We investigate the transformation of initial conditions for primordial curvature perturbations under two types of transformations of the associated action: field-redefinitions and the addition of surface terms. We consider a subset of these transformations that preserve the form of the equation of motion and the commutator structure of the theory, making them canonical transformations. Actions related to each other via such transformations are physically equivalent (both classically and in the quantum sense), and choosing between the equivalent actions can be thought of as a gauge choice. Under these transformations we find that initial conditions derived via minimising the vacuum expectation value of the Hamiltonian and those obtained using the Danielsson vacuum prescription are not invariant, whereas those obtained by minimising the local energy density are invariant. We derive the range of physically distinct initial conditions obtainable by Hamiltonian diagonalisation, and illustrate their effect on the scalar primordial power spectrum and the Cosmic Microwave Background under the ‘just enough inflation’ model. We also generalise the analogy between the dynamics of a quantum scalar field on a curved, time-dependent spacetime and the gauge-invariant curvature perturbation.

I. INTRODUCTION

Anisotropies in the Cosmic Microwave Background (CMB) are thought to have been seeded during cosmic inflation by quantum fluctuations. To model the statistical properties of the CMB, one therefore needs either to assume a spectrum of such perturbations at the end of inflation, or compute one. To compute a spectrum, the relevant equations one needs to solve are the cosmological field equations \[1\], which describe the time-evolution of a homogeneous, expanding ‘background’ universe, alongside the Mukhanov–Sasaki equation \[2\], a second-order ordinary differential equation which governs the growth of small fluctuations in the metric and matter field(s) on this background. The gauge-invariant curvature perturbations ‘freeze out’ during inflation. They are therefore evolved numerically until well into inflation, and their frozen-out amplitudes are used to compute the primordial power spectrum. The numerical solution requires two initial conditions for the Fourier modes of perturbations (referred to as mode functions), which are usually motivated by quantum mechanical vacuum considerations. Traditionally, the vacuum is chosen so as to minimise the Hamiltonian density. In an expanding spacetime however, the Hamiltonian becomes time-dependent, leading to the vacuum state at a given time no longer being the ground state at a later time. The divergent Hamiltonian then yields infinite particle density at times other than the instant the vacuum is set \[3, 4\]. Handley \textit{et al.} \[4\] thus suggest minimisation of a quantity describing the local energy density instead, and derive a different set of conditions. There exist further choices of vacua, such as one proposed by Danielsson \[5\], or the \(\alpha\)-vacua \[6–9\].

In this work we review the aforementioned procedures for setting initial conditions from the perspective of invariance under a set of transformations that are canonical. Such transformations are purely mathematical and can be thought of as a gauge choice, and therefore should not alter any physics, including vacuum initial conditions set for the perturbation mode functions one can derive from each of the vacuum choices. If the initial conditions were to change, so would the frozen-out amplitude of the mode functions, and in turn the primordial power spectrum and the power spectrum of CMB anisotropies. However, as first observed by Fulling, S. A. \[3\] in 1979, canonical transformations do in fact change the initial conditions resulting from Hamiltonian diagonalisation (minimising the Hamiltonian density), a fact that he used to argue against this procedure. Weiss \[10\] then added field-redefinitions to the group of canonical transformations considered by Fulling, but instead came to the conclusion that a preferred Hamiltonian can be picked out for its desirable mathematical properties. This preferred Hamiltonian is the one written in terms of conformal time \(\eta\) and the Mukhanov variable \(v\). The preferred Hamiltonian coincides with the one considered conventionally, for its action describes a canonically normalised scalar field. A recent study \[11\] provides a thorough review of canonical transformations and their effect on scalar field fluctuations during inflation, observing that the transformations can be used to select out different vacuum states.

In our current work, in addition to reinforcing Fulling’s view of the Hamiltonian diagonalisation vacuum being a non-gauge-invariant (and hence unphysical) choice, we show that the Danielsson vacuum suffers the same
pathology, whereas minimising the local energy density through the renormalised stress–energy tensor does not. The latter two procedures were not available to Fulling at the time.

Section II covers the relevant mathematical and physical background, with Section II A summarising the classical theory of inflationary perturbations and Section II B reviewing how the vacuum choices considered arise. Section III then explains what transformations of the vacuum-setting procedures are carried out in this work. Results are presented in Section IV, broken into subsections to show the effect of the canonical transformations considered, under each vacuum prescription, of the vacuum-setting procedures are carried out in this work. Results are presented in Section IV, broken into subsections to show the effect of the canonical transformations considered, under each vacuum prescription.

The notation used throughout this paper is summarised in Table I. We use reduced Planck units such that $\hbar = c = k_B = 8\pi G = 1$. Greek indices can have any value from 0 to 3, with 0 reserved for time and 1–3 denoting spatial components. Latin indices indicate spatial components.

| symbol | meaning |
|--------|---------|
| $t$    | cosmic time |
| $\eta$ | conformal time |
| $\tau$ | an arbitrary independent variable |
| $f$    | $\frac{\partial f}{\partial t}$ |
| $f'$   | $\frac{\partial f}{\partial \eta}$ |
| $\partial_\tau f$ | $\frac{\partial f}{\partial \tau}$ |

II. BACKGROUND

A. Dynamics of primordial perturbations

1. The perturbed classical action

The dynamics of primordial curvature perturbations arise from perturbing the metric and matter fields around a homogeneous, isotropic, expanding background (for a thorough review, see e.g. V.F. Mukhanov and H.A. Feldman and R.H. Brandenberger [2], Maldacena [12], Baumann [13]). In an inflationary model with a single scalar field $\phi(t)$ and potential $V(\phi)$ on a Friedmann–Robertson–Walker (FRW) spacetime, the system can be described via the action

$$S = \frac{1}{2} \int d^4x \sqrt{-g} \left[ R - (\nabla \phi)^2 - 2V(\phi) \right],$$

where the metric $g_{\mu\nu}$ is the spatially flat FRW metric. Perturbing this action in the comoving gauge

$$\delta \phi = 0, \quad g_{ij} = a^2 \left[ (1 - 2\mathcal{R}) \delta_{ij} + h_{ij} \right], \quad \partial_i h_{ij} = h_i^i = 0,$$

yields, to second order in the gauge-invariant curvature perturbation $\mathcal{R}$,

$$S_2 = \frac{1}{2} \int d^4x a^2 \left[ \mathcal{R}^2 - a^{-2}(\partial_i \mathcal{R})^2 \right].$$

Traditionally this is then written in terms of the Mukhanov variable $v = z\mathcal{R} = \frac{a^2}{\mathcal{R}} \mathcal{R}$ and conformal time $\eta$ and integrated by parts to give

$$S_2 = \frac{1}{2} \int d\eta d^3x \left[ (v')^2 - (\partial_i v)^2 + \frac{z''}{z} v^2 \right].$$

The reason behind the variable choice and integration by parts is that in the resulting action $v$ is canonically normalised, i.e. it has a kinetic term of the form $\frac{1}{2} \partial_\mu v \partial^\mu v$, and thus yields an equation of motion of a particular form. Writing $v$ as a Fourier decomposition,

$$v(\eta, x) = \int \frac{d^3k}{(2\pi)^3} \tilde{v}_k(\eta) e^{ikx},$$

the action (4) gives the equation of motion of an oscillator:

$$v''_k + \left( k^2 - \frac{z''}{z} \right) v_k = 0,$$

where the vector notation on the wavevector $k$ has been removed due to the isotropy of the field $v$. The variables $(\eta, v)$ were thus chosen because they yield an oscillator’s equation of motion (without a ‘first-derivative term’ proportional to $v'$), allowing the classical field $v$ to be quantised by analogy with a time-dependent quantum harmonic oscillator.

