

Hamiltonian Formulation of General Relativity

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1 Introduction

The usual approach to treating general relativity as a field theory is based on the Lagrangian formulation. For some purposes (e.g. numerical relativity and canonical quantization), a Hamiltonian formulation is preferred. The Hamiltonian formulation of a field theory, like the Hamiltonian formulation of particle mechanics, requires choosing a preferred time variable. For a single particle, proper time may be used, and the Hamiltonian formulation remains manifestly covariant. For a continuous medium, the Hamiltonian formulation requires that a time variable be defined everywhere, not just along the path of one particle. Thus, the Hamiltonian formulation of general relativity requires a separation of time and space coordinates, known as a 3+1 decomposition. Although the form of the equations is no longer manifestly covariant, they are valid for any choice of time coordinate, and for any coordinate system the results are equivalent to those obtained from the Lagrangian approach.

It is convenient to decompose the metric as follows:

$$g_{00} = -\alpha^2 + \gamma^{ij} \beta_i \beta_j, \quad g_{0i} = \beta_i, \quad g_{ij} = \gamma_{ij}, \quad (1)$$

where γ^{ij} is the inverse of γ_{ij} , i.e. $\gamma^{ik} \gamma_{jk} = \delta^i_j$. This 3+1 decomposition of the metric replaces the 10 independent metric components by the **lapse function** $\alpha(x)$, the **shift vector** $\beta_i(x)$, and the symmetric **spatial metric** $\gamma_{ij}(x)$. The inverse spacetime metric components are

$$g^{00} = -\frac{1}{\alpha^2}, \quad g^{0i} = \frac{\beta^i}{\alpha^2}, \quad g^{ij} = \gamma^{ij} - \frac{\beta^i \beta^j}{\alpha^2}, \quad (2)$$

where $\beta^i \equiv \gamma^{ij}\beta_j$. From now on, except as noted otherwise, all Latin (spatial) indices are raised and lowered using the spatial metric. The determinant of the four-metric is $g = -\alpha^2\gamma$ where γ is the determinant of γ_{ij} .

The 3+1 decomposition separates the treatment of time and space coordinates. In place of four-dimensional gradients, we use time derivatives and three-dimensional gradients. **In these notes, the symbol ∇_i denotes the three-dimensional covariant derivative with respect to the metric γ_{ij} . We will not use the four-dimensional covariant derivative.** Thus,

$$\nabla_j A^i = \partial_j A^i + \gamma_{jk}^i A^k, \quad \gamma_{jk}^i \equiv \frac{1}{2}\gamma^{il}(\partial_j \gamma_{kl} + \partial_k \gamma_{jl} - \partial_l \gamma_{jk}) . \quad (3)$$

In these notes we choose units so that $16\pi G = 1$. We assume a coordinate basis throughout.

These notes first consider a general metric and then specialize to a perturbed Robertson-Walker spacetime.

2 Curvature and Gravitational Actions

In the 3+1 approach, spacetime is described by a set of three-dimensional hypersurfaces of constant time $t = x^0$ propagating forward in time. These hypersurfaces have **intrinsic curvature** given by the three-dimensional Riemann tensor,

$${}^{(3)}R^i{}_{lkm} = \partial_k \gamma_{lm}^i - \partial_m \gamma_{kl}^i + \gamma_{kn}^i \gamma_{lm}^n - \gamma_{mn}^i \gamma_{kl}^n . \quad (4)$$

Contractions define the three-dimensional Ricci tensor ${}^{(3)}R_{ij} = {}^{(3)}R^k{}_{ikj}$ and Ricci scalar, ${}^{(3)}R = \gamma^{ij}{}^{(3)}R_{ij}$. In addition to the intrinsic curvature, the hypersurface of constant time has an **extrinsic curvature** K_{ij} arising from its embedding in four-dimensional spacetime:

$$K_{ij} = \frac{1}{2\alpha} (\nabla_i \beta_j + \nabla_j \beta_i - \partial_t \gamma_{ij}) . \quad (5)$$

The full spacetime curvature is related to the intrinsic and extrinsic curvature of the constant-time hypersurfaces by the **Gauss-Codazzi equations**

$${}^{(4)}R^0{}_{jkl} = -\frac{1}{\alpha} (\nabla_k K_{jl} - \nabla_l K_{jk}) \quad (6)$$

and

$${}^{(4)}R^i{}_{jkl} = {}^{(3)}R^i{}_{jkl} - {}^{(4)}R^0{}_{jkl} \beta^i + K^i{}_k K_{jl} - K^i{}_l K_{jk} . \quad (7)$$

MTW and other sources give these relations assuming an orthonormal basis, for which $\beta^i = 0$ and $\alpha = 1$. Equations (6) and (7) are exact for any coordinate basis. The other components of the four-dimensional Riemann tensor follow from

$${}^{(4)}R^0{}_{i0j} = -\frac{1}{\alpha} \partial_t K_{ij} - K_i{}^k K_{jk} - \frac{1}{\alpha} \nabla_i \nabla_j \alpha + \frac{1}{\alpha} [\nabla_j (\beta^k K_{ik}) + K_{jk} \nabla_i \beta^k] \quad (8)$$

and

$${}^{(4)}R^k{}_{i0j} = {}^{(4)}R^k{}_{ilj}\beta^l + [{}^{(4)}R^0{}_{ilj}\beta^l - {}^{(4)}R^0{}_{i0j}] \beta^k + \alpha [\nabla^k K_{ij} - \nabla_i K^k{}_j] . \quad (9)$$

