} f_2\right) \frac{\nabla^4 \dot{h}}{a^4} = 0, \tag{100}
\]

stemming from the variation of the second-order Lagrangian function
\[
\mathcal{L} = \frac{M_p^2}{2} R + f_1 R_{\alpha\beta\mu\nu} + f_2 R_{\alpha\beta} + f_3 R^2 - \frac{4\pi}{3} \sqrt{|b|} \sigma \Box R + \frac{1}{2} \sigma \Delta \sigma, \tag{101}
\]

and we have set \( \rho = \rho_h \to 0 \) and \( \sigma_h \to 0 \) as the background depends only on time; the perturbation \( h(x, t) \) is the amplitude of the tensor mode \( h_{ij} \) for a given polarisation. In Eqs. (100) and (101), the coefficients \( f_1, f_2 \) and \( f_3 \) are time-dependent functions that take the values
\[
f_1 = a_1 + a_2 + \frac{|b| - \omega}{2\sqrt{|b|}} \sigma,
f_2 = -2a_1 - 4a_2 + \frac{\omega - 2|b|}{\sqrt{|b|}} \sigma,
f_3 = \frac{a_1}{3} + a_2 - \frac{3c - 2|b|}{36} + \frac{3|b| - \omega}{6\sqrt{|b|}} \sigma.
\]
By inspection of the combinations of $f$’s entering Eq. (100), one notes that the equation of motion does not depend on $a_2$, as expected from the fact that this comes from a surface term.

Eq. (100) was obtained by assuming the value (97) for the auxiliary field $\sigma(t)$ in terms of the background Hubble variable, and so can be used for any admissible solution for the scale factor, including the inflating case of (99). Expanding in Fourier modes, i.e. replacing $\nabla$ by $-k^2$, in principle permits to evaluate the gravitational wave stochastic spectrum in such a theory, with a catch: contrary to GR, the mode equation is no longer that of a parametric oscillator, so that its quantisation, and consequently the vacuum initial conditions, are not that well defined.

This issue, still under discussion, can be handled by assuming that our semiclassical framework provides a perturbation to GR, so that the extra (higher derivative) terms may be neglected while quantising in a regime in which one can manage to construct a consistent Hilbert space of state. Setting quantum vacuum fluctuation initial conditions exactly then allows setting initial values for the gravitational wave amplitude and its first three time derivatives.

Moreover, the presence of the higher derivative terms potentially implies instabilities. Setting initial conditions as discussed above, one finds [66, 67] that the time development, and hence the resulting predictions, is very sensitive to the properties of the background. Assuming, for instance, a de Sitter inflation phase with constant Hubble rate $H = H_{\text{inf}}$, initial trans-Planckian runaway solutions can be redshifted to become sub-Planckian and then rapidly damped by the expansion: the instabilities indeed present in the theory can end up harmless in a cosmological setup. We assume in what follows that this is indeed the case.

### 3.8 Primordial gravitational-wave background

Independently of the underlying quantum theory leading to the production of primordial tensor modes, one must now evolve them through the expanding universe to evaluate their current contribution. As we know GR to be valid for the most part of the FLRW evolution, we consider from now on that the higher derivative terms discussed above are either not present at all, or contribute only negligibly. In order to clearly distinguish classical from quantum effects, we include again the relevant factors of $\bar{h}$ when necessary.

In Sec. 3.6, we have laid out three equivalent ways to describe the evolution of perturbations for a general time-dependent background $a(\eta)$: the use of Bogoliubov transformations, mode functions and squeezing parameters. We now solve the dynamics of the gravitational wave field in a simplified model of the cosmological evolution to discuss the properties of the primordial gravitational waves generated and make a connection with observations.
3.8.1 Cosmological evolution

In FLRW the curvature of spacetime is contained in the scale factor $a$, whose dynamics is related to the matter content of the Universe through the Friedmann equations. In what follows, we first solve them in the standard approximation that there is always a single fluid dominating the energy budget of the Universe and that transitions between two phases are instantaneous. One can thus model the cosmological evolution as a succession of three eras: first an accelerated expansion phase for $\eta < \eta_r$, whose dynamics is that of a slow-roll inflation phase [68], then a radiation dominated phase for $\eta_r < \eta < \eta_m$ and finally a matter domination for $\eta > \eta_m$. For the sake of simplicity, we ignore the late-time accelerated expansion.

The evolution of the gravitational waves contained in the universe is controlled by Eq. (4) where the expansion enters through the scale factor $a(\eta)$ and its second derivative. Connecting the scale factor and its derivative continuously across the transitions, we have

$$
\frac{a(\eta)}{a_r} = \begin{cases} 
\eta r^{-1} & \text{for } -\infty \leq \eta \leq \eta_r, \\
\frac{\eta}{\eta_m} & \text{for } \eta_r \leq \eta \leq \eta_m, \\
\frac{\eta^2}{2\eta_r} & \eta \leq \eta_m,
\end{cases}
$$

(102)

where $\eta_r > 0$. The first expression in inflation is at first order in $\varepsilon = 1 - \dot{H}/H^2$ the first slow-roll parameter considered time-independent and we have also given the de Sitter limit $\varepsilon = 0$. From this, one computes the time-dependent part of the frequency $\omega_\varepsilon^2$ defined in Eq. (5)

$$
\frac{a''}{a} = \begin{cases} 
\frac{2 + 3\varepsilon}{4(2\eta_r - \eta)^2} & \text{for } -\infty \leq \eta \leq \eta_r, \\
0 & \text{for } \eta_r \leq \eta \leq \eta_m, \\
\frac{2}{\eta^2} & \eta \leq \eta_m,
\end{cases}
$$

(103)

Solving Eq. (4) with (103) yields reference mode functions in each era, namely

$$
u_k^{(\text{infl.})}(\eta) = \sqrt{-\frac{(\eta - 2\eta_r)}{4}} \frac{\eta^{(1)}_r}{2\eta_r} [-k(\eta - 2\eta_r)] \quad \text{for } -\infty \leq \eta \leq \eta_r,
$$

(104a)

$$
u_k^{(r)}(\eta) = \frac{e^{-ik\eta}}{2k} = u_k^{(m)}(\eta) \quad \text{for } \eta_r \leq \eta \leq \eta_m,
$$

(104b)

$$
u_k^{(m)}(\eta) = \frac{e^{-ik\eta}}{2k} \left(1 - \frac{i}{k\eta}\right) \quad \text{for } \eta \leq \eta_m.
$$

(104c)
where in the first line, $H^{(1)}_\kappa$ is the Hankel function of the first kind of index $\kappa$ and the approximation corresponds to the de Sitter limit. We refer to [69] for a recent textbook in which all details of the computations of the inflationary mode function can be found. Note that during radiation domination, the solution is given by the Minkowski mode function because $d'' = 0$. Since two solutions of (4) are related by a Bogoliubov transformation, a mode function solution of (4) for the whole cosmological evolution is related by a Bogoliubov transformation to the associate reference mode function (104c) in each era.

One can construct a global solution $u_k(\eta)$ starting in the inflationary period. The reference mode function there was chosen to match the Minkowski mode function $u_k^{(M)}$ in the asymptotic past $\eta \rightarrow -\infty$. This gives us an “in” region in which we can set the initial condition for the state of the system in terms of a well-defined particle content. We therefore pick $u_k(\eta) = u_k^{(M)}(\eta)$ during inflation. The expressions for the radiation and matter domination are then

$$u_k(\eta) = \begin{cases} 
\alpha_k^{(r)} u_k^{(r)}(\eta) + \beta_k^{(r)} u_k^{*(r)}(\eta) & \text{for } \eta_r \leq \eta \leq \eta_m, \\
\alpha_k^{(m)} u_k^{(m)}(\eta) + \beta_k^{(m)} u_k^{*(m)}(\eta) & \text{for } \eta_m \leq \eta,
\end{cases}$$

(105)

where the Bogoliubov coefficients are found by requiring that the mode function and its first time-derivative are continuous across the transition. Their expressions are worked-out in full in Ref. [45]. The mode $u_k(\eta)$ is then completely determined for both polarisations and, using (38), one achieves a fully quantum description of the evolution of the gravitational wave field.

The analysis is completed once one specifies the initial state of the gravitational waves as $k\eta \rightarrow -\infty$. The standard choice is to assume that, in the far past, the inflation phase somehow wiped out any initial perturbation, leaving no graviton to start with: this is the motivation behind choosing the vacuum state for every mode. This vacuum initial state is often referred to the Bunch-Davies vacuum [25], although it should be more appropriately be called Minkowski vacuum. This choice implies that the state of the perturbation consists of a collection of independent 2-mode squeezed states as discussed in Sec. 3.4.

For scalar perturbations, the above vacuum choice turns out to be in excellent agreement with the observations of the Cosmic Microwave Background [70]. For gravitational waves, we are so far short of equivalent observations so that other states could be chosen as initial condition [71]. Although such alternative choices do not modify our description of the subsequent evolution, they change the values of the Bogoliubov coefficients and therefore the prediction on the amplitude of gravitational waves or, equivalently, the number of gravitons produced.

We have explained in Sec. 3.6 that, most of the time, this number is ambiguous due to the time-dependent part of $\omega^2_k$. Let us explain how to make sense of it for primordial gravitational waves. First, in the sub-Hubble regime $k^2 \gg a''/a$ the frequency reduces to $\omega_k \sim k$ i.e. the mode $k$ does not feel the expansion of space and effectively oscillates as in flat spacetime. In this sub-Hubble limit, the reference mode functions (104c) reduce to the Minkowski one, and we can treat the mode as if
evolving in Minkowski. On the other hand, in the super-Hubble regime $k^2 \ll a''/a$, the mode behaves as an inverted harmonic oscillator $\omega_k \sim -a''/a < 0$. One therefore expects its amplitude to be amplified, and it is indeed where most of the squeezing happens, as illustrated in the first two panels of Fig. 5.