2. Scalar fields in curved spacetime

One could alternatively model the scalar inflationary perturbations as a scalar field with mass $m = 0$. This analogy holds true because the equation of motion for a massless scalar field in spatially flat FRW spacetime admits a similar equation of motion to (6). Starting from the action

$$S = \frac{1}{2} \int d^4x \sqrt{-g} \left( g^{|\mu\nu|} \partial_\mu \phi \partial_\nu \phi - m^2 \phi^2 \right),$$

which one traditionally considers in terms of the auxiliary field $y = a\phi$ and conformal time (for similar reasons as $v$ was considered in the previous section), one derives the Fourier space equation of motion

$$y''_k + \left( k^2 - \frac{a''}{a} + a^2 m^2 \right) y_k = 0.$$
The similarity between (6) and (8) means, as pointed out by Handley et al. [4], that the perturbation modes \( v_k \) behave like the modes \( y_k \) derived from a massless scalar field \( \phi \) in an alternative FRW spacetime, as long as the two background spacetimes satisfy

\[
\frac{a''}{a} = \frac{z''}{z}.
\]

The above holds true for a number of scenarios, the most important being slow-roll inflation, when \( z \approx a \). Therefore one could treat the Mukhanov variable in an inflating universe as if it was a scalar field \( \phi(\eta, x)/a(\eta) \) on the same background, obeying the action (7). The advantage of working with action (7) over (4) is that the former is in covariant form (once each \( \partial_\mu \) has been replaced by \( \nabla_\mu \)), and hence can be used to derive further covariant quantities such as the stress–energy tensor, the minimisation of which provides a definition of the ground state (see Section II B 3).

### B. Vacuum choices

In the above models of primordial perturbations there are multiple ways to define a vacuum or ground state. These result in expressions for the Fourier modes of the perturbations considered (\( v_k \) or \( y_k \)), which can then be used as initial conditions for the perturbation modes, and affect the form of the primordial power spectrum the modes admit. In this section we introduce three different definitions of the vacuum state: Hamiltonian diagonalisation, the Danielsson vacuum, and minimising the renormalised stress–energy tensor. We derive initial conditions each vacuum definition gives for the mode functions if applied in the conventional way. We then examine how the initial conditions change under a field-redefinition in the associated action and the addition of surface terms in Section IV A.

#### 1. Hamiltonian diagonalisation

To obtain a quantum theory from the semiclassical action (4), the field \( v \) is promoted to an operator:

\[
\hat{v}(\eta, x) = \int \frac{d^3k}{(2\pi)^3} \left[ a_k v_k(\eta)e^{ik \cdot x} + a_k^\dagger v_k^*(\eta)e^{-ik \cdot x} \right],
\]

where \( a_k^\dagger \) and \( a_k \) are the creation and annihilation operators, respectively. The momentum conjugate to \( v \) is

\[
\pi = \frac{\partial \mathcal{L}}{\partial v'} = v',
\]

(with \( \mathcal{L} \) being the Lagrangian density associated with the action) and is quantised accordingly. To impose canonical commutation relations

\[
\left[ a_k, a_{k'}^\dagger \right] = (2\pi)^3 \delta(k - k'),
\]

and to obey the equation of motion, the time-dependent part of the mode functions in (10) must satisfy the equation of motion and a normalisation constraint:

\[
v''_k + \left( k^2 - \frac{z''}{z} \right) v_k = 0,
\]

\[
-ikv'_k - v^*_kv_k = -i.
\]

The equations (13)–(14) do not fully determine the mode functions \( v_k(\eta) \). To fix the leftover degree of freedom, one needs to specify a vacuum, which obeys \( \hat{a}_k |0\rangle = 0 \). One popular definition of the ground state is that which minimises the vacuum expectation value of the Hamiltonian of the system. This choice of variables results in the expression

\[
\langle 0 | H | 0 \rangle \propto \int \frac{d^3k}{(2\pi)^3} \left[ |v'_k|^2 + \left( k^2 - \frac{z''}{z} \right)^2 |v_k|^2 \right].
\]

We must then minimise the contribution to the Hamiltonian separately for each \( k \)-mode, with respect to the mode functions belonging to that mode, subject to the constraint (14). This leads to the solutions

\[
|v_k|^2 = \frac{1}{2\sqrt{k^2 - \frac{z''}{z}}},
\]

\[
v'_k = -i \sqrt{k^2 - \frac{z''}{z}} v_k,
\]

which can be used to set initial conditions to the mode functions \( v_k \).

#### 2. Danielsson vacuum

Danielsson [5] proposed that the vacuum should be chosen such that

\[
|v_k|^2 = (2k)^{-1},
\]

\[
v'_k = \left( -ik + a'/a \right) v_k.
\]

This result is derived from ‘first principles’, working in the Heisenberg picture. For detailed reviews of the following, see [14–16].

In the Heisenberg picture, the operators carry time-dependence. When quantising the massless field \( y \) appearing in the action (7) with \( m = 0 \), we may write in Fourier space

\[
\hat{y}_k(\eta) = \frac{1}{\sqrt{2k}} \left[ \hat{a}_k(\eta) + \hat{a}_{-k}^\dagger(\eta) \right],
\]

and for its conjugate momentum \( \pi_k = y^*_k - \frac{a'}{a} y_k \),

\[
\hat{\pi}_k(\eta) = -i \frac{k}{2} \left[ \hat{a}_k(\eta) - \hat{a}_{-k}^\dagger(\eta) \right].
\]
The creation and annihilation operators mix over time via a Boguliubov transformation

\[
\hat{a}_k(\eta) = \alpha_k(\eta)\hat{a}_k(\eta_0) + \beta_k(\eta)\hat{a}^\dagger_{-k}(\eta_0),
\]

\[
\hat{a}^\dagger_{-k}(\eta) = \beta_k^*(\eta)\hat{a}_k(\eta_0) + \alpha_k^*(\eta)\hat{a}^\dagger_{-k}(\eta_0),
\]

where \(\alpha_k(\eta)\) and \(\beta_k(\eta)\) are time-dependent mixing coefficients. One can therefore isolate the time-dependent parts of the fields,

\[
\hat{y}_k(\eta) = f_k(\eta)\hat{a}_k(\eta_0) + f_k^*(\eta)\hat{a}^\dagger_{-k}(\eta_0),
\]

\[
i\hat{\pi}_k(\eta) = g_k(\eta)\hat{a}_k(\eta_0) - g_k^*(\eta)\hat{a}^\dagger_{-k}(\eta_0),
\]

with

\[
f_k(\eta) = \frac{1}{\sqrt{2k}}(\alpha_k(\eta) + \beta_k^*(\eta)),
\]

\[
g_k(\eta) = \sqrt{\frac{k}{2}}(\alpha_k(\eta) - \beta_k^*(\eta)),
\]

where the \(f_k\) now take the role of the mode functions \(y_k\) in the Schrödinger picture, because they carry all time dependence of the field operator. At \(\eta = \eta_0\), the creation and annihilation operators are by definition unmixed, therefore

\[
\beta_k(\eta_0) = 0 = \sqrt{\frac{k}{2}}f_k^*(\eta_0) - \frac{1}{\sqrt{2k}}g_k^*(\eta_0).
\]

Identifying the mode function \(y_k\) with \(f_k\) and the conjugate momentum \(\pi_k\) with \(-ig_k\), we obtain the Danielsson vacuum \((17)\).