These equations may be combined to give:

$${}^{(4)}R_{ijkl} = {}^{(3)}R_{ijkl} + K_{ik}K_{jl} - K_{il}K_{jk} , \quad (10a)$$

$${}^{(4)}R_{0jkl} = {}^{(4)}R_{ijkl}\beta^i + \alpha(\nabla_k K_{jl} - \nabla_l K_{jk}) = {}^{(4)}R_{kl0j} , \quad (10b)$$

$$\begin{aligned} {}^{(4)}R_{0i0j} &= \alpha\partial_t K_{ij} + \alpha^2 K_i{}^k K_{jk} + \alpha\nabla_i \nabla_j \alpha + \alpha\beta^k \nabla_k K_{ij} \\ &\quad - \alpha\nabla_i(\beta^k K_{jk}) - \alpha\nabla_j(\beta^k K_{ik}) + {}^{(4)}R_{kilj}\beta^k \beta^l , \end{aligned} \quad (10c)$$

and

$${}^{(4)}R^{ij}{}_{kl} = {}^{(3)}R^{ij}{}_{kl} + K^i{}_k K^j{}_l - K^i{}_l K^j{}_k + \frac{4}{\alpha} \beta^{[i} \nabla_{[k} K^{j]}{}_{l]} , \quad (11a)$$

$${}^{(4)}R^{0j}{}_{kl} = -\frac{1}{\alpha}(\nabla_k K^j{}_l - \nabla_l K^j{}_k) , \quad (11b)$$

$${}^{(4)}R^{0i}{}_{0j} = -\frac{1}{\alpha}\partial_t K^i{}_j + K^i{}_k K^k{}_j - \frac{1}{\alpha}\nabla^i \nabla_j \alpha + \frac{1}{\alpha}\nabla_j(\beta^k K^i{}_k) - \frac{1}{\alpha}(\nabla_k \beta^i) K^k{}_j . \quad (11c)$$

From these one obtains the four-dimensional Einstein tensor components

$$G^{00} = -\frac{\mathcal{H}}{2\alpha^2\sqrt{\gamma}} , \quad \mathcal{H} = \sqrt{\gamma} [K_{ij}K^{ij} - K^2 - {}^{(3)}R] , \quad (12a)$$

$$G^{0i} = \frac{\alpha\mathcal{H}^i + \beta^i\mathcal{H}}{2\alpha^2\sqrt{\gamma}} , \quad \mathcal{H}^i = 2\sqrt{\gamma}\nabla_j(K^{ij} - K\gamma^{ij}) , \quad (12b)$$

$$\begin{aligned} G^{ij} &= -\frac{\beta^i\beta^j\mathcal{H}}{2\alpha^2\sqrt{\gamma}} + \frac{1}{\alpha\sqrt{\gamma}}\partial_t(\sqrt{\gamma}P^{ij}) + {}^{(3)}R^{ij} - \frac{1}{2}{}^{(3)}R\gamma^{ij} \\ &\quad - \frac{1}{\alpha}(\nabla^i\nabla^j - \gamma^{ij}\nabla^2)\alpha + \frac{1}{\alpha}\nabla_k(\beta^i P^{jk} + \beta^j P^{ik} - \beta^k P^{ij}) \\ &\quad + 2P^i{}_k P^{jk} - P P^{ij} - \frac{1}{2}\left(P_{kl}P^{kl} - \frac{1}{2}P^2\right)\gamma^{ij} , \end{aligned} \quad (12c)$$

where $K \equiv \gamma_{ij}K^{ij}$ and

$$P^{ij} \equiv K\gamma^{ij} - K^{ij} , \quad P \equiv \gamma_{ij}P^{ij} . \quad (13)$$

(Components of the four-dimensional Riemann and Einstein tensors are raised and lowered using the four-dimensional metric; components of all other quantities, including K_{ij} and the three-dimensional Riemann tensor, are raised and lowered using γ_{ij} .) The four-dimensional Ricci scalar obeys

$$\sqrt{-g}{}^{(4)}R = \alpha\sqrt{\gamma} [K_{ij}K^{ij} - K^2 + {}^{(3)}R] - 2\partial_t(\sqrt{\gamma}K) + 2\partial_i[\sqrt{\gamma}(K\beta^i - \nabla^i\alpha)] . \quad (14)$$

Equation (14) provides an expression for the Einstein-Hilbert Lagrangian in the 3+1 decomposition. This expression includes two derivative terms that make no contribution to the equations of motion. We may therefore define a new action involving the intrinsic and extrinsic curvatures of the hypersurfaces of constant coordinate time. The result is the ADM action [1]:

$$S_{\text{ADM}}[\alpha, \beta_i, \gamma_{ij}] = \int d^4x \mathcal{L}_{\text{ADM}}(\alpha, \beta_i, \gamma_{ij}) , \quad \mathcal{L}_{\text{ADM}} = \alpha\sqrt{\gamma} [K_{ij}K^{ij} - K^2 + {}^{(3)}R] . \quad (15)$$

The intrinsic curvature term may be integrated by parts to give

$$\int {}^{(3)}R \alpha\sqrt{\gamma} d^3x = \int [(\gamma^{ij}\gamma_{jk}^k - \gamma^{jk}\gamma_{jk}^i)\nabla_i\alpha + \alpha\gamma^{ij}(\gamma_{li}^k\gamma_{kj}^l - \gamma_{ij}^k\gamma_{kl}^l)] \sqrt{\gamma} d^3x \quad (16)$$

plus a surface term $\oint \alpha(\gamma^{jk}\gamma_{jk}^i - \gamma^{ij}\gamma_{jk}^k)dS_i$, where dS_i is the covariant surface element.