The evolution (103) of the time-dependent piece $a''/a$ is plotted in Fig. 4 and is compared to the square of the comoving frequencies of two different modes $k_s^2$ and $k_l^2$. Note that at the beginning of inflation and during the radiation era, since $a'' = 0$, all modes are sub-Hubble and effectively living in Minkowski there$^{12}$. This second aspect is due to our simplistic modelling of the transition in Eq. (102). In a realistic cosmological model, $a''$ is continuous and part of the modes progressively reach the sub-Hubble regime. In Fig. 4, the mode $k_s$ has a short wavelength and is always sub-Hubble. It is not affected by the amplification process. The mode $k_l$ has a larger wavelength and becomes super-Hubble during inflation after $\eta_{k,1}$, is insensitive to the expansion during radiation domination, becomes super-Hubble again during matter domination, until $\eta_{k,2}$ where it settles in the sub-Hubble regime. The modes of interest for cosmological observations are of the second type (or become and stay super-Hubble during radiation domination).

The picture that we have just sketched for these modes, putting aside radiation domination, is reminiscent of the idealized situation described in Sec. 3.6 where the “in” region corresponds to $\eta \ll \eta_{k,1}$ and the “out” region to $\eta \gg \eta_{k,2}$. For such modes, we are thus justified in talking about graviton production.

---

$^{12}$ Recall that in this limiting case, the relation between the dominant term in the frequency and the wavelength size compared to the Hubble radius does not hold. One cannot, strictly speaking, employ the terminology sub or super-hubble here.
Two remarks are in order here. First, modes progressively reenter the Hubble radius during the neglected current accelerated expansion. For the modes of interest here, this is of no consequence. Second, one should be careful when discussing modes responsible for the B modes of polarisation in the CMB since some of them had not yet reached the sub-Hubble regime when generating polarisation.

To close this discussion, we compute the relevant quantities describing the gravitons in the different formalisms. For simplicity we only consider an inflationary period where most of the amplification occurs. For this estimate, we neglect slow-roll corrections and model inflation by a period of de Sitter expansion ending at $\eta_r$. After the transition to radiation domination, the mode does not feel the expansion any more, so that its particle content can be computed. In de Sitter, the covariance matrix elements can be computed exactly using the mode function in Eqs. (104c).

We evaluate them at $\eta_r$ [37]

$$
\gamma_{11} = 1 + \frac{1}{k^2 \eta_r^2} \approx e^{2N}, \quad \gamma_{12} = -\frac{1}{k \eta_r} \approx e^{N}, \quad \gamma_{22} = 1. \quad (106)
$$

where, since we are considering a mode which is in the super-Hubble regime during inflation, we have taken the limit $k \eta_r \ll 1$. These last expressions are given in terms of the number of $e$-folds $N$ defined by

$$
N = \ln \left[ \frac{a(\eta)}{a(\eta_{k})} \right] = \ln \left[ k (2 \eta_r - \eta) \right]
$$

where $a(\eta_k)$ is the scale factor evaluated at Hubble crossing time $k (2 \eta_r - \eta_k) = 1$.

At this point, one notes that

$$
\langle \left( \hat{\mu}_{\lambda, k} \hat{\mu}_{\lambda, -k} \right)^2 \rangle \propto \gamma_{22} / a^2(\eta),
$$

so that, for a super-Hubble mode, it decays exponentially during inflation. The fact that the matrix element $\gamma_{11} = 2k \langle \left( \hat{\mu}_k^R \right)^2 \rangle$ grows faster than $\gamma_{12}$ and $\gamma_{22}$ leads to squeezing in a direction close to that of the $\mu_k^R$ axis. This can be verified by computing explicitly the squeezing parameters: inverting Eq. (66), we deduce the squeezing parameters as

$$
r_k = \text{arcsinh} \left( \frac{1}{2k \eta_r} \right), \quad \phi_k = \frac{\pi}{2} - \frac{1}{2} \text{arctan} \left( 2k \eta_r \right), \quad (107)
$$

which, in the super-Hubble limit, yields

$$
r_k \approx \ln \left( \frac{1}{2k \eta_r} \right) \approx N, \quad \phi_k \approx \frac{\pi}{2} - k \eta_r \approx \frac{\pi}{2} - e^{-N}. \quad (108)
$$

$\phi_k \to \pi/2$ so that indeed the ellipse will be squeezed in a direction close to $\mu_k^R$.

For scales of cosmological interest, one typically expects $N = \ln (k \eta_r) \approx 50$ at the end of inflation so that $r \approx 50$. This is to be compared with the best quantum optics experiments where one can hardly achieve $r \approx 2$; the squeezing is extreme [72]. The resulting evolution of the Wigner function is plotted for a few $e$-folds after Hubble exit in Fig. 5 where the very large squeezing is manifest.

Finally, we compute the number of particles created and their pair correlation: Eq. (78b) in the de Sitter and super-Hubble limits gives
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Fig. 5 Phase space ellipse in the plane \((k^{3/2} \mu_s^k, k^{-1/2} \pi_k^k)\) at different instants during inflation, labelled by \(N = \ln[a/a(\eta_k)]\), i.e. the number of e-folds measured from the Hubble-crossing time of the mode under consideration. On sub-Hubble scales, the ellipse remains roughly a circle, while it gets squeezed and rotates in the super-Hubble regime.

\[
n_k = \frac{1}{4k^2 \eta^2} = \frac{e^{2N}}{4}, \quad (109)
\]

\[
c_k = \frac{1}{4k^2 \eta^2} - \frac{i}{2k \eta} \approx \frac{e^{2N}}{4}. \quad (110)
\]

The number of pairs and their correlation grow at the same rate; squeezing necessarily creates entangled pairs. After 50 e-folds of inflation, one finds \(n_k \sim 10^{43}\). This number might appear very large, but the physical field \(h_{ij}\) is diluted by the inverse of the scale factor that will keep acting even when the creation process stops, following Eq. (3). In addition, the number of gravitons is not directly observable; we observe gravitational waves or their imprint on other fields, e.g. the electromagnetic field in the CMB, but not individual gravitons. One therefore needs to compute the physical quantities that are more directly relevant in forecasting future observations.

3.8.2 Connection to observations

There is hope that observable signatures of these primordial gravitational waves will be found either in the B-modes of the CMB or directly in future gravitational wave interferometers. We refer to Ref. [73] or Chapter 19, 20 and 23 in Ref. [33] for a detailed account. The waves we have described are stochastic in nature owing
to their quantum origin. They account for part of the stochastic gravitational-wave background (SGWB), the rest being produced by unresolved astrophysical sources or possibly other high-energy phenomena such as topological defects. The SGWB is usually assumed to be statistically homogeneous and isotropic, as the FLRW background metric, Gaussian, either due to the sum of a large number of independent sources or because it is sourced by a Gaussian state as considered here, and unpolarised (same content in both polarisations and polarisations are uncorrelated)\(^\text{13}\) because there is no significant source of parity violation in the Universe \[73\]. All these assumptions only have to be made on the initial state as the dynamics is the same for both fields \(\mu_{\lambda}^{\mu}\) and preserves isotropy and homogeneity. They are in particular satisfied for primordial gravitational waves produced from the Bunch-Davies vacuum. A typical quantity used to characterize a stochastic ensemble of waves is their power spectrum which, within the gaussianity assumption, contains all the information. The power spectrum \(\mathcal{P}_T\) of gravitational waves \(h_{ij}\) at time \(\eta\) is then defined (working classically for the moment) by

\[
\langle \mu_{\lambda} (k, \eta) \mu_{\lambda'}^{\mu} (k', \eta) \rangle = \frac{\pi a^2(\eta)}{16 G_N k^2} \delta^{(3)}(k-k') \delta_{\lambda,\lambda'} \mathcal{P}_T(k, \eta),
\]

where the Dirac delta comes from homogeneity, and \(\mathcal{P}_T\) only depends on \(k\) since the background is isotropic and unpolarised. The index “\(T\)” stands for “tensor”, to differentiate the latter from the scalar power spectrum \(\mathcal{P}_S\). Using (3), (15) and the orthogonality relations of the tensors below (16), one finds the two-point correlation function of the Fourier coefficients of \(h_{ij}\)

\[
\langle h^{ij}(k, \eta) h^{ij}_*(k, \eta) \rangle = \delta^{(3)}(k-k') \frac{4 \pi^2}{k^3} \mathcal{P}_T(k, \eta),
\]

as well as the two-point correlation of \(h_{ij}\) in real space, namely

\[
\langle h^{ij}(x, \eta) h_{ij}(x, \eta) \rangle = 2 \int \ln(k) \mathcal{P}_T(k, \eta).
\]

The power spectrum \(\mathcal{P}_T(k, \eta)\) corresponds to the typical squared amplitude of the wave, per logarithm of \(k\), and per polarisation, at the time \(\eta\). For perturbations made of sub-Hubble modes \(k \gg |\mathcal{H}|\), the time dependent term of (4) can be neglected and the energy density of gravitational waves reads\(^\text{14}\)

\[
\rho_{GW} = \frac{1}{32 \pi G_N} \langle h^{ij}(x, \eta) h_{ij}(x, \eta) \rangle.
\]

---

\(^{13}\) It can be checked using (17) that the assumptions that the waves are both unpolarised \(\langle \mu, \mu_* \rangle = \langle \mu, \mu_* \rangle\) and that polarisations uncorrelated \(\langle \mu, \mu_* \rangle = 0\) in terms of the \(+, -\) helicity basis is equivalent to the same two assumptions on the \(+, \times\) basis.