Immediately it is clear that since the Danielsson vacuum relates a field and its conjugate momentum, the initial conditions derived from it will generally change under transformations that change that relationship, e.g. the addition of a surface term to the action, described in Section III B.

### 3. Minimising the renormalised stress–energy tensor

Handley et al. \cite{4} have proposed to minimise the vacuum expectation value of the local energy density as the ground state to avoid the excessive particle production of the Hamiltonian diagonalisation approach. The local energy density is computed as the 00 component of the stress–energy tensor of the system \((7)\). General relativity requires a symmetric stress–energy tensor, as it appears on the right-hand side of the Einstein equations. It is defined as \cite{17}

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

with the subscript \(m\) signalling the matter part of the action. Just like the expectation value of the Hamiltonian, the stress–energy tensor is divergent, and has to be renormalised to yield finite quantities. There exist several procedures of renormalisation of the stress–energy tensor, and in Handley et al. \cite{4} the Hadamard pointsplitting method is used (thoroughly described in \cite{17}).

In summary, this consists of first quantising the field \(y\) from Section II A 2, writing down an expression for the Hadamard Green function,

\[
G^{(1)}(x, x') = \frac{1}{2} \langle 0\{\phi(x), \phi(x'), \}\{0
\]

then applying the bi-scalar derivative \(D_{\mu\nu}\) to the function

\[
G^{(1)}(x, x') - G^{(1)}_{DS}(x, x'),
\]

where the second term denotes the de-Witt Schwinger geometrical terms. The geometrical terms do not depend on the variables with respect to which one minimises the stress–energy tensor, and will therefore be summarised as \(\tilde{T}\) and ignored in the minimisation process. The coincidence limit \(x \rightarrow x'\) is then taken to yield \(\langle 0| T_{\mu\nu} |0\rangle_{\text{ren}}\). Altogether,

\[
\langle 0| T_{\mu\nu} |0\rangle_{\text{ren}} = \lim_{x \rightarrow x'} \frac{1}{2} G^{(1)}(x, x') \left[ (\nabla_\mu \nabla_\nu + \nabla_\nu \nabla_\mu) - g_{\mu\nu} \nabla_\alpha \nabla^\alpha + g_{\mu\nu} m^2 \right] \tilde{T},
\]

which is a functional to be minimised with respect to the mode functions \\{\(y_k, y_k', y_k', y_k'^{\prime}\)\} treated as independent variables, subject to the normalisation constraint on \(y_k\) arising from the canonical commutation relations. The minimisation process yields the solutions

\[
|y_k|^2 = \frac{1}{2\sqrt{(k^2 + m^2 a^2)}},
\]

\[
y_k' = \left( -i \sqrt{k^2 + m^2 a^2 + \frac{\alpha'}{a}} \right) y_k,
\]

which, under the circumstances described in Section II A 2, can be used to set

\[
|v_k|^2 = (2k)^{-1},
\]

\[
v_k' = \left( -ik + \frac{z'}{z} \right) v_k
\]

for the Mukhanov variable.

### III. METHODS

In the theories of primordial perturbations reviewed in the previous section, the standard choices of variables was explained by the simple form of equation of motion they admitted, more specifically that the modes involved behaved like harmonic oscillators, so their quantisation was known.
However, as we shall show, one can always make a canonical transformation of the action of the system by redefining the independent and dependent variables simultaneously such that the resulting equation of motion is first-derivative-free and appropriate commutation relations are satisfied. The new, redefined field will then still be quantisable by analogy with the harmonic oscillator. Apart from the conveniently ‘bare’ $k^2$ term in the associated equation of motion (originating from the canonically normalised scalar field in the action), there is nothing that makes the standard choice of variables $(\eta, v)$ special. In fact there is no choice of variables for which the action is canonically normalised in the case of a non-flat universe [18]. In addition to field-redefinitions, one could always add a surface term to the Lagrangian, equivalent to performing an integration by parts, and obtain an equivalent system (so long as the boundary terms vanish). This has been shown [19] to be true in the quantum limit as well, as addition of surface terms leaves the expectation values of observables unchanged. This section summarises the procedures described above by which the vacuum prescriptions will be transformed.

### A. Field redefinition

For all vacuum-setting methods involving the quantisation of a field, we consider quantising an alternative field related to the conventional choice by a time-dependent, scalar-valued, homogeneous function $h$, and the redefinition of time to a new independent variable $\tau$, whilst keeping in mind how the form of the metric changes. We then derive the vacuum conditions in analogy with the conventional procedures. For Hamiltonian diagonalisation this redefinition will thus be

$$ t \rightarrow \tau(t), \quad R \rightarrow \chi(x, \tau) \equiv \frac{R}{h(\tau)}, \quad (30) $$

and for minimising the renormalised stress–energy tensor, we shall consider instead

$$ t \rightarrow \tau(t), \quad \phi \rightarrow \chi(x, \tau) \equiv \frac{\phi}{h} = \frac{y}{ah}, \quad (31) $$

as the field being quantised is $\phi$.

We shall derive a constraint linking $\tau$ and $h$ for each action considered to ensure it yields the equation of motion of an oscillator, as this is not guaranteed by the transformation (30). This generally leaves an unconstrained integration constant $C_0$. The field-redefinition also does not necessarily conserve the commutator structure. For all transformations considered, this will be ensured via an additional constraint that needs to be satisfied during the minimisation of the vacuum expectation value of the Hamiltonian density or the 00-component of the renormalised stress–energy tensor.

### B. Surface terms

In the conventional Hamiltonian diagonalisation approach, one performs an integration by parts to obtain the action (4). This is equivalent to adding the total derivative

$$ \left(\frac{z'}{z} v^2\right)' \quad (32) $$

to the associated Lagrangian density, or a vanishing surface or boundary term to the action. Under the field redefinition of the previous section, the action changes such that the appropriate boundary term to add will be

$$ -\partial_\tau \left(\chi^2 \frac{\partial_t h}{h}\right). \quad (33) $$

It is clear that (i) there are infinitely many choices of vanishing boundary terms one could add; and that (ii) the boundary terms modify the form of the action and in turn the field-conjugate momentum relationship. For Hamiltonian diagonalisation and the Danielsson vacuum we shall investigate how the addition of the boundary term (33) alters the initial conditions, and we shall show that minimising the renormalised stress–energy tensor is invariant under the addition of boundary terms by construction.