3 ADM Formulation

In the Lagrangian approach, the classical equations of motion follow from extremizing the total action with respect to the metric fields $\alpha(x)$, $\beta_i(x)$, $\gamma_{ij}(x)$ and any matter fields. The matter action S_{M} also depends on the metric fields. The functional derivative is defined by the integrand of a variation, neglecting any boundary terms arising from total derivatives, e.g.

$$\delta S[\gamma_{ij}] \equiv \lim_{\delta\gamma_{ij} \rightarrow 0} S[\gamma_{ij}(x) + \delta\gamma_{ij}(x)] - S[\gamma_{ij}(x)] \equiv \int d^4x \left(\frac{\delta S}{\delta\gamma_{ij}} \right) \delta\gamma_{ij}(x) , \quad (17)$$

where there variation is carried to first order in $\delta\gamma_{ij}$. The four-dimensional stress-energy tensor is given by

$$T^{\mu\nu} = \frac{2}{\sqrt{-g}} \frac{\delta S_{\text{M}}}{\delta g_{\mu\nu}} . \quad (18)$$

Using equation (1), this gives

$$\frac{\delta S_{\text{M}}}{\delta\alpha} = -\alpha^2\sqrt{\gamma} T^{00} , \quad (19a)$$

$$\frac{\delta S_{\text{M}}}{\delta\beta_i} = \alpha\sqrt{\gamma} \gamma^{ij} T^0_j , \quad (19b)$$

$$\frac{\delta S_{\text{M}}}{\delta\gamma_{ij}} = \frac{1}{2}\alpha\sqrt{\gamma} (T^{ij} - \beta^i\beta^j T^{00}) . \quad (19c)$$

(Note that four-dimensional components are always used for $T^{\mu\nu}$ and $G^{\mu\nu}$. Their components are raised and lowered using the full spacetime metric.) Varying the ADM action

with respect to the metric fields gives

$$\frac{\delta S_{\text{ADM}}}{\delta \alpha} = -\mathcal{H} = 2\alpha^2 \sqrt{\gamma} G^{00}, \quad (20a)$$

$$\frac{\delta S_{\text{ADM}}}{\delta \beta_i} = -\mathcal{H}^i = -2\alpha \sqrt{\gamma} \gamma^{ij} G^0_j, \quad (20b)$$

$$\begin{aligned} \frac{\delta S_{\text{ADM}}}{\delta \gamma_{ij}} &= -\partial_t(\sqrt{\gamma} P^{ij}) - \alpha \sqrt{\gamma} \left[{}^{(3)}R^{ij} - \frac{1}{2} {}^{(3)}R \gamma^{ij} \right] \\ &\quad + \sqrt{\gamma} (\nabla^i \nabla^j - \gamma^{ij} \nabla^2) \alpha - \sqrt{\gamma} \nabla_k (\beta^i P^{jk} + \beta^j P^{ik} - \beta^k P^{ij}) \\ &\quad - \alpha \sqrt{\gamma} \left[2P^i_k P^{jk} - P P^{ij} - \frac{1}{2} \left(P_{kl} P^{kl} - \frac{1}{2} P^2 \right) \gamma^{ij} \right] \\ &= -\alpha \sqrt{\gamma} (G^{ij} - \beta^i \beta^j G^{00}). \end{aligned} \quad (20c)$$

Combining equations (19) and (20) with $\delta S_{\text{ADM}} + \delta S_{\text{M}} = 0$ yields the Einstein equations

$$G^{\mu\nu} = \frac{1}{2} T^{\mu\nu}. \quad (21)$$

In the mechanics of a system of finitely many degrees of freedom, $S = \int L(q, \dot{q}, t) dt$ where q are generalized coordinates and $\dot{q} = dq/dt$ are coordinate velocities. The transition to a Hamiltonian formulation begins with the definition of canonical momenta, $p \equiv \partial L / \partial \dot{q}$. In field theory, there are infinitely many degrees of freedom; the Lagrangian $L = \int \mathcal{L} d^3x$ sums over every field variable. The discrete variables q are, in effect, replaced by infinitely many variables $\alpha(x) d^3x$, and so on. The field Lagrangian is now regarded as a function of both the generalized coordinates $(\alpha, \beta, \gamma_{ij})$ and their velocities $(\dot{\alpha}, \dot{\beta}, \dot{\gamma}_{ij})$, where a dot denotes ∂_t . Note that the coordinate time t must be singled out to define generalized momenta, and the Hamiltonian formulation regards time and space derivatives in very different ways — time derivatives act on individual generalized coordinates (the field values at fixed spatial position) while space derivatives relate different field values. Using equations (5) and (15), one finds the momenta conjugate to α , β_i , and γ_{ij} are, respectively,

$$\pi_\alpha \equiv \frac{\partial \mathcal{L}_{\text{ADM}}}{\partial \dot{\alpha}} \approx 0, \quad (22a)$$

$$\pi^i \equiv \frac{\partial \mathcal{L}_{\text{ADM}}}{\partial \dot{\beta}_i} \approx 0, \quad (22b)$$

$$\pi^{ij} \equiv \frac{\partial \mathcal{L}_{\text{ADM}}}{\partial \dot{\gamma}_{ij}} = \sqrt{\gamma} (K \gamma^{ij} - K^{ij}) = \sqrt{\gamma} P^{ij}. \quad (22c)$$

(The matter Lagrangian is assumed to be independent of the time derivative of the metric so it makes no contribution to the momenta.) In the classical theory, the momenta conjugate to α and β_i vanish because the Lagrangian is independent of $\dot{\alpha}$ and $\dot{\beta}$. In

quantum field theory, π_α and π^i vanish “weakly,” i.e. on shell (denoted by ≈ 0). In the language of Dirac [2], equations (22a) and (22b) are called **primary constraints**.