\(^{14}\) Averaging is necessary even for a deterministic source of gravitational waves to make sense of their energy. The averaging can either be performed over a certain volume or a certain duration, see \[33\]. In the context of this review, the averaging in (112) refers to an ensemble average.
For sub-Hubble modes, $h_{ij}(k, \eta) \propto e^{i(kx - k\eta)/a(\eta)}$ so that neglecting terms in $\mathcal{H}$ with respect to $k$ we get

$$\langle h^{ij}(k, \eta) h_{ij}(k, \eta) \rangle \approx k^2 \frac{\langle h^{ij}(k, \eta) h_{ij}(k, \eta) \rangle}{a^2(\eta)}.$$  \hfill (113)

Note that, since $h_{ij}$ dilutes as $a^{-1}$, $\rho_{GW}$ dilutes as $a^{-4}$, i.e. sub-Hubble modes dilute as standard radiation. Expanding the energy density in Fourier space and normalising by the critical energy density $\rho_c = \frac{3H^2}{8\pi G_N}$, we get the energy fraction per logarithm of $k$ that is directly expressed as a function of the power spectrum

$$\Omega_{GW}(k, \eta) = \frac{1}{\rho_c} \frac{d\rho_{GW}}{d\ln k} = \frac{k^2}{6H^2 a^2(\eta)} \mathcal{P}_T(k, \eta).$$  \hfill (114)

The power spectrum (111) and the energy density fraction (114) are the two quantities customarily used to assess the observability and constrain the models of primordial gravitational waves. More precisely, we often estimate the primordial power spectrum, i.e. the power spectrum at the beginning of radiation domination. The rest of the evolution is encoded in so-called transfer functions; these can be estimated using the previous computations. For actual comparison with observations, they have to be computed numerically by solving Boltzmann-like equations.

Let us then evaluate the primordial power spectrum by considering only the initial phase of single field slow-roll inflation in the cosmological evolution Eq. (102) and assuming Bunch-Davies vacuum for both polarisations $\pm$. Using (38), the power spectrum is straightforwardly expressed in terms of the mode function for $\hat{\mu}_k$

$$\mathcal{P}_T(k, \eta) = \left| \frac{32G_N k^3}{\pi a^2(\eta)} \right|^2 \left| \hat{\mu}^{(\text{infl.})}_k(\eta) \right|^2.$$  \hfill (115)

Making use of (104c) and expanding all the quantities at first order in the slow-roll parameter $\varepsilon$, we get

$$\mathcal{P}_T(k, \eta) = H_k^2 (1 - 2\varepsilon) \left| -k(\eta - 2\eta_r) \right|^{3 + 2\varepsilon} \left| H_r^{(1)}[-k(\eta - 2\eta_r)] \right|^2,$$  \hfill (116)

where $H_k = H(\eta_k)$ and $\eta_r$ is the Hubble crossing time $k/a(\eta_k) = H(\eta_k)$. This time is often taken in the super-Hubble limit $|k(\eta_k - 2\eta_r)| \ll 1$ relevant for cosmological scales. We get

$$\mathcal{P}_T(k, \eta) = \frac{2H_k^2}{\pi} \left[ 1 + 2(1 + \log 2 + 2 + \gamma_e) \varepsilon(\eta_k) \right],$$  \hfill (117)

where $\gamma_e$ is the Euler-Mascheroni constant. The exact magnitude of (117) depends on the values of $\varepsilon$ and $H$ at Hubble crossing, which are model-dependent quantities.

Current experiments have not been able to detect the primordial gravitational-wave background but the combined (non)-observations of Planck and BICEP experiments allow us to put bounds on the tensor-to-scalar ratio in single-field slow-roll
inflation [74]. A discussion of its potential observability in future gravitational wave interferometers and with future CMB experiments can be found in [73, 75, 76]. Notice that different models of the very early universe would change the prediction (116): initially excited states [71], temporary departures from the single field slow-roll scenario [77] or coupling with extra fields [78] might for instance be able to generate larger signatures than single-field slow-roll inflation, while modifications of gravity in the high energy regime could also lead to changes in the spectrum at high frequencies, e.g. through introduction of a cut-off in theories of lower dimensionality in the ultraviolet [79]. Finally, we want to emphasise that the toy model of cosmological evolution of Eq. (102) makes the unrealistic assumption of an instantaneous reheating. Adding a period of reheating is known to significantly modify the resulting spectrum, e.g. the frequency at which it starts to decay, thereby modifying observational perspectives [80].

3.8.3 Quantum origin of the primordial gravitational waves

To close this part, we want to comment on how quantumness enters the prediction (116).

First, a subtle point hidden in (111) is the meaning of the averaging $\langle \rangle$. In the discussion of the dynamics of perturbations, we have been computing averages in the sense of expectation value for observables in a given quantum state. It is a basic assumption of quantum mechanics that this would be the expected average value of the physical quantity after repeated measurements of it when the system is prepared in the same state. Unfortunately, we only have one realisation of the history of the Universe. Yet, using statistical isotropy, we can treat each (sufficiently large) patch of sky as an independent realisation of the same underlying random process and compute average values over this ensemble of patches. Under an ergodicity assumption, the resulting correlation functions can then be compared to (116), a procedure applied to CMB data analysis [81]. Additional arguments to justify trading quantum averages for classical ones will be discussed in Sec. 4.

Second, as we repeatedly emphasised, since the linear evolution is the same in the classical and quantum settings, the quantum aspect has to be confined to the choice of initial state. The result (116) reflects the choice that the waves emerged from initial vacuum fluctuations. For primordial gravitational waves, we are short of observational data to test this prediction. Still, if we were to insist on having a purely classical treatment, then a classical vacuum of gravitational waves, i.e. $a_{\pm \mathbf{k}}(\eta_m) = 0$ would persist throughout the evolution. There would simply be no primordial gravitational waves. On the contrary, initial gravitational waves would be classically amplified by cosmological expansion, but we then have to motivate a specific choice for the initial distribution of perturbations. For scalar perturbations, the CMB observations already demonstrated a tremendously good agreement with the predicted power spectrum $P_\mathcal{S}$ of initial vacuum fluctuations for the modes observed [74, 82]. Giving up on a quantum treatment in the inflationary paradigm would then require providing an ad hoc classical theory that yields the same initial conditions as the
quantum vacuum. We could therefore argue that observations of the scalar sector give indirect proof that gravitational degrees of freedom should be quantised.

Yet, third, it is sometimes argued see e.g. [33, 83], that the verification of the prediction (116) would provide additional insights on the quantum aspect of gravity with respect to the observation of the scalar perturbations. In the treatment of scalar perturbations in single-field slow-roll inflation, the appropriate gauge-invariant variable is the Mukhanov-Sasaki (MS) field related to the perturbations of the inflaton $\delta \phi$ and the gravitational potential $\Psi$ through

$$v_{\text{MS}} = \frac{z}{\kappa} \left( \Psi + \mathcal{H} \frac{\delta \phi}{\phi_0} \right),$$  \hspace{1cm} (118)

where $z = a \sqrt{2 \varepsilon}$, $\varepsilon$ being the first slow-roll parameter, $\phi_0$ the homogeneous background inflaton field and $\kappa$ the reduced Planck mass. This is a scalar field whose Lagrangian is the same as (22) upon substituting $a \rightarrow z$, and up to normalisation. The MS field is then quantised in exactly the same manner as the two polarisations of the graviton and the power spectrum evaluated by initially choosing the Bunch-Davies vacuum. However, in the absence of perturbations $\delta \phi$ for the scalar field, the equation of motion of the scalar part of the metric perturbations show that they can be set to zero. This is the so-called synchronous gauge [84]. The existence of scalar perturbations then requires the presence of the scalar field $\delta \phi$ and is not intrinsic to the gravitational degrees of freedom. Even when $\delta \phi \neq 0$, in the synchronous gauge $\Psi = 0$ and only the scalar field contributes to the perturbations. In this gauge, the whole quantification process and evaluation of the power spectrum only deals with the physics of a quantum scalar field that is not related to gravitational degrees of freedom. This could therefore cast some doubt on whether some gravitational degrees of freedom were even quantised in the first place. Such ambiguity does not exist when dealing with gravitational waves. In the absence of any anisotropic stress, the gravitational waves persist, and the quantisation procedure is undeniably a perturbative quantisation of the gravitational field. Verification of (116) would then be an indirect observational proof that the gravitational field must be quantised.

Finally, to mitigate the above discussion, let us also mention an argument against our line of reasoning, as discussed, e.g. in Ref. [35]. The argument made above can be reversed, as one can also find a gauge in which the perturbation of the field vanishes altogether, with $\delta \phi = 0$, while the metric part is $\Psi \neq 0$; in this gauge, the quantisation is then over an element of the metric only. In addition, since perturbations of matter and geometry appear on each side of Einstein equations (however, note that their quantum counterpart is unknown), it is inconsistent to quantise only one degree of freedom. The observational verification of the prediction for the scalar power spectrum thus can be argued to be an indirect proof that the gravitational field should be quantised.
4 Quantum features in primordial gravitational waves?

Given the quantum origin of primordial gravitational waves, it may seem natural to wonder about their state’s quantum or classical character at present. While it is expected that we will never be able to detect the signal produced by a single graviton [85], a discrete spectrum of excitations is not the only specific feature of a quantum theory. For instance, entanglement is a statistical quantum feature that can be experimentally verified using Bell inequalities [86, 87]. The exciting possibility that primordial gravitational waves exhibit such features has been investigated since this idea was first put forward by Grishchuk and Sidorov in [30]. These discussions have gradually introduced many concepts borrowed from low-energy quantum physics, particularly quantum optics: squeezing, quasi-probability distribution, decoherence, quantum discord. In this section, we will review this line of research following a historical approach and trying to show the progress brought by each contribution.

This section is structured as follows. First, arguments based on the very squeezed character of the state are used to justify a classical treatment to compute cosmological observables [45]. This approach, sometimes called “decoherence without decoherence” [39], and its critics are reviewed in Sec. 4.1. It turns out, however, that the classicality identified by these works does not do away with all the quantum features of the state; the state of the perturbations could for instance violate a Bell inequality [88]. We review these “quantum information” approaches in Sec. 4.2. Lastly, taking into account the weak interactions of the perturbations is necessary as they would induce decoherence which might erase the quantum features exhibited at the linear level. This aspect is reviewed in Sec. 4.3.