Detailed calculations of initial conditions arising from systems subject to field-redefinitions and addition of surface terms can be found in Appendices A and B.

### IV. RESULTS

#### A. Initial conditions

1. **Hamiltonian diagonalisation**

Under the field redefinition (30), minimising the vacuum expectation value of the Hamiltonian (15) gives the generalised initial conditions

$$ |\chi_k|^2 = (2C_0 \omega_k)^{-1}, \quad \partial_\tau \chi_k = -i\omega_k \chi_k, \quad (34) $$

where $\omega_k$ is the time-dependent frequency of the equation of motion in terms of $(\tau, \chi_k)$, and $C_0 = 1$.

As a sanity check, substituting $h = z^{-1}$ and $C_0 = 1$, corresponding to quantising the Mukhanov variable in terms of conformal time, we recover the conventional initial conditions (16). However, changing variables to $(\eta, v)$ in the generalised initial conditions (34) yields

$$ |v_k|^2 = \frac{1}{2\left(k^2 + h'' \frac{2}{h} + 2 \frac{h' z'}{k z}ight)}, \quad (35) $$

$$ v'_k = \left(-i \sqrt{k^2 + h'' \frac{2}{h} + 2 \frac{h' z'}{k z}} \right) v_k, \quad (36) $$
which carry the arbitrary function \( h \). This means that one can derive a family of initial conditions for \( v_k(\eta) \) depending on the field in terms of which the action was written.

Under addition of the boundary term defined in Section III B and the field re-definition that led to (35), one can derive another set of conditions:

\[
|v_k|^2 = \frac{1}{2\sqrt{k^2 - \left(\frac{h'}{h}\right)^2}},
\]

\[
v'_k = -i\sqrt{k^2 - \left(\frac{h'}{h}\right)^2} - \frac{h'}{h} + \frac{z'}{z} v_k.
\]

(36)

Not only is this another family of solutions depending on the function \( h \), it is a different set to (35)! This can be seen by noting that for all values of \( h'/h \) in (36) there will be a lower limit for \( k \) below which the expression under the square root becomes negative, which is not allowed (for the squared magnitude of the perturbation has to be real). This ‘forbidden region’ is different for (35).

Since we could have chosen any action connected to (4) via a canonical transformation, we could have arrived at a range of different Hamiltonians yielding different quantum initial conditions for the perturbations. Hamiltonian diagonalisation is inherently ambiguous (gauge-dependent).

The two example solution families obtained via Hamiltonian diagonalisation are parametrised by a time-dependent function \( h \). If we choose to use the solutions as initial conditions, and the spacetime slice we set them on is chosen such that all modes (i.e. all \( k \)) are set simultaneously at a conformal time \( \eta_0 \), the shape of the function \( h(\eta) \) only matters in the vicinity of \( \eta_0 \). We can determine how much freedom this gives by Taylor-expanding \( h \) near \( \eta_0 \):

\[
h(\eta) = \sum_{n=0}^{\infty} \frac{1}{n!} h_n(\eta - \eta_0)^n,
\]

(37)

substituting into (35), then finally evaluating at \( \eta = \eta_0 \). This gives

\[
|v_k|^2 = \frac{1}{2\sqrt{k^2 + \frac{h_2}{h_0} + 2\left(\frac{h_1 z'}{h_0 z}\right)}},
\]

\[
v'_k = \left(-i\sqrt{k^2 + \frac{h_2}{h_0} + 2\frac{h_1 z'}{h_0 z} + \frac{h_1}{h_0} + \frac{z'}{z}}\right) v_k,
\]

(38)

showing that there are two real degrees of freedom in this set of initial conditions \( (h_2/h_0 \) and \( h_1/h_0 \)), whereas (36) only depends on \( h_1/h_0 \):

\[
|v_k|^2 = \frac{1}{2\sqrt{k^2 - \left(\frac{h_1}{h_0}\right)^2}},
\]

\[
v'_k = -i\sqrt{k^2 - \left(\frac{h_1}{h_0}\right)^2} + \frac{h_1}{h_0} + \frac{z'}{z} v_k.
\]

(39)

It is worth noting that there exist prescriptions that do not set initial conditions for all perturbations simultaneously. \([5]\) for example chooses a finite \( v_0(k) \) for each \( k \) such that the physical momentum corresponding to the mode is given by some fixed scale, and it is common to initialise the perturbations when their lengthscales are a fixed fraction of the Hubble horizon. These prescriptions may lead to more degrees of freedom in the initial conditions.

In \([20]\), the authors do not attempt to find the preferred choice of vacuum (if that exists), rather they parametrise a general choice of initial conditions by two complex scalars, \( X \) and \( Y \) (\( Y \) being purely imaginary), that characterise the choice of vacuum:

\[
v_k(\eta_0) = \frac{e^{i\phi_1}}{\sqrt{k}} \left[ 1 + \frac{X + Y}{2} \theta_0 + O(\theta_0^2) \right].
\]

(40)

\[
v'_k(\eta_0) = -i\sqrt{k} e^{i\phi_2} \left[ 1 + \frac{Y - X}{2} \theta_0 + O(\theta_0^2) \right].
\]

(41)

Their initial conditions are the solutions of the mode equation (6) in the limit where the metric is Minkowski, with added corrections due to expansion as a power series in the small, dimensionless parameter \( \theta_0 \):

\[
\theta_0 = \left. aH \right|_{\eta = \eta_0}.
\]

(42)

In terms of this parametrisation, the solutions (38) represent a subset with

\[
X = -Y, \quad Y \text{ arbitrary},
\]

(43)

which can be seen by factoring out \( 1/\sqrt{k} \) from the expression for \( v_k \), expanding the rest in powers of \( 1/k \), and observing that there is no term linear in \( 1/k \).

2. Danielsson vacuum

It is easily seen that Danielsson’s result, for a different choice of field (31), generalises as

\[
\pi_\chi(\tau) = -ik\chi(\tau),
\]

(44)

where \( \pi_\chi \) is the momentum conjugate to \( \chi \). Using the action (7) under the field redefinition (31) to compute the conjugate momentum, this gives for \( y_k \):

\[
|y_k|^2 = \frac{(ah)^2}{2k},
\]

\[
y'_k = \left( -\frac{ik}{(ah)^2} + \frac{a'}{a} \right) y_k.
\]

(45)

Under the addition of the surface term (33) to the action (which has the effect of eliminating the \( \partial_\tau \chi \) term), the momentum conjugate to the field \( \chi \) changes, and the initial conditions become

\[
|y_k|^2 = \frac{(ah)^2}{2k},
\]

\[
y'_k = \left( -\frac{ik}{(ah)^2} + \frac{a'}{a} + \frac{h'}{h} \right) y_k.
\]

(46)
Since canonical transformations by addition of surface terms only change the relationship between the field and its conjugate momentum, infinitely many solution families like (45) and (46) exist that differ in $y_k'(y_k)$. There is no theoretical guidance as to which action one should consider, and hence which set of initial conditions is the correct one in the Danielsson prescription.