The Hamiltonian follows from Legendre transformation of the action:

$$\begin{aligned}
H &= \int \left[\dot{\alpha}\pi_\alpha + \dot{\beta}_i\pi^i + \dot{\gamma}_{ij}\pi^{ij} - \mathcal{L}_{\text{ADM}} - \mathcal{L}_{\text{M}} \right] d^3x \\
&= \int \left[\dot{\alpha}\pi_\alpha + \dot{\beta}_i\pi^i + 2\pi^{ij}\nabla_{(i}\beta_{j)} - 2\alpha K_{ij}\pi^{ij} - \mathcal{L}_{\text{ADM}} - \mathcal{L}_{\text{M}} \right] d^3x \\
&= \int \left[\dot{\alpha}\pi_\alpha + \dot{\beta}_i\pi^i - \alpha \left(\frac{\mathcal{L}_{\text{ADM}}}{\alpha} + 2K_{ij}\pi^{ij} \right) \right. \\
&\quad \left. - \beta_i(\partial_j\pi^{ij} + \partial_j\pi^{ji} + 2\gamma_{jk}^i\pi^{jk}) - \mathcal{L}_{\text{M}} \right] d^3x .
\end{aligned}$$

In the second line we have used equation (5) and in the last line we have integrated by parts the $\partial_{(i}\beta_{j)}$ terms and dropped the irrelevant boundary terms. Writing K_{ij} in terms of π^{ij} using equations (13) and (22c), we obtain the **ADM Hamiltonian**,

$$H(\alpha, \beta_i, \gamma_{ij}, \pi_\alpha, \pi^i, \pi^{ij}) = \int \left(\dot{\alpha}\pi_\alpha + \dot{\beta}_i\pi^i + \alpha\mathcal{H} + \beta_i\mathcal{H}^i - \mathcal{L}_{\text{M}} \right) d^3x , \quad (23)$$

where

$$\mathcal{H} = \frac{1}{\sqrt{\gamma}} \left(\gamma_{ik}\gamma_{jl} - \frac{1}{2}\gamma_{ij}\gamma_{kl} \right) \pi^{ij}\pi^{kl} - \sqrt{\gamma} {}^{(3)}R , \quad (24)$$

$$\mathcal{H}^i = -(\partial_j\pi^{ij} + \partial_j\pi^{ji} + 2\gamma_{jk}^i\pi^{jk}) = -2\sqrt{\gamma} \nabla_j \left(\frac{\pi^{ij}}{\sqrt{\gamma}} \right) . \quad (25)$$

These are exactly the same quantities introduced in equations (12a)–(12b) except that now they are expressed in terms of the canonical fields and momenta. The three-dimensional Ricci scalar is a function of the fields γ_{ij} only (it contains no time derivatives) and its spatial integral should be integrated by parts to eliminate the spatial derivatives. Note that the Hamiltonian densities \mathcal{H} and \mathcal{H}^i must be regarded as functions of the canonical variables γ_{ij} and π^{ij} and not, for example, $\pi^i{}_j \equiv \gamma_{jk}\pi^{ik}$ or $\pi \equiv \gamma_{ij}\pi^{ij}$.

The ADM Hamiltonian includes terms $\dot{\alpha}\pi_\alpha + \dot{\beta}_i\pi^i$ that would seem to depend on velocities. In fact, $\dot{\alpha}$ and $\dot{\beta}_i$ are Lagrange multipliers which enforce the primary constraints $\pi_\alpha \approx 0$ and $\pi^i \approx 0$. These Lagrange multipliers are arbitrary and will be constrained later by gauge-fixing. General covariance (diffeomorphism-invariance) allows us to replace $\dot{\alpha}$ and $\dot{\beta}_i$ by any functions of the metric variables $(\alpha, \beta_i, \gamma_{ij})$. This procedure amounts to making a gauge choice. For now we impose no gauge conditions.

We can obtain the equations of motion using equal-time Poisson brackets, which are defined by

$$\{A, B\} = \int \left[\frac{\delta A}{\delta\gamma_{ij}(\mathbf{x}, t)} \frac{\delta B}{\delta\pi^{ij}(\mathbf{x}, t)} - \frac{\delta A}{\delta\pi^{ij}(\mathbf{x}, t)} \frac{\delta B}{\delta\gamma_{ij}(\mathbf{x}, t)} \right] d^3x . \quad (26)$$

The fundamental Poisson brackets are

$$\{\alpha(\mathbf{x}), \pi_\alpha(\mathbf{x}')\} = \delta^3(\mathbf{x} - \mathbf{x}') , \quad (27a)$$

$$\{\beta_j(\mathbf{x}), \pi^i(\mathbf{x}')\} = \delta^i_j \delta^3(\mathbf{x} - \mathbf{x}') , \quad (27b)$$

$$\{\gamma_{kl}(\mathbf{x}), \pi^{ij}(\mathbf{x}')\} = \delta^i_{(k} \delta^j_{l)} \delta^3(\mathbf{x} - \mathbf{x}') . \quad (27c)$$

Using them, we may obtain the time evolution of the canonical variables:

$$\dot{\alpha} = \{\alpha, H\} = \dot{\alpha}(\alpha, \beta_i, \gamma_{ij}) , \quad (28a)$$

$$\dot{\beta}_i = \{\beta_i, H\} = \dot{\beta}_i(\alpha, \beta_i, \gamma_{ij}) , \quad (28b)$$

$$\dot{\gamma}_{ij} = \{\gamma_{ij}, H\} = \nabla_i \beta_j + \nabla_j \beta_i + \frac{\alpha}{\sqrt{\gamma}} (2\pi_{ij} - \pi \gamma_{ij}) , \quad (28c)$$

$$\dot{\pi}_\alpha = \{\pi_\alpha, H\} = -\mathcal{H} + \frac{\delta S_M}{\delta \alpha} = -\mathcal{H} - \alpha^2 \sqrt{\gamma} T^{00} \approx 0 , \quad (28d)$$

$$\dot{\pi}^i = \{\pi^i, H\} = -\mathcal{H}^i + \frac{\delta S_M}{\delta \beta_i} = -\mathcal{H}^i + \alpha \sqrt{\gamma} \gamma^{ij} T_{0j} \approx 0 , \quad (28e)$$