For the most part, these works are based on analysing the state of a quantum scalar field, which can either represent the MS field of scalar perturbations or one of the polarisations of the tensor perturbations. The mechanisms and arguments being the same for both, we do not distinguish when citing works which refers to which and are only specific when necessary.

4.1 Classicalisation of perturbations without decoherence

In [30], the authors argue that the perturbations exhibit non-classical features due to the fact that the relevant quantum state is strongly squeezed. In order to make the discussion precise yet simple, we focus again on the inflationary period modeled by a de Sitter phase of expansion and assume initial Bunch-Davies vacuum [15]; the relevant equations were derived at the end of Sec. 3.8.1, and the squeezing is shown in Fig 5.

One of the arguments developed in [30] is that the trajectory in phase space of a classical system with given initial conditions is represented by a point moving on a single curve. The situation is different for a quantum system. Due to the intrinsic

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15 The reasoning can also be extended to certain non-vacuum initial states [89].
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uncertainty stemming from the Heisenberg principle, the trajectory is represented by a moving surface. The quantum state that comes closest to mimicking a classical trajectory would then be a coherent state. Indeed, its trajectory in phase space is represented by a circle moving along a single curve: the system is located within a tube of minimal uncertainty around the classical trajectory. On the contrary, the surface representing an increasingly squeezed state is stretched around its centre delocalising the position of the system away from any single curve. Therefore, they argue, a very squeezed state like that of the cosmological perturbations is a very quantum state.

In a couple of works written in response [45, 39], the authors reproduce and complement the computations made in [30], but give a different interpretation of the result. The gist of their arguments, which we reproduce below, is that the properties of a system in an extremely squeezed state are indistinguishable from that of a classical system whose state is represented by a classic stochastic distribution; an argument borrowed from [90]. In other words, although the intrinsic quantum uncertainty on the outcome of a measurement dramatically spreads due to the evolution of the system, this uncertainty cannot be distinguished from a purely classical one. To demonstrate this, let us consider the wavefunction of the perturbations in the modes $\pm k$ decomposed in the $\mathcal{R}/\mathcal{I}$ sector and given by Eq. (63). Discarding the indices “$k$”, we recall that this is the wavefunction of a 1-mode squeezed state. We can show that for large $r$, it satisfies very well the conditions of the WKB approximation. For a general wavefunction $\Psi(\mu) = C(\mu) \exp[iS(\mu)/\hbar]$ the WKB approximation is valid when the amplitude $C$ varies slowly compared to the phase $S$: $|\partial S/\partial \mu| \gg |C^{-1}\partial C/\partial \mu|$. Since the WKB approximation is generally understood as a semi-classical limit, this property is sometimes referred to as the “WKB-classicality” of the state. Using the wavefunction (63), we have

$$C(\mu) = \left(\frac{1}{\pi \gamma_1}\right)^{1/4} e^{-\frac{i\mu^2}{2\gamma_1}},$$

$$S(\mu) = k\mu^2 \frac{\gamma_2}{2\hbar \gamma_1},$$

where we have dropped the exponent $S$ and the index $k$ for simplicity. We get

$$\left| \frac{C}{\partial C/\partial \mu} \frac{\partial S/\partial \mu}{\hbar} \right| = |\sin(2\varphi_k) \sinh(2r_k)|.$$  

(120)

In the de Sitter case, using Eq. (107), one has $\sin(2\varphi_k) \sinh(2r_k) \approx e^N$; the condition is perfectly satisfied. We then compute the action of $\hat{\mu}$ and $\hat{\pi}$ on such a state

$$\hat{\mu}\Psi(\mu) = \mu \Psi(\mu),$$

$$\hat{\pi}\Psi(\mu) = -i\hbar \frac{\partial \Psi}{\partial \mu} = \frac{\partial S}{\partial \mu} \left(1 - i\hbar \frac{\partial C/\partial \mu}{C\partial S/\partial \mu}\right) \Psi(\mu) \approx \frac{\partial S}{\partial \mu}(\mu) \Psi(\mu),$$

(121a)  

(121b)
where in the last line we have used Eq. (120). This last equality suggests that, neglecting sub-dominant contributions, we could attribute an unambiguous value to the “momentum” $\pi$ through the relation $\pi \approx \partial S / \partial \mu$ [45] while the value of the position $\mu$ would be controlled by the probability distribution given by the $\mu$-representation of the wavefunction, namely

$$P(\mu) = C(\mu)^2 = \left( \frac{k}{\pi \hbar \gamma_1} \right)^{1/2} e^{-\frac{\mu^2}{2\gamma_1}}.$$ (122)

To make this intuition rigorous, which is not always possible as we explain at the end of the section, we have to use a phase space representation of the state. The Wigner function $W^S(\mu, \pi)$ can be factorised

$$W^S(\mu, \pi) = \sqrt{\frac{k}{\pi \hbar \gamma_1}} e^{-\frac{\mu^2}{2\gamma_1}} \sqrt{\frac{\gamma_1}{k\pi \hbar}} e^{-\frac{\gamma_1}{2\gamma_2} (\pi - \frac{\gamma_2}{\gamma_1} k\mu)^2},$$ (123)

where the relation $\det(\gamma) = \gamma_{11} \gamma_{22} - \gamma_{21}^2 = 1$ (we are using a pure state) was used. The first piece is the probability distribution (122). The second piece controls the value of $\pi - \gamma_2 k\mu / \gamma_1 = \pi - \partial S / \partial \mu$, i.e. the difference between the actual value of $\pi$ and that attributed to it following the WKB-classicality approach. It can be read out from the above, or shown by a straightforward computation using covariance matrix elements, that

$$\left\langle \left( \pi - \frac{\gamma_2}{\gamma_1} k\mu \right)^2 \right\rangle = \frac{k}{2} \frac{1}{\gamma_1} \approx \frac{k}{2} e^{-2N},$$ (124)

where we have taken the super-Hubble limit in the last equality. Since the state is Gaussian, and $\hat{\pi}, \hat{\mu}$ are centred, this is the only quantity that controls the error induced by replacing $\hat{\pi}$ by its WKB counterpart $\gamma_2 k\mu / \gamma_1$ in the expectation values. As inflation proceeds, this error becomes exponentially small while the fluctuations of $\hat{\mu}$ get exponentially large, and that of $\gamma_2 k\mu / \gamma_1$ tends to a constant. Therefore, to compute the expectation value of any operator which is a polynomial in $\hat{\pi}$ and $\hat{\mu}$, one can safely make the WKB replacement. We emphasise that, to have meaningful operators, the coefficients of these polynomials must not depend on the state of the system. In such polynomials, when expanding $\hat{\pi}$ as $(\hat{\pi} - \gamma_2 k\mu / \gamma_1) + \gamma_2 k\mu / \gamma_1$, the coefficients of $\hat{\mu}$ and $\hat{\pi}$ cannot conspire to yield an expression depending only on the subdominant combination $\hat{\pi} - \gamma_2 k\mu / \gamma_1$ since it explicitly depends on the squeezing parameters. The translation of this approximation in terms of the Wigner function is to take the limit of infinite $r_k$, with $\gamma_1 \to \infty$, and to replace the Gaussian over $\pi - \partial S / \partial \mu$ by a Dirac delta [21, 45, 39]

$$W^S(\mu, \pi) \approx P(\mu) \delta \left( \pi - \frac{\gamma_2}{\gamma_1} k\mu \right),$$ (125)
The interpretation of this equation is straightforward: when computing expectation values using the Wigner function and Eq. (54), up to very sub-dominant contributions, we can replace $\pi$ by $\frac{\partial S}{\partial \mu}$ in the Weyl transform and take the average on $\mu$ using the classical stochastic variable of distribution Eq. (122). In the limit of Eq. (125), the contour levels of the Wigner function are squashed from ellipses to lines, and this implies that the size of the sub-fluctuant mode has been neglected. This line-like limit of the Wigner function is visible in the last panels of Fig. 5.

We conclude with a series of remarks on this result. First, it is clear that the replacement $\hat{\pi} \rightarrow \frac{\partial S}{\partial \mu}$ cannot be exact as it implies $[\hat{\mu}, \hat{\pi}] = 0 \neq i\hbar$, thus violating the canonical commutation relations, although those must be verified irrespective of the state of the system. Yet, the contribution of this non-vanishing commutator to the expectation value of operators $O(\hat{\mu}, \hat{\pi})$ which are polynomial in $\hat{\mu}$ and $\hat{\pi}$ is negligible.

The second remark is that, as explained in [72], we want to emphasise that the Wigner function of a WKB state does not in general give rise to a Dirac delta; in fact, it needs not even be positive everywhere. The naive intuition is only verified here because the state is also Gaussian. In addition, the fact that the Wigner function can be negative suggests taking with a grain of salt the idea that any WKB state is understandable as an approximate classical state.

Thirdly, as stressed in [83], the distribution (125) has some undesirable features for a Wigner function. For instance, computing the purity using the function (125) and Eq. (54) yields an infinite result. This is obviously incorrect since for any quantum state $p_k \leq 1$, and, in this pure case, we had derive earlier $p_k = 1$. Geometrically, by squeezing the ellipse to a line, one looses the information on the area that encodes the purity and the non-commutation of the variables through the Heisenberg uncertainty principle. This additionally informs us that there exist quantities of interest that crucially depend on the sub-leading contributions that were neglected, and so on the sub-fluctuant mode.

The fourth point we want to stress concerns classicality. The part of the argument based on analysing the phase space distribution does not actually require large squeezing to be formulated. Indeed, even before taking any limit, the Wigner function of the state is everywhere positive and obeys the classical equations of motion (59), so that using Eq. (54), any observable can be computed using a classical stochastic distribution.