3. **Minimising the renormalised stress–energy tensor**

Working from the action (7) under a canonical field redefinition, and minimising the expression (27) fixes the mode functions $\chi_k$ fully as

$$|\chi_k|^2 = \frac{1}{2\sqrt{h^4a^2(k^2 + m^2a^2)}},$$

$$\partial_\tau \chi_k = \left(-i \frac{\sqrt{h^4a^2(k^2 + m^2a^2)}}{C_0} - \frac{\partial_\tau h}{h}\right)\chi_k.$$  (47)

Converting back to conformal time and $y$ gives the solutions

$$|y_k|^2 = \frac{1}{2\sqrt{(k^2 + m^2a^2)}},$$

$$y_k' = \left(-i \sqrt{k^2 + m^2a^2} + \frac{a'}{a}\right)y_k,$$  (48)

independent from the choice of $h(\tau)$ and $\tau$, and in agreement with solutions derived using the conventional treatment, (28).

From the definition (24), it can be shown that an added 4-divergence (involving the field and the metric) to the Lagrangian does not change the form of the stress–energy tensor as long as the added surface term does not break covariance of the existing Lagrangian. Not only has the stress–energy tensor been constructed in a covariant way, Yargic et al. [21] have recently shown that one can define a ground state family, with respect to which its expectation value is covariantly conserved. This possibility was also pointed out in Fulling, S. A. [3]. All that matters in the minimisation process is the form of the field-dependent part of $T_{\mu\nu}$ (the geometrical terms do not come into play as they do not depend on the field), and therefore the initial conditions derived via minimisation of the renormalised stress–energy tensor are invariant under the addition of surface terms.

Minimising the 00-component of the renormalised stress–energy tensor is therefore invariant under canonical field-redefinitions and addition of surface terms. The stress–energy tensor was defined to be covariant, therefore its invariance under the addition of surface terms comes as no surprise, but it has not been constructed to be invariant under field-redefinitions. In taking the 00-component however, covariance has been broken, and we must ensure that the same results hold when a coordinate-independent quantity is minimised.

To make sure this is the case, one should consider the eigenvalue belonging to a timelike eigenvector of the tensor. Let us therefore generate the off-diagonal components of $\langle 0| T_{\mu\nu} |0\rangle$, ignoring those arising from the geometrical terms:

$$\langle 0| T_{0} |0\rangle_{\text{ren}} = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{k}{\tau a z^2},$$  (49)

$$\langle 0| T_{ij} |0\rangle_{\text{ren}} = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} 2h^2 \chi_k \chi_k' k_i k_j,$$  (50)

with $i \neq j$. All the above components include integrals with integrands odd in $k_i$, and so they vanish. The de Witt–Schwinger terms in the off-diagonal elements can also be shown to vanish due to the metric $g_{\mu\nu}$ being diagonal \(^1\). Consequently the expectation value of the renormalised stress–energy tensor is diagonal, and its eigenvalues are just the diagonal entries. The eigenvalue corresponding to the timelike eigenvector is the 00 element, confirming the results of this section.

4. **Generalised analogy between a scalar field on a curved spacetime and the curvature perturbation**

In Section II B 3, we derived initial conditions for the Mukhanov variable in an inflating background from the solutions for $y_k$ in (28) by drawing an analogy between their equations of motion, (6) and (8). For the two equations to be the same, we required $a''/a = z''/z$. We now derive similar requirements for the two equations of motion to have the same form, after having performed the field-redefinitions

$$\mathcal{R} \rightarrow \chi_1 = \frac{\mathcal{R}}{h_1},$$  (51)

and

$$\phi \rightarrow \chi_2 = \frac{\phi}{h_2} = \frac{y}{ah_2},$$  (52)

respectively. The first, obvious requirement is that the redefined field in (8) has to be massless, $m = 0$. For the classical perturbed action we then have the equation of motion

$$0 = \partial_{\tau^2} \chi_1 + \left[\left(\frac{kh_2^2a^2}{C_2^2}\right)^2 + \frac{\partial_{\tau^2} h_1}{h_1} - 2\left(\frac{\partial_{\tau} h_1}{h_1}\right)^2\right] \chi_1,$$  (53)

whereas from the massless scalar field we get

$$0 = \partial_{\tau^2} \chi_2 + \left[\left(\frac{kh_2^2a^2}{C_2^2}\right)^2 + \frac{\partial_{\tau^2} h_2}{h_2} - 2\left(\frac{\partial_{\tau} h_2}{h_2}\right)^2\right] \chi_2.$$  (54)

\(^1\) For an explicit expression for $\langle 0| T_{\mu\nu} |0\rangle_{\text{ren}}$ that confirms this, see [17].
We are free to choose \( h_1, h_2 \), and the constants \( C_1 \) and \( C_2 \). We first have to set
\[
\frac{h_1 z}{C_1} = \frac{h_2 a}{C_2}
\]
(55)
for the first term in the frequency to be the same, then we need to satisfy
\[
\frac{h_1''}{h_1} - 2 \left( \frac{h_1'}{h_1} \right)^2 = \frac{h_2''}{h_2} - 2 \left( \frac{h_2'}{h_2} \right)^2 ,
\]
(56)
where prime denotes differentiation with respect to the function’s argument. This differential equation admits the solution
\[
\frac{h_1}{h_2} = A \exp \left( \int dt \frac{h_2^2}{B - \int dt h_2^2} \right).
\]
(57)
One can always choose \( h_1/h_2 \) such that (55) holds. One can then calculate \( h_2 \) by inverting (57). This means that if \( h_1, h_2 \) are chosen appropriately, one can always map the solution of the scalar-field action onto the cosmological perturbations.

Alternatively, for an arbitrary choice of \( h_1 \) and \( h_2 \), if \( z \propto a \), the equations of motion take the same form. Therefore the conclusion that we may use the solutions (47) as initial conditions for the associated perturbation mode in inflation is still valid.

B. Primordial power spectra

Primordial power spectra show the power in the Fourier modes of gauge-invariant curvature perturbations \( (R_k) \) after horizon exit – when their characteristic length-scale \( k^{-1} \) first exceeds the size of the comoving Hubble horizon \((aH)^{-1}\) during inflation. When this happens, the amplitude of fluctuations becomes constant, as shown in Fig. 1 alongside definitions of quantities used in this section. Primordial power spectra are not directly observable\(^2\), but are the first physical quantities one can derive from the perturbations, and hence the first physical objects affected by the existence of a range of quantum initial conditions. To compute them, first the ‘cosmological background’ quantities such as the scale factor and Hubble horizon are computed by solving the cosmological field equations [1], which are derived from the action (1) using Einstein’s field equations. The numerical solution is initiated at the start of inflation, which is assumed to be preceded by a *kinetically dominated* [23–25] phase. In kinetic dominance the inflaton particle’s kinetic energy dominates over its potential energy, causing the comoving Hubble horizon to grow and reach a maximum as the universe enters slow-roll inflation. The universe has been proven to emerge from the Big Bang into a period of kinetic dominance under very broad assumptions [23]. Although the assumption of a start of inflation is not a common one, it is necessary in this case for the different initial conditions considered here to yield distinct observable spectra. If all perturbations were initialised when they are deep inside the comoving Hubble horizon, such as in an eternal inflation scenario, the primordial power spectrum would take a power-law form irrespective of vacuum prescription. The result concerning the invariance of vacuum choices under field-redefinitions and addition of surface terms would be theoretically important nonetheless. For simplicity, we consider a single-field inflationary model with a potential that is quadratic in the field,
\[
V(\phi) = \frac{1}{2} \mu^2 \phi^2.
\]
(58)
For convenience, we choose the number of e-folds, \( N \equiv \ln a \) to be the independent variable in the field equations. With this choice, they become
\[
\frac{d \ln D}{dN} = 4 + D \left( 4K - 2e^{2N}V(\phi) \right),
\]
(59)
\[
\left( \frac{d \phi}{dN} \right)^2 = 6 + D \left( 6K - 2e^{2N}V(\phi) \right),
\]
(60)
where \( D = (aH)^{-2} \) and \( K \) is the spatial curvature that can take values 0, ±1 for flat, closed, and open universes, respectively [26]. We set \( K = 0 \) when calculating the primordial power spectra and all subsequent computations.