$$\begin{aligned} \dot{\pi}^{ij} = \{\pi^{ij}, H\} = & -\alpha \sqrt{\gamma} \left[{}^{(3)}R^{ij} - \frac{1}{2} {}^{(3)}R \gamma^{ij} \right] \\ & + \sqrt{\gamma} (\nabla^i \nabla^j - \gamma^{ij} \nabla^2) \alpha - \sqrt{\gamma} \nabla_k \left[\frac{2\beta^{(i} \pi^{j)k} - \beta^k \pi^{ij}}{\sqrt{\gamma}} \right] \\ & - \frac{\alpha}{\sqrt{\gamma}} \left[2\pi^i{}_k \pi^{jk} - \pi \pi^{ij} - \frac{1}{2} \left(\pi_{kl} \pi^{kl} - \frac{1}{2} \pi^2 \right) \gamma^{ij} \right] + \frac{\delta S_M}{\delta \gamma_{ij}} . \end{aligned} \quad (28f)$$

Equations (28a)–(28b) contain no dynamical content whatsoever; they arise as Lagrange multipliers. Equations (28d)–(28f) are equivalent to equations (19)–(21). Equation (28c) reproduces equation (22c). Equations (28d) and (28e) are called **secondary constraints** or dynamical constraints, as they enforce the primary constraints $\pi_\alpha \approx 0$ and $\pi^i \approx 0$. In the quantum theory, they imply that the wave function does not depend on α and β [2]. The last equation, (28f), contains the actual dynamics of the gravitational field. From equations (28c) and (28f), we see that γ_{ij} (unlike α and β_i) obeys a second-order differential equation in time.

We now wish to eliminate the non-dynamical degrees of freedom from the Hamiltonian. This is done following the prescription given by Dirac [2] and detailed by Weinberg [4]. The first step is to solve the secondary constraints for the non-dynamical variables α and β . The results depend on the matter fields. For a scalar field $\phi(x)$ with Lagrangian density

$$\mathcal{L}_M = \sqrt{-g} \left[-\frac{1}{2} g^{\mu\nu} (\partial_\mu \phi) (\partial_\nu \phi) - V(\phi) \right] , \quad (29)$$

varying the action yields

$$\frac{\delta S_M}{\delta \alpha} = -\sqrt{\gamma} \left[\frac{1}{2\alpha^2} (\dot{\phi} - \beta^k \partial_k \phi)^2 + \frac{1}{2} \gamma^{ij} (\partial_i \phi) (\partial_j \phi) + V(\phi) \right] , \quad (30a)$$

$$\frac{\delta S_M}{\delta \beta_i} = -\frac{\sqrt{\gamma}}{2\alpha} (\dot{\phi} - \beta^k \partial_k \phi) \gamma^{ij} (\partial_j \phi) , \quad (30b)$$

$$\frac{\delta S_M}{\delta \gamma_{ij}} = \frac{\alpha \sqrt{\gamma}}{2} \gamma^{ik} \gamma^{jl} (\partial_k \phi) (\partial_l \phi) . \quad (30c)$$

Solving equations (28d) and (28e) for α and β_i gives the following constraints:

$$C_\alpha \equiv \alpha^2 \left[\frac{2\mathcal{H}}{\sqrt{\gamma}} + \gamma^{ij} (\partial_i \phi) (\partial_j \phi) + 2V(\phi) \right] + (\dot{\phi} - \beta^k \partial_k \phi)^2 \approx 0 , \quad (31a)$$

$$C_i \equiv (\dot{\phi} - \beta^k \partial_k \phi) (\partial_i \phi) + \frac{2\alpha \mathcal{H}_i}{\sqrt{\gamma}} \approx 0 , \quad (31b)$$

where \mathcal{H} and \mathcal{H}_i are the functions of γ_{ij} and π^{ij} given by equations (24) and (25).

4 Eliminating non-dynamical degrees of freedom

Equations (31) are insufficient to fix α and β_i . They must be supplemented by gauge conditions. For example, the following conditions are equivalent in the weak-field limit to the transverse gauge conditions:

$$\chi_0 \equiv \nabla_i \beta^i \approx 0 , \quad \chi^i \equiv \partial_j (\gamma^{1/3} \gamma^{ij}) \approx 0 . \quad (32)$$

(Yes, that really is $\gamma^{1/3}$.) These constraints include what Dirac called **second-class constraints**, i.e. those whose Poisson brackets with the primary and secondary constraints do not vanish. We must follow the procedure outlined by [2] and [4], using the algebra of second-class constraints to modify the Poisson brackets. With the modified brackets, the commutators of constraints will lead to no new constraints and thereby provide a Lie algebra. **This section remains to be completed.**

5 Perturbed Robertson-Walker Spacetime

To clarify the treatment of constraints and gauge-fixing, it is useful to analyze a perturbative example. We choose the perturbed Robertson-Walker spacetime because of its cosmological relevance and because it has been studied extensively using the Lagrangian formulation.

The perturbed Robertson-Walker metric may be written

$$ds^2 = a^2(t) \left[-e^{2\Phi} dt^2 + 2w_j E^j{}_i dx^i dt + {}^0\gamma_{ik}(\mathbf{x}) E^k{}_l E^l{}_j dx^i dx^j \right] , \quad (33)$$

where the time-independent background Robertson-Walker spatial metric ${}^0\gamma_{ij}$ and its inverse ${}^0\gamma^{ij}$ are used to raise and lower all spatial indices unless otherwise noted. The time coordinate is called conformal time and the spatial coordinates are called comoving coordinates. We have introduced a spatial triad matrix E^i_j , which may be written

$$E^i_j = (e^{-\Psi})^i_j = \delta^i_j - \psi^i_j + \frac{1}{2!}\psi^i_k\psi^k_j + \dots \quad (34)$$

We require that Ψ be symmetric, i.e. $\psi_{ij} \equiv {}^0\gamma_{ik}\psi^k_j = \psi_{ji}$. The determinant of the spatial metric is $\gamma = {}^0\gamma a^6 \exp(-2\psi^i_i)$ where ${}^0\gamma$ is the determinant of ${}^0\gamma_{ij}$.