As a fifth point, let us note that the above statement has to be made more precise because it hides several subtle points. To start with, as pointed out in [37], beyond quadratic order, the Weyl transform of an observable $O(\hat{\mu}, \hat{\pi})$ is, in general, not obtained by replacing the operators $\hat{\mu}$ and $\hat{\pi}$ by the corresponding phase space variables i.e. $O(\mu, \pi) \neq \tilde{O}(\mu, \pi)$. For instance

$$\tilde{\mu}_k^2 \tilde{\pi}_k^2 + \tilde{\pi}_k^2 \tilde{\mu}_k^2 = 2\mu_k^2 \pi_k^2 - \hbar,$$

so that, using Eq. (54)

$$\langle \mu_k^2 \pi_k^2 + \pi_k^2 \mu_k^2 \rangle = 2\mathbb{E}(\mu_k^2 \pi_k^2) - \hbar.$$


This extra $\hbar$ is a contribution of the commutator that the Wigner-Weyl formalism takes into account. Therefore, despite the Wigner function being everywhere positive and acting as a measure in Eq. (54), these terms introduce a slight difference with classical stochastic distributions. The culprit is the Weyl transform of the operators rather than the Wigner function. As argued above, in the large squeezing limit, these extra contributions to the Weyl transform of $\hat{\mu}$ and $\hat{\pi}$ are expected to become negligible. The second subtle point is precisely that these distortions will not become negligible for all observables so that the classicality argument does not apply to these. The fact that certain quantum features persist should not be a surprise since we have shown that the gravitons produced by the evolution remain in entangled pairs in the absence of other interactions [83].

The findings of this section can be summarised as follows: as long as we measure only $\hat{\mu}$ and $\hat{\pi}$, or observables which are polynomials of it, super-Hubble modes behave classically since their expectation values can be completely reproduced by a classical stochastic distribution [88, 37].

4.2 Quantum information approaches

It has to be mentioned that the authors of Ref. [45] do recognise the possibility that other operators would exhibit quantum features since squeezed states are known to possess such features in quantum optics experiments. However, they dismiss this possibility by arguing that, contrary to quantum optics, one can only perform measurements of the values of the fields $\hat{\mu}_k$ and $\hat{\pi}_k$ and not, say, of the number of particles $\hat{n}_k$. Therefore the ‘decoherence without decoherence’ argument is sufficient to claim that the perturbations are practically classical. Setting temporarily aside the question of their observability, we now derive examples of operators revealing non-classicality features in the state of primordial gravitational waves.

We have already mentioned that the purity of the state cannot be computed if the sub-dominant contributions of the non-vanishing commutators are dropped. In [91], the authors showed that in order to correctly compute the entropy of the state using the von Neumann entropy $S(\hat{\rho}) = -\text{Tr} [\hat{\rho} \log(\hat{\rho})]$ the sub-dominant contributions have to be restored. For a 2-mode mode squeezed state , the von Neumann entropy reads [92]

$$S(\hat{\rho}) = 2f [\det(\gamma)] ,$$

(128)

where the growing function $f$ is defined for $x \geq 1$ by

$$f(x) = \left( \frac{x+1}{2} \right) \log_2 \left( \frac{x+1}{2} \right) - \left( \frac{x-1}{2} \right) \log_2 \left( \frac{x-1}{2} \right) .$$

(129)

The entropy and purity are both controlled by the determinant of the covariance matrix, which requires the inclusion of sub-dominant contributions to be correctly
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evaluated. For the pure 2-mode squeezed state of perturbations, one gets \( \det(\gamma) = 1 \)
and the definition of \( f \) gives \( f(1) = 0 \), so we recover that the entropy vanishes.

We have so far only shown that, for certain operators, it is not appropriate to
ignore the sub-fluctuant mode. We now go further and exhibit quantities whose
values cannot be accounted for if the system is described by a classical stochastic
distribution. The prime example of such quantities is the combinations of expectation
values of spin operators entering the famous Bell inequalities [86]. To design
a Bell inequality, one has to exhibit a combination of operators \( C(\hat{O}_1, ..., \hat{O}_n) \) such
that, if the expectation values of the \( \hat{O}_i \)'s are described by a stochastic probability
distribution\(^{16}\), then \( C \) is bounded by a real number \( c \)

\[ C(O_1, ..., O_n) \leq c. \]  

As a consequence, if a quantum state is such that \( \langle C(\hat{O}_1, ..., \hat{O}_n) \rangle > c \), then we have
proven that not all expectation values of this state can be accounted for by a classical
probabilistic theory.

A necessary condition for a state to violate a Bell inequality is that it is not
separable [94]. A state \( \hat{\rho} \) of a system that can be partitioned in two subsystems \( A \) and \( B \) is said to be separable in this partition if its density matrix can be written as

\[ \hat{\rho} = \sum_i p_i \hat{\rho}_i^A \otimes \hat{\rho}_i^B, \]  

where \( p_i \geq 0 \) and \( \sum p_i \geq 0 \). Such a state can be constructed using a classical protocol
[94]. The interpretation of Eq. (131) is that \( p_i \) is the probability of finding the system
in the sector \( \hat{\rho}_i^A \otimes \hat{\rho}_i^B \) where the subsystems \( A \) and \( B \) are independent since the
density matrix is factorised. The correlations between the subsystems are thus con-
trolled only by the probabilities \( \{p_i\} \) and deemed classical. Non-separable states are
generally called \textit{entangled} states. In general, it is very difficult to determine whether
a state is separable. Fortunately, for Gaussian states, the Peres-Horodecki criterion
allows us to check separability using the covariance matrix elements only [95]. This
method was first applied to cosmological perturbations by Campo and Parentani in
[44]. We explain their result in the terms used in this review.

We first need to choose a partition of the system. The separable character of the
state or not depends on the subsystems considered; for a general discussion of the
notion of partition, see [46]. Using the vectors of conjugate operators introduced in
Sec. 3.5, we define a (bi)partition of the system by sorting the operators into two
vectors of smaller dimensions

\[ \hat{X} = \hat{X}_A \bigoplus \hat{X}_B. \]  

To represent the state of the perturbations we have used the \( R/I \) partition defined by
\( \hat{X}_{R/I} = (k^{1/2}\hat{r}_k, k^{-1/2}\hat{r}_k, k^{1/2}\hat{\mu}_k, k^{-1/2}\hat{\mu}_k) \) where the two subsystems decouple.
These operators will, however, mix the creation/annihilation operators (28) defining

\(^{16}\) The precise assumption is that their values are described by a local realistic theory. For a discus-
sion of this subtle and important point we refer to [93].
the modes $\pm k$. If we are interested in the correlations between these modes we have to build separate hermitian operators describing the mode $k$ and $-k$. This is readily done by considering

$$\hat{q}_{\pm k} = \sqrt{\frac{\hbar}{2k}} (\hat{a}_{\pm k} + \hat{a}_{\pm k}^\dagger) \quad \text{and} \quad \hat{p}_{\pm k} = -i \sqrt{\frac{\hbar k}{2}} (\hat{a}_{\pm k} + \hat{a}_{\pm k}^\dagger). \quad (133)$$

These operators define the $\pm k$ partition $\hat{X}_{\pm k} = (k_{1/2} \hat{q}_{k}, k_{1/2} \hat{p}_{k}, k_{1/2} \hat{q}_{-k}, k_{1/2} \hat{p}_{-k})$.

We compute the covariance matrix in this partition

$$\gamma = \begin{pmatrix} \gamma_k & \gamma_{-k} \\ \gamma_{-k} & \gamma_k \end{pmatrix}, \quad (134)$$

with

$$\gamma_k = \gamma_{-k} = \cosh(2r_k) \mathbb{I}_2 = \left( n_k + \frac{1}{2} \right) \mathbb{I}_2, \quad (135)$$

where $\mathbb{I}_2$ is the 2-dimensional identity matrix and

$$\gamma_{-k} = \gamma_{k} = -\sinh(2r_k) \begin{pmatrix} \cos 2\varphi_k & \sin 2\varphi_k \\ \sin 2\varphi_k & -\cos 2\varphi_k \end{pmatrix} = \begin{pmatrix} \Re e(c_k) - \Im m(c_k) \\ \Im m(c_k) - \Re e(c_k) \end{pmatrix}. \quad (136)$$

Unlike in the $R/I$ partition, this covariance matrix is not block-diagonal. It shows that the $k$ and $-k$ particles are correlated. The Peres-Horodecki applied to this covariance matrix reduces to [44]

$$\hat{\rho} \text{ separable in } \pm k \text{ partition } \iff |c_k| \leq n_k. \quad (137)$$

This criterion lends itself to a very simple interpretation, the state will be separable if and only if the correlation of the pairs is larger than their number. When is this satisfied? The condition (137) is straightforwardly expressed in terms of the squeezing parameters. We find that the state is separable if only if $e^{-r_k} \geq 1$, i.e. for the vacuum $r_k = 0$. Therefore, the primordial gravitons pairs $\pm k$ are always entangled. We have found a first quantum feature of their distribution. Notice that the same analysis could be repeated in the $R/I$ partition, but since these sectors are not correlated, it would trivially lead to the conclusion that the state is always separable in this partition. This illustrates clearly the dependence of the (non)-separable character of the state on the choice of subsystems.

The state of the perturbations we have considered so far is pure. It was shown that, for any entangled pure state, one can build a Bell inequality that the state violates [94]. The separability criterion is, in this case, sufficient. How can we find operators able to violate a Bell inequality for the gravitons? The considerations of Sec. 4.1 already demonstrated that, in order to reveal the quantumness of the distribution, we have to use operators which are non-polynomials in $\hat{\mu}^S_k$ and $\hat{\pi}^S_k$. In [96],
Revzen further introduces a distinction between what he calls proper and improper operators.