\(^2\) They are, however, reconstructable [22].
At the start of inflation, the field equations give
\[
D = D_i = \frac{2\epsilon^{-2N_i}}{V(\phi_i)},
\]  
leaving \(N_i\) and \(\phi_i\) as adjustable parameters. In a flat universe we can set \(N_i = 0\) without loss of generality, so the only free parameter left in the background initial conditions is the initial field strength, \(\phi_i\). This determines \(N_{\text{tot}}\), the total number of e-folds during inflation, and \(N_f\), the number of e-folds between the start of inflation and a ‘pivot’ perturbation mode with lengthscale \(k^{-1} = 0.05\ \text{Mpc}^{-1}\) exiting the Hubble horizon. Observations constrain the value of \(N_s\), the number of e-folds between the pivot scale existing the Hubble horizon and the end of inflation, to be between 50 and 60. We pick a value for \(\phi_i\) consistent with the ‘just enough inflation’ scenario \([27]\), where \(N_s \approx N_{\text{tot}}\). In the inflationary potential, \(\mu\) denotes the inflaton mass, which determines the overall ‘normalisation’ of the primordial power spectrum and can be calculated using the slow-roll approximation from \(N_s\) and \(A_s\) to yield the observed normalisation. The primordial parameters and the cosmological parameters used in the following sections are summarised in Table II.

Once the cosmological field equations have been solved, the perturbations \(\mathcal{R}_k\) are initialised simultaneously at the start of inflation with two arbitrary sets of initial conditions (e.g. \(\{\mathcal{R}_k = 1, d\mathcal{R}_k/dN = 0\}, \{\mathcal{R}_k = 0, d\mathcal{R}_k/dN = 1\}\)) and for each \(k\)-mode the Mukhanov–Sasaki equation is solved to obtain their evolution in \(N\). We use the numerical solver \texttt{oscode} \([26]\) to carry out this computation efficiently. The amplitude of each perturbation is read off when they are well outside the Hubble horizon, \(k < 10^{-2}aH\). The two solutions for \(\mathcal{R}_k\) can then be linearly combined to satisfy any initial condition from the sets derived, without having to re-compute the evolution of perturbations. Finally, the primordial power spectrum is constructed according to
\[
\mathcal{P}_\mathcal{R}(k) = \frac{k^3}{2\pi^2}|\mathcal{R}_k|^2. 
\]

Fig. 2 shows example primordial power spectra generated using conventional Hamiltonian diagonalisation \((16)\) and renormalised stress–energy tensor \((29)\) initial conditions, and the corresponding CMB angular \(TT\) spectra. The details of how the latter kind of spectra are computed can be found in Section IV.C. Note the dual \(x\)-axis shows both the wavenumber \(k\) and the multipole \(\ell\). The conversion between the two is performed using the Limber approximation,
\[
\ell \approx KD_{\text{rec}} = \frac{r_s}{\theta_s}, 
\]  
where \(D_{\text{rec}}\) is the distance to the last scattering surface at recombination, \(r_s\) is the sound horizon at recombination, and \(\theta_s\) is the angular parameter. The latter two can be derived from the Planck baseline CMB parameters listed in Table II.

| parameter       | fiducial value | parameter       | fiducial value |
|-----------------|----------------|-----------------|----------------|
| \(\Omega_b h^2\) | 0.02236        | \(A_s\)         | 2.101 \times 10^{-9} |
| \(\Omega_c h^2\) | 0.1202         | \(n_s\)         | 0.9649         |
| \(h\)           | 0.6727         | \(\phi_i\)      | 16 m_p         |
| \(\tau_{\text{reio}}\) | 0.0544       | \(N_s\)         | 55             |

To show the full range of primordial power spectra achievable using Hamiltonian diagonalisation initial conditions \((38)\), we need to consider the two-dimensional space spanned by the two initial condition parameters, \(h_2/h_0\) and \(h_1/h_0\). Since it is difficult to visualise individual spectra in this two-dimensional space, we opt to show instead contour plots of different features in the power spectra. The features considered are listed below.
FIG. 3. Dependence of features of the primordial power spectrum derived from Hamiltonian Diagonalisation initial conditions (38) on the parameters $h_1/h_0$ and $h_2/h_0$. The cutoff position is measured as the wavenumber $k_c$ where the power spectrum drops below a value of $10^{-10}$ towards large scales. The oscillation amplitude is measured as the log-difference between a peak and the following trough. The three coloured points correspond to parameter pairs considered in Section IV C, their individual primordial power spectra are shown in Fig. 5.
1. **Cutoff position**: position of the low-$k$ cutoff present in all primordial power spectra considered. The cutoff is a result of considering kinetic dominance instead of eternal inflation, and is caused by perturbation modes that do not enter the Hubble horizon. We define the cutoff as the position where the amplitude of the power spectrum drops below $10^{-10}$.

2. **Amplitude of first oscillation**: calculated as the logarithmic difference between the first peak and the following trough.

3. **Average amplitude of the first 10 oscillations**.

4. **Ratio of the first to second peak**: defined as $(A_1 - A_2)/(A_1 + A_2)$, where $A_{1,2}$ are the amplitudes of the first and second peaks, respectively.

5. **Frequency of oscillations**: the leading frequency in the Fourier transform of $P_R(k)$ was also considered as a feature initially. However, the frequency was not expected to change with $(h_1/h_0, h_2/h_0)$, which was indeed what has been found, and therefore the resulting contour plot is not shown.

Figs. 3a to 3d show contour plots of the features 1–4 in primordial power spectra in $(h_1, h_2)$-space, with the three coloured points corresponding to parameter pairs considered in Section IV C. The empty ‘forbidden’ region in all plots is a result of $h_2/h_0$ and $h_1/h_0$ appearing under a square root in (38), causing there to be a lower limit to

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**FIG. 4.** Zoom-in of the centre region of the contour plots in Figs. 3b and 3d. The dotted horizontal and vertical lines correspond to the line collections of primordial power spectra in the lower panels. The sharp lines in the contour plot correspond to the (dis-)appearance of the first peak.
possible $k$ values if

$$h_2/h_0 + 2 h_1 z' / h_0 z < 0.$$  (64)

Figs. 3b and 3d exhibit an interesting feature around $h_1/h_0 = 1.5$, $h_2/h_0 = 3.5$: the emergence of a new peak from the low-$k$ region of the primordial power spectrum. The phenomenon is shown in Figs. 4a to 4d: Fig. 4a and Fig. 4b mark the region of interest in parameter space and the extent of inversion, while Fig. 4c and Fig. 4d show the emergence of the new peak along orthogonal directions in parameter space.