The metric of equation (33) has been parameterized in a fully general form but we will treat (Φ, w_i, ψ^k_j) as being small perturbations and will compute the Hamiltonian to second order in these variables. The translation of our new metric variables to those of equation (1) is

$$\begin{aligned} \alpha &= a (e^{2\Phi} + {}^0\gamma^{ij}w_iw_j)^{1/2} = a \left[1 + \Phi + \frac{1}{2}(\Phi^2 + w^2) + \dots \right], \\ \beta_i &= a^2 w_j E^j_i = a^2 (w_i - w_j \psi^j_i + \dots), \\ a^{-2}\gamma_{ij} &= {}^0\gamma_{ik}E^k_l E^l_j = {}^0\gamma_{ij} - 2\psi_{ij} + 2\psi_{ik}\psi^k_j + \dots, \\ a^2\gamma^{ij} &= {}^0\gamma^{ik}\tilde{E}^l_k \tilde{E}^j_l = {}^0\gamma^{ij} + 2\psi^{ij} + 2\psi^i_k\psi^kj + \dots, \end{aligned} \quad (35)$$

where $\tilde{\mathbf{E}} = \exp(\Psi)$ is the matrix inverse of $\mathbf{E} = \exp(-\Psi)$, i.e. $\tilde{E}^i_k E^k_j = E^i_k \tilde{E}^k_j = \delta^i_j$.

The connection coefficients with respect to γ_{ij} are

$$\gamma^k_{ij} = {}^0\gamma^k_{ij} + \tilde{E}^k_l \left[{}^0\nabla_{(i} E^l_{j)} + \tilde{E}^{lm} E_{n(i} {}^0\nabla_{j)} E^n_m - \tilde{E}^l_m E_{n(i} {}^0\nabla^m E^n_{j)} \right], \quad (36)$$

where ${}^0\gamma^k_{ij}$ is the connection and ${}^0\nabla_i$ is the covariant derivative, both taken with respect to ${}^0\gamma_{ij}$. Taylor expanding \mathbf{E} to second order in Ψ , we get

$$\gamma^k_{ij} = {}^0\gamma^k_{ij} + {}^1\gamma^k_{ij} + {}^2\gamma^k_{ij} + \dots, \quad (37)$$

where

$${}^1\gamma^k_{ij} = {}^0\nabla^k \psi_{ij} - {}^0\nabla_i \psi^k_j - {}^0\nabla_j \psi^k_i, \quad (38a)$$

$${}^2\gamma^k_{ij} = 2\psi^k_l \left[{}^0\nabla^l \psi_{ij} - {}^0\nabla_{(i} \psi^l_{j)} \right] + 2\psi^l_{(i} {}^0\nabla_{j)} \psi^k_l - 2\psi_{l(i} {}^0\nabla^k \psi^l_{j)}. \quad (38b)$$

Notice that the perturbations to the connection are three-tensors on the constant-time hypersurfaces.

The extrinsic curvature, to second order in the perturbations, is given by

$$\begin{aligned} a^{-1}K_{ij} &= -\eta \left[1 - \Phi + \frac{1}{2}(\Phi^2 - w^2) \right] {}^0\gamma_{ij} + \left[{}^0\nabla_{(i} w_{j)} + \frac{1}{a^2} \partial_t (a^2 \psi_{ij}) \right] (1 - \Phi) \\ &\quad - \psi^k_{(i} {}^0\nabla_{j)} w_k + \left[{}^0\nabla_{(i} \psi^k_{j)} - {}^0\nabla^k \psi_{ij} \right] w_k - \frac{1}{a^2} \partial_t (a^2 \psi_{ik} \psi^k_j), \end{aligned} \quad (39)$$

where $\eta \equiv \dot{a}/a$. This gives the following extrinsic curvature contribution to the ADM action:

$$\begin{aligned} \frac{\alpha\sqrt{\gamma}(K_{ij}K^{ij} - K^2)}{a^2\sqrt{{}^0\gamma}} &= -6\eta^2 + 2\eta [2B^i{}_i + \eta(3\Phi - \psi)] \\ &+ \tilde{K}_{ij}\tilde{K}^{ij} - (\tilde{K}^i{}_i)^2 - 4\eta \left[\Phi\tilde{K}^i{}_i + \psi^{ij}\psi_{ij} + w^i({}^0\nabla_i\psi - {}^0\nabla_j\psi^j{}_i) \right] \\ &- \eta^2 [3(\Phi^2 - w^2) - 2\Phi\psi - \psi^2 + 4\psi_{ij}\psi^{ij}] , \end{aligned} \quad (40)$$

where $\psi \equiv \psi^i{}_i$ and

$$\tilde{K}_{ij} = {}^0\nabla_{(i}w_{j)} + \frac{1}{a^2}\partial_t(a^2\psi_{ij}) \quad (41)$$

reduces to the extrinsic curvature when $\dot{a} = 0$. Cosmic expansion ($\dot{a} \neq 0$) introduces many terms. The second and third lines of equation (40) give the second-order contributions.