Proper operators are defined as those that cannot be used to violate a CSH-type Bell inequality when the Wigner function of the state is positive. He shows that any operator $\hat{O}$ whose Weyl transform $\tilde{O}$ takes values in the set of its eigenvalues is proper. Indeed, the Wigner function then provides an appropriate local hidden variable theory to describe its expectation values. Therefore, we have to use operators that do not fall in this category to build a Bell inequality that can be violated by primordial gravitational waves. In fact, these operators are not uncommon. Consider, for example, the number operator

$$\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k = \frac{k}{2\hbar} \hat{j}_k^2 + \frac{1}{2\hbar} \hat{p}_k^2 + \frac{1}{2}.$$  \hspace{1cm} (138)

It has a discrete spectrum, while its Weyl transform $\tilde{\hat{n}}_k = \frac{k}{2\hbar} \mu^2 + \frac{1}{2\hbar} \pi^2 + \frac{1}{2}$ is a continuous function of the phase space variables. In [44], Campo and Parentani were the first to exhibit Bell inequalities violated by cosmological perturbations. They emphasise the necessity to use non-polynomial operators in the field operator and they use as a building block the probability of finding the system in a certain 2-mode coherent state

$$Q(v, w) = \text{Tr} \left( \hat{\rho} \hat{N}_{k,-k} \right),$$

$$= \frac{1}{\Delta_k} \exp \left\{ - \frac{1}{\Delta_k} \left[ (n_k + 1) \left( |v|^2 + |w|^2 \right) - 2\text{Re}(c_k^*vw) \right] \right\},$$  \hspace{1cm} (139)

where $\Delta_k = (n_k + 1)^2 - |c_k|^2$ and $\hat{N}_{k,-k} = |v, k\rangle \langle v, k| \otimes |w,-k\rangle \langle w,-k|$ projects the subsystem $k$ (respectively $-k$) on the coherent state associated to $v \in \mathbb{C}$ (resp. $w \in \mathbb{C}$). The bounds given on $n_k$ and $c_k$ in Sec. 3.4 ensure that $\Delta_k$ is a positive quantity. This real and positive function of $v$ and $w$ is called the Husimi Q-representation of the state [98].

For the purpose of building a Bell inequality, it can be simplified by re-parametrising the arbitrary phase of $v$ to absorb that of $c_k$. We take $\text{arg} v = \text{arg} c_k$ so that $2\text{Re}(c_k^*vw) = 2|c_k|^2\text{Re}(v^*w)$. For a 2-mode squeezed state $|c_k| = \sqrt{n_k(n_k+1)}$ so that, upon rearranging,

$$Q(v, w) = \frac{1}{n_k+1} \exp \left( - \frac{|v|^2}{n_k+1} \right) \exp \left( - |w - v\sqrt{n_k/(n_k+1)}|^2 \right).$$  \hspace{1cm} (140)

Since the Husimi representation is also the expectation value of an operator, it can be used in a Bell inequality. The authors then use the Bell inequality demonstrated by [99] over $Q(v, w)$. 

17 Like the Wigner function, it is a phase-space representation of the state but using coherent states as a basis rather than eigenstates of the field operators. The authors discuss the quantumness of the perturbation using its properties and that of the related Glauber Sudarshan P-representation. They argue that the state not admitting a P-representation can be considered a non-classical feature. For brevity, we will not discuss these aspects here and refer to [44, 98] for details.
C(v, w) = [Q(0, 0) + Q(v, 0) + Q(0, w) - Q(v, w)] \left( \frac{n_k + 1}{2} \right) \leq 1. \hspace{1cm} (141)

They argue that C is maximal for w = -v in which case it only depends on |v|^2 and

\[ C_{\text{max}}(|v|^2) = \frac{1}{2} \left[ 1 + 2e^{-|v|^2} - e^{-2\left(1 + \sqrt{\frac{n_k + 1}{2}}\right)|v|^2} \right]. \hspace{1cm} (142) \]

One can show that, provided we are not in the vacuum n_k = 0, C_{\text{max}} is always larger than unity in the vicinity of v = 0, as illustrated in Fig. 7; the Bell inequality is violated. As expected, we have recovered the separability condition. In a later work [100], the authors proved that another inequality, built using operators, also defined in [101], that are complementary (in the sense that their sum is the identity) to the projectors ˆΠ_{kkk}, ˆΠ_{-kkk}, is violated. They also build other inequalities using the (GKM and Larsson) pseudo-spin operators in the same work. They explicitly show that all these operators belong to the subclass of improper operators identified by Revzen. Since the Weyl transform of the identity is just the number 1, we can infer from their complementary with the projectors ˆΠ_{kkk}, ˆΠ_{-kkk} that the operators ˆΠ_{kkk}, ˆΠ_{-kkk} also belong to this subclass.

We now introduce a last non-classicality criterion, the quantum discord. We start by giving the intuition behind its definition and reviewing some important properties. Technical details in definitions and proofs are skipped and can be found in [102, 103]. The idea of quantum discord is also to show that correlations between two subsystems are stronger than allowed classically. Two measures of the information attached to these correlations are introduced to that end. These measures are based on the von Neumann entropy, which, as we have shown, is highly sensitive to terms that can be neglected when computing field expectation values. The first measure is the mutual information

\[ J(A, B) = S(A) + S(B) - S(A, B), \hspace{1cm} (143) \]

where S(A, B) is the von-Neumann entropy of the full system while S(A) and S(B) are the entropies of the subsystems. The latter are defined by computing the entropy of the reduced density matrices when one of the subsystems is traced out, e.g. ˆρ_A = Tr_B( ˆρ) for the subsystem A. They are also called the entanglement entropy of the state. The second measure

\[ D(A, B) = S(A) - S(A|B), \hspace{1cm} (144) \]

where S(A|B) measure the information gained on A by measuring B. Its precise definition in the quantum setting must therefore include the system state after measuring the system B. It is obtained by minimising the density matrix residual entropy after having measured a complete set of projections on B, i.e. by maximising the information gain. For a quantum state, we then define the quantum discord as their difference

\[ D(A, B) = J(A, B) - J(A, B), \hspace{1cm} (145) \]
which is shown to be in general non-negative. The key observation is that, by the Bayes theorem, \( I \) and \( J \) coincide for a classical system so that the discord vanishes. A non-vanishing discord \( D(A, B) > 0 \) is therefore taken as a non-classical feature. As the other criteria introduced, the quantum discord depends on the choice of partition \( \mathcal{R} = \mathcal{R}_A \oplus \mathcal{R}_B \). However, it does not depend on the operators chosen to represent them, i.e. it is invariant under any change of operators within the sectors \( A \) and \( B \). We call such a quantity a local symplectic invariant. On the contrary, a Bell inequality is not necessarily a local symplectic invariant. A last important property of the discord is that, for a pure state, it reduces to the entanglement entropy \( D(A, B) = S(A) = S(B) \), and, for a pure state still, being entangled is equivalent to a non-vanishing entanglement entropy. Therefore, all criteria introduced (separability, Bell inequality, quantum discord) are equivalent for pure states. The cosmological perturbations must therefore have a non-vanishing quantum discord.

The quantum discord of cosmological perturbations was computed in [37] for the \( \pm k \) partition\(^{18} \). It reads

\[
D_{\pm k} = f \left[ \cosh \left( 2r_k \right) \right],
\]

where \( f \) was defined in Eq. (129). We immediately verify that the discord is non-vanishing provided that \( r_k > 0 \), i.e. that we are not in the vacuum. Taking the de Sitter limit of the above expression, we find \( D_{\pm k} \approx 2r_k / \ln 2 \approx 2N / \ln 2 \), the discord grows linearly with the number of e-folds.

The results of this section demonstrate that, as suspected, the primordial gravitational waves are only classical if we restrict our attention to field operators \( \hat{\mu} \) and \( \hat{\pi} \). We showed, using several criteria, that their state exhibits in principle quantum features: it is entangled, violates Bell inequalities and has a non-vanishing quantum discord. We additionally verified that these three criteria are equivalent for pure states like the 2-mode squeezed state considered here. Still, in any realistic model of the early Universe, this assumption of purity has to be given up. What has allowed us so far to simply consider a couple of modes \( \pm k \) of the field is that we have neglected all interactions of the gravitational waves, in particular their intrinsic non-linearities. We were justified in doing since the latter are weak. Yet, it is well known that even very weak interactions can lead to an erasure of non-classical features by inducing decoherence of the system. The most famous example of this is probably that a grain of dust whose spatial superposition would be turned into a classical superposition in a fraction of an instant simply by the scattering of photons from the CMB [105]. The importance of decoherence in the discussion of quantum features of cosmological perturbations was quickly realised [106, 107]. We now investigate how it affects the state, in general, and in particular the quantum features we have just exhibited.

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\(^{18}\) The quantum discord was already used in a work on cosmological perturbations in [104] but the author considered correlation of another nature, namely that of the perturbations and their environment.
4.3 Decoherence of cosmological perturbations

We start by briefly recalling some basic concepts of decoherence and refer to [108] for details. The 2-mode squeezed state of a coupled of modes ±\(k\) is a pure state represented by the ket (46). One can easily compute its density matrix and express it in the graviton 2-mode number basis

\[
\hat{\rho}_{2\text{MSS}} = \frac{1}{\cosh^2(2r_k)} \sum_{n,n'=0}^{\infty} \left[ -\tanh(2r_k) \right]^{n+n'} e^{2i(n-n')\phi_k} |n_k, n_{-k} \rangle \langle n_k', n'_{-k} | . \tag{147}
\]

The coefficients on the diagonal \(q_n = \frac{\tanh^{2n}(2r_k)}{\cosh^2(2r_k)}\) give a classical probability distribution over the 2-mode number states, while the non-diagonal reflects the quantum interferences between them. If we discard these terms, the density matrix reads

\[
\hat{\rho}_{\text{th}} = \frac{1}{\cosh^2(2r_k)} \sum_{n=0}^{\infty} \tanh^{2n}(2r_k) |n_k, n_{-k} \rangle \langle n_k, n_{-k} | . \tag{148}
\]

The state now represents a classical superposition of different number states with the same probabilities as \(\hat{\rho}_{2\text{MSS}}\). Such states are called statistical mixtures and are indeed mixed states (except if all coefficients but one vanish) since \(p_k = \sum_n q_n^2\) and \(q_n \leq 1\). The general idea of decoherence is that interactions of the system with a large number of unobserved degrees of freedom, referred to as the environment, precisely diagonalises the density matrix, driving the state to a statistical mixture. Equation (148) is actually the density matrix of a thermal state with, on average, \(n_k\) particles in both modes. Since it is fully diagonal, it is considered the result of a complete decoherence process. A very important point is that the (non)-diagonal character of the matrix depends on the basis, e.g. the matrix is originally diagonal in the 2-mode squeezed state basis. The basis in which decoherence makes the density matrix diagonal is called the pointer basis. Once again, we see that the choice of basis and operators to analyse the state of the system is crucial. For cosmological perturbations, several pointer basis were considered: coherent state basis [109, 44], field amplitude basis [110, 111, 106, 107], number basis [110], and others [112].