It is to be noted that one can arrive at the renormalised stress–energy tensor initial conditions (29) from Hamiltonian diagonalisation, by choosing the field to be quantised as $\mathcal{R}$, i.e. choosing $h = 1$. This choice translates to $h_1/h_0 = 0$, $h_2/h_0 = 0$ in Figs. 3, 4 and 8. The ‘standard’ Danielsson prescription leads to the same initial conditions as minimising the renormalised stress–energy tensor, and so corresponds to $h_1/h_0 = 0$, $h_2/h_0 = 0$. Conventional Hamiltonian diagonalisation is equivalent to choosing $h = z^{-1}$, or $h_1/h_0 \approx 0.82$, $h_2/h_0 \approx 1.37$ in Figs. 3, 4 and 8.

C. Cosmic Microwave Background

We generate the angular CMB $TT$, $TE$, and $EE$ power spectra starting from primordial power spectra using the Boltzmann code \textsc{CLASS} [29–32], with Planck 2018 baseline [28] cosmological parameters as presented in Table II.

There are no obvious choices of physical features in the range of angular spectra observable today that would allow their visualisation in contour plots, therefore without any claim to completeness, we show the primordial power spectra and the corresponding $TT$, $TE$ and $EE$ spectra of three points in $(h_1/h_0, h_2/h_0)$-space marked in colour in Figs. 3a to 3d and 4a to 4d. The primordial power spectra and the $TT$ spectra are shown in Fig. 5, while Fig. 6 shows the $TE$ and $EE$ spectra. The low-$\ell$ region of all the above CMB spectra are shown separately in Fig. 7.

Immediately it is clear that in the ‘just enough inflation’ case, the choice of the function $h$ (through the values $h_1/h_0$ and $h_2/h_0$) can influence the CMB we observe today, despite $h$ being a gauge choice. Again we must stress that in the eternal inflation case, the different initial conditions discussed would yield the same observable

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**FIG. 5.** Primordial power spectrum (top panel) and angular CMB power spectrum of temperature anisotropies (bottom panel) for three different combinations of $h_1/h_0$ and $h_2/h_0$ as used in (38).

**FIG. 6.** CMB angular power spectra of the TE cross-spectrum and the EE auto-spectrum for three different combinations of $h_1/h_0$ and $h_2/h_0$ as in Fig. 5.
The question of whether observations could theoretically rule out certain regions of the \((h_1/h_0, h_2/h_0)\) parameter space is worth investigating, even though the inflationary potential used in this work, \(V(\phi) \propto \phi^2\) has mostly been ruled out by the Planck 2015 results [33], and is only used here for the sake of simplicity. The posterior probability of \((h_1/h_0, h_2/h_0)\) given the Planck 2018 low-\(\ell\) (\(\ell \leq 30\)) temperature-only likelihood [34] is shown in Fig. 8, where a uniform prior was used over the range \(-10 \leq h_1/h_0 \leq 10, -10 \leq h_2/h_0 \leq 30\), excluding the forbidden region. The posterior has been explored using the PolyChord sampler [35, 36]. The low-\(\ell\) data was used because Figs. 5 and 6 suggest that it is the low-\(\ell\) region the different initial conditions have the most effect on.

It is clear that data can be used to select a preferred region of the initial condition parameters, but the point we would like to emphasise in this section is that of the wide-range effects the gauge choice can have on observations when using Hamiltonian diagonalisation to define the vacuum.

V. CONCLUSION

In part, this work serves to highlight some points made by Fulling, S. A. [3] regarding the lack of robustness of Hamiltonian diagonalisation under canonical transformations, in that we have shown that this procedure yields physically distinct vacua, and different initial conditions for the scalar curvature perturbations. We have shown that all sets of initial conditions derived this way can be cast into the general form proposed by [20], and therefore could be argued to be physically sensible. We have however illustrated the effect that the choice of initial conditions has on the primordial power spectrum and the CMB angular power spectra under the ‘just enough inflation’ assumption, noting that in the eternal inflation scenario, all initial conditions considered would yield the same results. We subjected two other choices of vacuum to the same transformations: one obtained by minimising the 00-component of the renormalised stress-energy tensor [4], and the Danielsson vacuum [5]. In doing so we found that the Danielsson vacuum is inherently sensitive
to canonical field-redefinitions and addition of surface terms, but the renormalised stress–energy tensor minimisation is not, despite not having been constructed to be invariant in this manner.

Many pieces of work since Fulling, S. A. [3] acknowledge the existence of Hamiltonians related via canonical transformations, but suggest that there is a preferred Hamiltonian which leads to the conventionally used initial conditions. We noted that the initial conditions derived via the renormalised stress–energy tensor, which have thus been shown to be invariant under canonical transformations, differ from the initial conditions associated with this preferred Hamiltonian.

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1. Field redefinition

Changing variables in the perturbed action (3) leads to

$$S = \int d^3x d\tau \frac{C}{2} \left[ (\partial_\tau \chi)^2 + 2\chi (\partial_\tau \chi) \frac{\partial_\tau h}{h} + \chi^2 \left( \frac{\partial_\tau h}{h} \right)^2 - (\nabla \chi)^2 \left( \frac{h^2 z^2}{C} \right) \right],$$

(A1)

with $C = h^2 r a z^2$. This will in general yield the equation of motion of an oscillator with a non-zero first-derivative term. If the field $\chi$ is to be quantised as an oscillator, the first-derivative term needs to vanish, which holds if

$$C = C_0 = \text{const.}$$

(A2)

Setting $C$ to be constant, the equation of motion in terms of the Fourier modes of $\chi$ becomes

$$0 = \partial_{\tau \tau} \chi_k + \left[ \frac{kh^2 z^2}{C_0} \right]^2 + \frac{\partial_\tau h}{h} - 2 \left( \frac{\partial_\tau h}{h} \right)^2 \chi_k.$$  

(A3)

To follow the conventional procedure, we integrate (A1) by parts to eliminate the term linear in $\partial_\tau \chi$ to get

$$S = \int d^3x d\tau \frac{C_0}{2} \left[ (\partial_\tau \chi)^2 + \chi^2 \left( \frac{\partial_\tau h}{h} \right)^2 - 2 \left( \frac{\partial_\tau h}{h} \right)^2 \right] - (\nabla \chi)^2 \left( \frac{h^2 z^2}{C_0} \right)^2.$$  

(A4)

The momentum conjugate to $\chi$ is then

$$\pi_\chi = C_0 \partial_\tau \chi.$$  

(A5)