Expanding the intrinsic curvature to second order in the perturbations gives

$$\begin{aligned} {}^{(3)}R a^2 &= 6K + 4K(\psi + \psi_{ij}\psi^{ij}) + 2({}^0\nabla^2\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij}) \\ &- ({}^0\nabla_i\psi)({}^0\nabla^i\psi) - ({}^0\nabla_k\psi^{ij})({}^1\gamma_{ij}^k) \\ &- {}^0\nabla_i [2\psi^{ij}\partial_j\psi - 2\psi^{jk}({}^1\gamma_{jk}^i) - {}^0\gamma^{jk}({}^2\gamma_{jk}^i)] , \end{aligned} \quad (42)$$

where K is the three-dimensional curvature of the background Robertson-Walker space and has nothing to do with \tilde{K}_{ij} . The intrinsic curvature contribution to the ADM action is then:

$$\begin{aligned} \frac{{}^{(3)}R \alpha\sqrt{\gamma}}{a^2\sqrt{{}^0\gamma}} &= 6K[1 + (\Phi - \psi)] + 4K\psi + 2({}^0\nabla^2\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij}) \\ &+ 3K[(\Phi - \psi)^2 + w^2] + 4K(\Phi - \psi)\psi + 4K\psi_{ij}\psi^{ij} + 2(\Phi - \psi)({}^0\nabla^2\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij}) \\ &- ({}^0\nabla_i\psi)({}^0\nabla^i\psi) - ({}^0\nabla_k\psi^{ij})({}^1\gamma_{ij}^k) - {}^0\nabla_i [2\psi^{ij}\partial_j\psi - 2\psi^{jk}({}^1\gamma_{jk}^i) - {}^0\gamma^{jk}({}^2\gamma_{jk}^i)] . \end{aligned} \quad (43)$$

The second and third lines give the second-order contributions and a total derivative term that may be discarded.

The ADM Lagrangian follows from combining equations (40) and (43). The zeroth-order part is

$${}^0\mathcal{L}_{\text{ADM}}(a, {}^0\gamma_{ij}) = a^2\sqrt{{}^0\gamma} \left(-6\eta^2 + {}^0\gamma^{ij}{}^0A_{ij} \right) , \quad {}^0A_{ij} = {}^0\gamma_{li}^k{}^0\gamma_{jk}^l - {}^0\gamma_{ij}^k{}^0\gamma_{kl}^l . \quad (44)$$

Varying the total action with respect to $a(\tau)$ and ${}^0\gamma_{ij}(\mathbf{x})$ gives the Friedmann and energy conservation equations for homogeneous matter at rest in comoving coordinates. We assume henceforth that the zeroth-order metric functions are known, and examine the first-order and second-order Lagrangians.

The first-order ADM Lagrangian is

$$\begin{aligned} \frac{{}^1\mathcal{L}_{\text{ADM}}}{a^2\sqrt{{}^0\gamma}} &= 2\eta \left[2\tilde{K}^i{}_i + \eta(3\Phi - \psi) \right] + ({}^0\gamma^{ji} - {}^0\gamma^{ij})\partial_i(\Phi - \psi) \\ &+ [(\Phi - \psi) {}^0\gamma^{ij} + 2\psi^{ij}] {}^0A_{ij} - 2 \left[{}^0\gamma^{kij} - {}^0\gamma^{l(i} {}^0\gamma^{j)k} \right] {}^0\nabla_k\psi_{ij} . \end{aligned} \quad (45)$$

Extremizing the first-order action with respect to Φ gives the Friedmann equation

$$\frac{1}{a^2\sqrt{{}^0\gamma}} \frac{\delta({}^1S_{\text{ADM}})}{\delta\Phi} = 6(\eta^2 + K) = 2a^4G^{00} = -\frac{1}{a^2\sqrt{{}^0\gamma}} \frac{\delta S_{\text{M}}}{\delta\Phi} = a^4T^{00} = 16\pi Ga^2\rho_0 . \quad (46)$$

Here, ρ_0 is the unperturbed density. Extremizing the first-order action with respect to w_i gives the consistency condition ${}^0\nabla_j {}^0\gamma^{ij} = 0$. Extremizing the first-order action with respect to ψ_{ij} gives

$$\begin{aligned} \frac{1}{a^2\sqrt{{}^0\gamma}} \frac{\delta({}^1S_{\text{ADM}})}{\delta\psi_{ij}} &= -2(2\dot{\eta} + \eta^2 + 3K) {}^0\gamma^{ij} + 2 {}^0A^{ij} + \frac{2}{\sqrt{{}^0\gamma}} \partial_k \left[\sqrt{{}^0\gamma} ({}^0\gamma^{kij} - {}^0\gamma^{l(i} {}^0\gamma^{j)k}) \right] \\ &+ 4 {}^0\gamma^{kl(i} {}^0\gamma^{j)kl} - 2 {}^0\gamma^{(ij)k} {}^0\gamma^l{}_{kl} - 2 {}^0\gamma^{k(i} {}^0\gamma^{j)l}{}_l \\ &= -2(2\dot{\eta} + \eta^2 + K) {}^0\gamma^{ij} = 2a^4G^{ij} \\ &= -\frac{1}{a^2\sqrt{{}^0\gamma}} \frac{\delta S_{\text{M}}}{\delta\psi_{ij}} = a^4T^{ij} = 16\pi Ga^2p_0 {}^0\gamma^{ij} . \end{aligned} \quad (47)$$

Here, p_0 is the unperturbed pressure. In summary, extremizing the first-order action gives the unperturbed Einstein equations. This repeats what happened with the zeroth-order action. If we define $a(\tau)$ and ${}^0\gamma_{ij}(\mathbf{x})$ to be the classical solutions for the Robertson-Walker spacetime, then the zeroth-order and first-order action both vanish identically. In the quantum theory, a and ${}^0\gamma_{ij}$ equal the classical functions multiplied by the identity operator so that they commute with all observables.