Ultimately, in a realistic model, the pointer basis is given by the eigenstates of the interaction Hamiltonian selected. The basis thus bears a double physical sense: it tells us for which type of measurements the system appears classical, e.g. measures of field amplitude or of number of particles, and also to which operators of the system is the environment sensitive. In their follow-up articles [106, 107] to [39], the group of authors (Kiefer, Lesgourgues, Starobinski, Polarski) considered the effect of decoherence. They argued that the correct pointer basis should be the field amplitude basis on the ground that self-interactions of pure gravity are local in the field basis.

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19 Notice that some of these, [111, 110], predate works referred to in the last section. Decoherence was, in fact, already investigated in the context of the early Universe before the argument of 'decoherence without decoherence' was made. It was especially used to try to make sense of the solutions of quantum cosmology, where both the background and the perturbations are treated as quantum fields [113].
i.e. $H_{\text{int}} \propto \hat{\mu}^n(x, \eta) \hat{\pi}^m(x, \eta)$. Since these interactions are contained in the Einstein-Hilbert action, they constitute a minimal and well-defined source of decoherence. They were then taken into account in a more realistic model of decoherence for the first time in [114, 115]. There, the system considered is made up of the observed large wavelengths while the environment is made-up of the rest of the short unobserved wavelengths like in stochastic inflation [116]. This approach was originally performed for scalar perturbations and was later generalised to tensor perturbations [117].

How is their influence on the state of $\pm k$ modes concretely accounted for? In [114, 115] the process is followed in time, rather than assumed to have completed [109, 118, 112], using a master equation. Earlier papers [111, 110] had also used an equivalent formalism, the Feynman-Vernon influence functional, but only in solvable toy models with two scalar fields interacting quadratically. The two formalisms were also used in [119], using the short-long wavelengths splitting and considering a quartic self-interaction of the scalar field. To derive a master equation, one starts by postulating that the couple system-environment evolves under a Hamiltonian

$$H_{\text{tot}} = \hat{H} \otimes \hat{I}_{\text{env}} + \hat{I} \otimes \hat{H}_{\text{env}} + g \hat{H}_{\text{int}},$$

where the Hamiltonian of interaction is taken to be an integral of a product of operators acting on the system and the environment

$$\hat{H}_{\text{int}} = \int d^3x \hat{A}(\eta, x) \otimes \hat{E}(\eta, x).$$

Under certain assumptions, essentially perturbative coupling and a “large” enough environment unperturbed by the action of the system, the von Neumann equation over the full density matrix $\hat{\rho}_{\text{tot}}$ can be reduced to a master equation over the reduced density matrix of the system $\hat{\rho} = \text{tr}_{\text{env}}(\hat{\rho}_{\text{tot}})$. Master equations became a standard tool to analyse the decoherence of cosmological perturbations and are very often considered to be of the Lindblad-type, e.g. [114, 115, 108, 120],

$$\frac{d\hat{\rho}}{d\eta} = -i [\hat{H}, \hat{\rho}] - g^2 \eta_c \int d^3x d^3y \langle \hat{E}(\eta, x) \hat{E}(\eta, y) \rangle [\hat{A}(x), [\hat{A}(y), \hat{\rho}]],$$

where $\eta_c$ is the auto-correlation time of the environment. This is a Markovian master equation; it assumes that the environment is effectively stationary with respect to the system, i.e. $\eta_c \ll \delta \eta$ where $\delta \eta$ is the typical time-scale of evolution of the system. In addition, the interaction term is often considered linear in the system field operators $H_{\text{int}} \propto (\alpha \hat{\mu} + \beta \hat{\pi}) \otimes \hat{O}_{\text{env}}$, where $\hat{O}_{\text{env}}$ acts only on the environment [39, 120]. It is the so-called Caldeira-Legget model [121]. Such interactions can also be identified as the dominant term when considering pure gravity [114, 117] and has the great advantage of preserving gaussianity and homogeneity. The result of the evolution can therefore be simply analysed by considering a Gaussian decohered homogeneous density matrix (GHDM). This class of state was introduced in [122, 44] to study decoherence finely, without having to assume any specific master equation, and still preserving a “partially” decohered state rather than assuming
from the on-set the density matrix diagonal. This class also encompasses the density matrices obtained by the common ansatz that its non-diagonal terms are suppressed by a Gaussian, e.g. [123, 100]. For all these reasons, we will in this section analyse the effect of decoherence using the GHDM and follow [44, 46].

To define the GHDM, we work in Fourier space. First, to avoid a preferred direction all 1-point correlation functions have to vanish. The Gaussian state is then completely characterised by its covariance matrix (58) made of 2-point correlation functions. By homogeneity, the only non-vanishing 2-point correlation functions involve $\mathbf{k}$ and $-\mathbf{k}$, and we can work with a single couple of modes $\pm \mathbf{k}$. A priori we have a $4 \times 4$ matrix, but, as mentioned below Eq. (63), homogeneity further imposes that the matrix is block diagonal in the $R/I$ partition. We are left with a $2 \times 2$ covariance matrix like that of Eq. (64). The state is then fully characterised by the three real covariance matrix elements $\gamma_{ij}$ in Eq. (65), or alternatively the number of pairs $n_k$ and their pair correlation $c_k$ (one complex and one real number) defined in Eq. (78b).

The only difference with the previous analyses is that the constraint imposed by the purity of the state $p_k = 1$ is now relaxed to $p_k \leq 1$, i.e. $\det(\gamma) = \gamma_{11} \gamma_{22} - \gamma_{12}^2 \geq 1$, or equivalently $|c_k| \leq \sqrt{n_k (n_k + 1)}$. Notice that these numbers can still not be arbitrarily chosen in order to keep a bona fide quantum state with purity bounded by one. Finally, to be able to have a simple geometrical representation, we can use the purity as an effective extra squeezing parameter and write [46]

$$\gamma_1 = p_k^{-1/2} \left[ \cosh (2r_k) - \cos (2\varphi_k) \sinh (2r_k) \right], \quad (152)$$
$$\gamma_2 = \gamma_2 = p_k^{-1/2} \sin (2\varphi_k) \sinh (2r_k), \quad (153)$$
$$\gamma_3 = p_k^{-1/2} \left[ \cosh (2r_k) + \cos (2\varphi_k) \sinh (2r_k) \right]. \quad (154)$$

One can check that this is a fully general parametrisation of a $2 \times 2$ symmetric matrix, that indeed $\det(\gamma) = p_k^{-2}$ and that for $p_k = 1$, we recover Eq. (66). How is the geometrical representation affected by this additional parameter? It is readily seen that the eigenvectors of $\gamma$ are unchanged, and its eigenvalues simply increased by $p_k^{-1/4} \geq 1$. The effect on the $\sqrt{2} - \sigma$ contour levels is thus simply a dilation by $p_k^{-1/4}$. This increased width of the Gaussian was already noticed as an effect of decoherence in [123] and before in a different context by [124]. An important remark is that the existence of a sub-fluctuant mode due to squeezing is not guaranteed anymore since the semi-minor axis is now of length $B_k = p_k^{-1/4} e^{-r_k}$ which can always be made larger than one, the vacuum value, provided that decoherence is strong enough at a given value of squeezing $r_k$. Fig. 6 illustrates the ellipse corresponding to the state in Fig. 3 after having lost purity to $p_k = 0.17$; there is no sub-fluctuant direction. We mention an alternative parametrisation, used in [44, 88], where the extent of the breaking of the relation between $n_k$ and $|c_k|$ is used to interpolate between a 2-mode squeezed state and a thermal state at fixed $n_k$. We define $\delta_k$ such that

$$|c_k| = (n_k + 1) (n_k - \delta_k). \quad (155)$$
\[ \delta_k = 0 \] is a 2-mode squeezed state and \( \delta_k = n_k \), the maximal value, is a thermal state. This parameter is easily related to the purity and the squeezing via

\[ \delta_k = \frac{1}{2\sqrt{\bar{p}_k}} \frac{1 - p_k}{\cosh(2r_k) + \sqrt{\bar{p}_k}}. \] (156)

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**Fig. 6** \( \sqrt{2} \sigma \) contour level of the Wigner function \( W^S \) for \( \varphi_k = \pi/4, r_k = 1, p_k = 0.12 \) (blue ellipse) or \( p_k = 1 \) (green ellipse) and the vacuum state \( n_k = 0 \) (pink circle).

Let us investigate the effect of decoherence using this class of state. To start with, how is the level of decoherence of the state estimated? Several criteria have been used in the literature: the so-called rate of de-separation [106], evaluating the suppression of non-diagonal terms [115, 114, 123], the positivity time if the initial state is assumed to be non-Gaussian [108], \( \delta_k \) [44] or simply the purity \( p_k \) [120]. We will use the latter since it directly enters our definition of the GHDM (154). The purity can also be conveniently related to the entropy by Eq. (128), which still applies for decohered states. Since the purity has decreased, the entropy increases and becomes non-vanishing. For instance, a thermal state in the 2-mode particle number basis (148) gives \( c_k = r_k = 0 \) and \( p_k = (2n_k + 1)^{-1} \).