We now quantise $\chi$ in the same way as $v$ in (10). Imposing canonical commutation relations on the creation and annihilation operators results in the constraint

$$(\partial_\tau \chi_k)\chi_k - (\partial_\tau \chi^*_k)\chi_k = -\frac{i}{C_0},$$

(A6)

because the momentum conjugate to $\chi$ was scaled by $C_0$. This is a necessary condition for the field redefinition to be a canonical transformation. The normal-ordered Hamiltonian then takes the general form

$$H = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \left[ \hat{a}_k \hat{a}_{-k} F_k(\tau) + \hat{a}_k^\dagger \hat{a}_{-k}^\dagger F_k^*(\tau) + (2\hat{a}_k^\dagger \hat{a}_k + \delta^{(3)}(0)) E_k(\tau) \right],$$

(A7)
with
\[ E_k(\tau) = |\partial_\tau \chi_k|^2 + \omega_k^2 |\chi_k|^2, \]
\[ F_k(\tau) = (\partial_\tau \chi_k)^2 + \omega_k^2 \chi_k^2, \]
\[ \omega_k^2 = \left( \frac{k^2 h^2 z^2}{C_0} \right)^2 + \left( \frac{\partial_\tau h}{h} \right)^2 - 2 \left( \frac{\partial_\tau h}{h} \right)^2. \]

Minimising the vacuum expectation value of the Hamiltonian for each \( k \)-mode separately, subject to the constraint (A6) thus gives the generalised initial conditions
\[ |\chi_k|^2 = \left( 2C_0 \omega_k \right)^{-1}, \]
\[ \partial_\tau \chi_k = -i \omega_k \chi_k. \] (A9)

2. Surface terms

In order to get to the form of the Hamiltonian (A7), we integrated by parts once and discarded a boundary term:
\[ S \supset \int d^3 x \, d\tau \frac{C_0}{2} \left[ 2 \chi (\partial_\tau \chi) \frac{\partial_\tau h}{h} + \chi^2 \left( \frac{\partial_\tau h}{h} \right)^2 \right] \]
\[ = \left[ \chi^2 \frac{\partial_\tau h}{h} \right] - \int d^3 x \, d\tau \left[ \frac{\partial_\tau h}{h} \chi^2 - 2 \left( \frac{\partial_\tau h}{h} \right)^2 \chi^2 \right]. \] (A10)

This is equivalent to adding the surface term
\[ - \partial_\tau \left( \chi^2 \frac{\partial_\tau h}{h} \right). \] (A11)

If we instead kept the action in its original form, (A1), the momentum conjugate to \( \chi \) would be
\[ \pi = C_0 \left( \partial_\tau \chi + \frac{\partial_\tau h}{h} \chi \right), \] (A12)
and the normal-ordered Hamiltonian would take the same form as (A7), but now with
\[ E_k(\tau) = |\partial_\tau \chi_k|^2 + \sigma_k^2 |\chi_k|^2, \]
\[ F_k(\tau) = (\partial_\tau \chi_k)^2 + \sigma_k^2 \chi_k^2, \]
\[ \sigma_k^2 = \left( \frac{k^2 h^2 z^2}{C_0} \right)^2 - \left( \frac{\partial_\tau h}{h} \right)^2. \] (A13)

As seen by symmetry, this yields initial conditions for \( (\tau, \chi) \) of the same form as (35), but with \( \omega_k \) replaced with \( \sigma_k \). Switching back to \( (\eta, \nu) \), they are
\[ |v_k|^2 = \frac{1}{2} \sqrt{k^2 - \left( \frac{\nu}{h} \right)^2}, \] (A14)
\[ v'_k = \left( -i \sqrt{k^2 - \left( \frac{\nu}{h} \right)^2} + \frac{h'}{h} + \frac{z'}{z} \right) v_k. \]

Appendix B: Minimising the renormalised stress–energy tensor under field redefinitions

We generalise the results (28)–(29) in analogy with Appendix A 1. We rewrite the action (7) in terms of the generalised perturbed classical action in Appendix A 1, and is therefore given by
\[ t \rightarrow \tau, \ \phi \rightarrow \chi(x, \tau) \equiv \phi = \frac{y}{ah}, \] (B1)
keeping in mind that the metric then changes to \( g_{\mu\nu} = \text{diag}(\tau^{-2}, -a^2, -a^2, -a^2). \) This yields
\[ S = \int d^3 x \, d\tau \frac{C_0}{2} \left[ \left( \partial_\tau \chi \right)^2 + 2 \left( \partial_\tau \chi \right) \frac{\partial_\tau h}{h} \chi \right. \]
\[ + \chi^2 \left( \frac{\partial_\tau h}{h} \right)^2 - \left( \nabla \chi \right)^2 \left( \frac{h^2 a^2}{C_0} \right)^2 \]
\[ - \chi^2 m^2 \left( \frac{h^2 a^2}{C_0} \right)^2, \] (B2)
with \( C = h^2 a^3. \) As before, the equation of motion resulting from the variation of this action can be made first-derivative-free by setting
\[ C = C_0 = \text{const}, \] (B3)
in which case it becomes, in Fourier space,
\[ \partial_\tau \chi_k + \left[ \left( \frac{k^2 h^2 a^2}{C_0} \right)^2 + \left( \frac{\partial_\tau h}{h} \right)^2 \right] \chi_k = 0. \] (B4)

The field \( \chi \) is then quantised, which makes \( \phi \) take the form
\[ \phi(x) = \int \frac{d^3 k}{(2\pi)^3} h(\tau) \left[ \hat{a}_k \chi_k(\tau)e^{i k \cdot x} + \hat{a}^\dagger_k \chi_k(\tau)e^{-i k \cdot x} \right]. \] (B5)

The Hadamard Green function can then be written
\[ G^{(1)}(x, x') = \int \frac{d^3 k}{(2\pi)^3} h(\tau) h(\tau') \left[ \chi_k(\tau) \chi_k^*(\tau') e^{i k \cdot (x-x')} \right. \]
\[ + \left. \chi_k^*(\tau) \chi_k(\tau') e^{-i k \cdot (x-x')} \right]. \] (B6)

Acting on this with the bi-scalar derivative function and taking the 00 component thus gives
\[ \langle 0 | T_{00} | 0 \rangle_{\text{ren}} = \tilde{T} + \frac{1}{2} \int \frac{d^3 k}{(2\pi)^3} \tilde{h} \left[ \left( \partial_\tau \chi_k + \frac{\partial_\tau h}{h} \chi_k \right) \right. \]
\[ \cdot \left. \left( \chi_k + \frac{\partial_\tau h}{h} \chi_k^* \right) + \left( \frac{k^2}{a^2} + \frac{m^2}{\tau^2} \right) \chi_k \chi_k^* \right]. \] (B7)
Minimising the expression (B7) subject to this constraint gives for the mode functions $\chi_k$

$$|\chi_k|^2 = \frac{1}{2\sqrt{h^4a^4(k^2 + m^2a^2)}},$$

$$\partial_\tau \chi_k = \left(-\frac{i}{C_0} \sqrt{h^4a^4(k^2 + m^2a^2)} - \frac{\partial_\tau h}{h}\right)\chi_k.$$  (B8)