Our focus is on how a certain level of decoherence, represented by \( p_k \), can lead to a classical state in the sense of the criteria discussed in the previous section. As we now show, for mixed states, the different criteria are, in general, inequivalent and give different answers [122]. The separability condition Eq. (131) is also still valid for the partially decohered distribution [44]. It has a very elegant interpretation
when rewritten in terms of the effective squeezing parameter

\[ B_k h^{-1/2} = p_k^{-1/4} e^{-\tau_k} \leq 1, \]

i.e. the state becomes separable when there is no sub-fluctuant mode anymore due to a sufficient level of decoherence \( p_k \ll e^{\tau_k} \). The condition can also be written as \( \delta_k \geq n_k / (n_k + 1) \) which, for the very large number of primordial gravitons expected \( n_k \gg 1 \), becomes \( \delta_k \geq 1 \) \[44\].

Let us now turn to the Bell inequality of Eq. (141). Its form, its maximisation procedure, and the formula Eq. (139) are still valid for our partially decohered state. We plot the value of \( C_{\text{max}} \) for a modest number of gravitons in each polarisation \( n_k = 100 \) and different values of \( \delta_k \) in Fig. 7. We see that the maximum of \( C_{\text{max}} \) gradually recedes away from violation as \( \delta_k \) increases, and that for \( \delta_k = 0.1 \), the inequality is not violated anymore. In \[88\], the authors give an approximation in the limit \( \delta_k \ll n_k \), which is equivalent to \( \cosh^2 (r_k) \gg 1 \), i.e. in the limit of a very squeeze state. In this limit, we have

\[ C_{\text{max}} (|v|^2) = \frac{1}{2(1 + \delta_k)} \left[ 1 + \frac{3}{2^{4/3}} + O \left( \frac{1 + \delta_k}{n_k} \right) \right]. \]  

(158)

so that inequality is violated when

\[ \delta_k < 0.095. \]

(159)

The threshold is an order of magnitude smaller than that of separability. This condition is unfortunately not easily expressed in a comparison between \( p_k \) and \( r_k \). The perturbations loose their quantum character in the sense of the Bell inequality Eq. (141) faster than in the sense of separability. This is expected since we recall that separability is a necessary condition for Bell inequality violation, and here we see that it is not a sufficient condition anymore; the criteria are inequivalent for mixed states.

Finally, let us examine the behaviour of the quantum discord. The formula (146) was generalised in \[46\] for partially decohered states. A similar computation in presence of decoherence, although less general, was previously carried out in \[125\]. The generalisation reads

\[ D_{\pm k} = f \left[ p_k^{-1/2} \cosh (2r_k) \right] - 2f \left( p_k^{-1} \right) + f \left[ \frac{p_k^{-1/2} \cosh (2r_k) + p_k^{-1}}{p_k^{-1/2} \cosh (2r_k) + 1} \right]. \]  

(160)

One notes that the discord does not depend on the squeezing angle \( \phi_k \). This angle can always be modified by a local symplectic transformation, and the discord is a local symplectic invariant, so it must not depend on it. In Fig. 8, we plot this formula as a function of \( p_k \) and \( r_k \), and draw the line delimiting separable from non-separable states. Its complexity prevents us from giving a simple threshold for the discord to be, say, larger than 1 and to compare with separability and Bell inequality. Figure 8 shows clearly that, as for separability, the value of the discord is dictated by the
result of a competition between the level of squeezing $r_k$ and that of decoherence $p_k$. These two criteria, along with a Bell inequality of the type considered in [100], were recently compared in [126].

The overall result of this discussion is that decoherence, if large enough, does, in the sense of different inequivalent criteria, erase the quantum features of the state. To be able to complete the analysis, the only thing necessary is to get a realistic estimation of the loss of purity in the early universe. Can we get observational constraints
on the interactions generating decoherence and on its level? Unfortunately, not for primordial gravitational waves since they were not detected yet. However, for scalar perturbations, the observation of the baryonic acoustic oscillation (BAO) actually imposes that during inflation, decoherence cannot modify too much the squeezing parameters \[ r_k \gg 1 \] and \[ \phi_k \approx -\pi/2 \]. In particular, this implies that complete decoherence during inflation, leading to a thermal state like Eq. (148), is excluded. Indeed, the squeezing parameter \( r_k \) would vanish [106]. Note that the purity \( p_k \) is not constrained by this argument. This relation between the oscillations and strong squeezing had initially led to label the former a quantum feature [30]. As we have explained, the squeezing, in its dynamical aspect, can be understood as the presence of a growing and a decaying mode so that this result can be understood completely classically as pointed in [45]. This ‘temporal coherence’ of the perturbations is explained in detail (using a classical point of view) in [82]. In addition of this general argument, for precise models of decoherence, other constraints can be obtained as discussed, for instance, in Ref. [120].

Let us close this section by coming back to the important question of the observability of the features. Even in the absence of decoherence, are the operators that we have used in the discussion measurable? For the Bell inequality Eq (141) they have derived in [88], Campo and Parentani argue that each of the four terms is, in principle, measurable. However, one needs to measure a difference of order 1 between these while the intrinsic fluctuations of the factor \( n_k \) is of order \( n_k \), which is of order \( 10^{86} \). The measure is, in practice, impossible. The authors of [100] argue that having only access to the growing mode makes it impossible to measure two of their three pseudo-spin operators. Verifying their Bell inequality necessitates measuring at least two, and so is experimentally impossible. To address this difficulty, they suggest that one could try to build Legget-Garg inequalities [127] that rely on correlation in time of a single operator and do not require to measure two non-commuting operators at a given time. Ref. [128] also proposed a “baroque”, to use the term of the author, inflationary model in which Bell operators are measured during inflation by another field rather than at later times by observer. The field stores the result in classical, robust variables that could be read out at later times by observers. Finally, the separability and quantum discord, being directly attached to properties of the density matrix, seem harder to measure. The possibility of measuring them directly in the cosmological case has not, to the best of our knowledge, been analysed. In [37], the authors took another approach and showed that if the perturbations were in a quantum non-discordant state, and reproduced the power spectrum measured for scalar perturbations, then they have to be in the thermal state (148). As we have just explained, this is ruled out. Note that this argument assumes that the system is described by a quantum state rather than proves it.
5 Some perspectives and critics

To conclude this review, we mention a few perspectives and possible criticisms of the previously developed issues.

First, the estimation of the minimal level of decoherence of cosmological perturbations keeps being refined see, e.g. [129, 117, 130]. Most authors conclude that decoherence has completed by the end of inflation, and the state is classical when the modes become sub-Hubble again. However, an application of the precise level of decoherence obtained to a concrete non-classicality criterion is still missing. Such computation would be essential since we have shown that the threshold for the emergence of classicality given by the different criteria depends on both the purity and the level of squeezing. In addition, some authors have also suggested that the use of Markovian approximation is not well-justified in the cosmological context and that a more general master equation is required to achieve a correct prediction [131, 132].

Second, the discussion of Sec. 4 applies to the tensor and scalar perturbations. However, primordial gravitational waves have the important specificity that they could be directly detected, not only indirectly in the temperature anisotropies of the CMB, as scalar ones. Direct detection (although futuristic see [73]) would bring about exciting possibilities to search for quantum signatures in gravitational wave detectors. Several authors, e.g. [133, 134, 135], have investigated these. The squeezed states of gravitons could produce noise in gravitational wave interferometers, and some of the authors argued that its quantum character might be revealed by measuring the decoherence it would induce between two entangled mirrors.

Another possibility that we have not discussed is to use the interactions of the perturbations, not as a mere source of decoherence, but as giving new signals in the form of non-gaussianities that could be used. Focusing on scalar perturbations, the authors of Ref. [136] showed that substituting the initial quantum vacuum fluctuations by a Gaussian stochastic field with the same two-point functions would lead to enhanced non-gaussianities akin to those generated by initial excited states. Not measuring such an enhancement was then suggested to be a sign of non-classicality of the initial state (see also [137]). With a different approach to non-gaussianities, the Wigner function of primordial gravitational waves was calculated in Ref. [138], taking into account the intrinsic non-linearities of gravity. Its regions of negativity were then explored as a means of exhibiting a signature of quantumness of the state. Other works such as Refs. [139, 140] took yet another route and provided some constraints on decoherence based on the level of non-gaussianities.

Finally, some authors criticised the standard approach of analysing correlations between \( \pm k \) modes. The authors of [141, 122] have argued that discussing correlations between \( \pm k \) modes is not appropriate as these two modes do not exist separately outside of Minkowski, in particular during inflation, and keep being mixed. Just as there is no preferred choice of vacuum (Sec. 3.6), there is no preferred choice of partition to unambiguously discuss levels of squeezing and correlations. These critics, we believe, would not apply to sub-Hubble modes, e.g., in our toy model radiation domination where \( a' = 0 \). Some recent works [142, 143] do not suffer from these shortcomings since they perform similar computations for quantum discord.
and Bell inequalities, but use real space correlation functions. Unfortunately, their results tend to show that, even in the absence of decoherence, no quantum features appear in real space. Lastly, the formalism presented here does not address the so-called “quantum measurement problem” in cosmology. In our approach, we used an ergodicity assumption to justify equating the quantum expectation values to average values over different patches of the sky. However, one could argue that we did not discuss how the perturbations “collapsed” from a homogeneous quantum state to an inhomogeneous distribution with different values in each patch. For a discussion of this point, see [144].

To conclude, it is fair to say that the current status regarding the quest for quantum features in the primordial gravitational wave background is not entirely settled. First, on the observational side, the waves themselves, even in their classical aspects, have yet to be detected [145]. Experiments in preparation [75, 76] might manage to detect signatures of the waves in the $B$-modes of the CMB. However, direct detection via gravitational wave interferometers seems so far out of reach [73]. On the theoretical side, in recent years, several quantum features of the quantum state for the primordial gravitational waves predicted in the simplest models have been exhibited. Unfortunately, no currently available experimental protocol has yet been designed to detect these features. In addition, the effect of decoherence has been increasingly more precisely characterised, and the latest findings tend to show that it might have erased all the potentially detectable features by the end of inflation. At this time, most analyses have been restricted to the simplest inflationary models and at the Gaussian level. More recently, some promising suggestions and proposals have been made concerning non-gaussianities, discussing the possible signatures of decoherence, or other possible hints of a quantum origin of the perturbations.

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