The dynamics of the perturbations (Φ, w_i, ψ_{ij}) follow from the second-order Lagrangian density,

$$\begin{aligned} \frac{{}^2\mathcal{L}_{\text{ADM}}}{a^2\sqrt{{}^0\gamma}} &= \tilde{K}_{ij}\tilde{K}^{ij} - (\tilde{K}^i{}_i)^2 - 4\eta \left[\Phi\tilde{K}^i{}_i + \psi^{ij}\dot{\psi}_{ij} + w^i({}^0\nabla_i\psi - {}^0\nabla_j\psi^j{}_i) \right] \\ &+ (K - \eta^2)(3\Phi^2 - 2\Phi\psi - \psi^2 + 4\psi_{ij}\psi^{ij}) + 3(\eta^2 + K)w^2 \\ &+ 2(\Phi - \psi)({}^0\nabla^2\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij}) - ({}^0\nabla_i\psi)({}^0\nabla^i\psi) - ({}^0\nabla_k\psi^{ij})({}^1\gamma^k{}_{ij}) , \end{aligned} \quad (48)$$

where we have discarded the boundary terms of equation (48). Varying this Lagrangian

with respect to the metric fields gives

$$\begin{aligned} \frac{1}{2a^2\sqrt{{}^0\gamma}} \frac{\delta({}^2S_{\text{ADM}})}{\delta\Phi} &= ({}^0\nabla^2 + 2K)\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij} - 2\eta(\dot{\psi} + 3\eta\Phi + {}^0\nabla_i w^i) \\ &\quad + 3(\eta^2 + K)(\Phi - \psi) , \end{aligned} \quad (49a)$$

$$\begin{aligned} \frac{1}{2a^2\sqrt{{}^0\gamma}} \frac{\delta({}^2S_{\text{ADM}})}{\delta w_i} &= -\frac{1}{2}({}^0\nabla^2 + 2K)w^i + \frac{1}{2}{}^0\nabla^i({}^0\nabla_j w^j) - {}^0\nabla_j\dot{\psi}^{ij} + {}^0\nabla^i(\dot{\psi} + 2\eta\Phi) \\ &\quad + 3(\eta^2 + K)w^i , \end{aligned} \quad (49b)$$

$$\begin{aligned} \frac{1}{2a^2\sqrt{{}^0\gamma}} \frac{\delta({}^2S_{\text{ADM}})}{\delta\psi_{ij}} &= -(\partial_t^2 + 2\eta\partial_t - {}^0\nabla^2 + 2K)\psi^{ij} - (\partial_t + 2\eta) \left[{}^0\nabla^{(i} w^{j)} - ({}^0\nabla_k w^k) {}^0\gamma^{ij} \right] \\ &\quad + \left[\ddot{\psi} + 2\eta(\dot{\Phi} + \dot{\psi}) + 2(2\dot{\eta} + \eta^2)\Phi + {}^0\nabla_k{}^0\nabla_l\psi^{kl} \right] {}^0\gamma^{ij} \\ &\quad - ({}^0\nabla^i{}^0\nabla^j - {}^0\gamma^{ij}{}^0\nabla^2)(\Phi - \psi) - 2{}^0\nabla^{(i}\nabla_k\psi^{j)k} \\ &\quad - (2\dot{\eta} + \eta^2 + K)(\Phi - \psi) {}^0\gamma^{ij} . \end{aligned} \quad (49c)$$

In deriving these we used the commutators

$$\begin{aligned} ({}^0\nabla_k{}^0\nabla_l - {}^0\nabla_l{}^0\nabla_k)w^i &= K(\delta_k^i{}^0\gamma_{nl} - \delta_l^i{}^0\gamma_{nk})w^n , \\ ({}^0\nabla_k{}^0\nabla_l - {}^0\nabla_l{}^0\nabla_k)\psi^{ij} &= K(\delta_k^i{}^0\gamma_{nl} - \delta_l^i{}^0\gamma_{nk})\psi^{nj} + K(\delta_k^j{}^0\gamma_{nl} - \delta_l^j{}^0\gamma_{nk})\psi^{in} . \end{aligned} \quad (50)$$

Equations (49) (with $\psi^{ij} = \phi^0\gamma^{ij} - h^{ij}$) reproduces the Einstein tensor components given in Ref. [5]. As we will see, the last line of each of equations (49) arises from the unperturbed Einstein tensor and will disappear when we add the matter action terms to the Lagrangian.

To show this, we write the Lagrangian for scalar field matter (29) in a perturbed Robertson-Walker spacetime by letting $\phi \rightarrow \phi_0(t) + \phi(x)$ and using the perturbed metric to second order. The result is

$$\begin{aligned} \frac{\mathcal{L}_M}{a^2\sqrt{{}^0\gamma}} &= \frac{1}{2}\dot{\phi}_0^2 - \tilde{V}(\phi_0, a) + \dot{\phi}_0\dot{\phi} + \frac{1}{2}\dot{\phi}^2 - \tilde{V}(\phi_0 + \phi, a) + \tilde{V}(\phi_0, a) - \frac{1}{2}{}^0\gamma^{ij}(\partial_i\phi)(\partial_j\phi) \\ &\quad - \frac{1}{2}(\Phi + \psi)(\dot{\phi}_0 + \dot{\phi})^2 - (w^i\partial_i\phi)(\dot{\phi}_0 + \dot{\phi}) - (\Phi - \psi)\tilde{V}(\phi_0 + \phi, a) \\ &\quad - \frac{1}{2}[(\Phi - \psi) {}^0\gamma^{ij} + 2\psi^{ij}] (\partial_i\phi)(\partial_j\phi) \\ &\quad + \frac{1}{4}[(\Phi + \psi)^2 - w^2] (\dot{\phi}_0 + \dot{\phi})^2 + (\Phi + \psi)(\dot{\phi}_0 + \dot{\phi})(w^i\partial_i\phi) \\ &\quad + \frac{1}{2}(w^i\partial_i\phi)^2 - (\dot{\phi}_0 + \dot{\phi})\psi^{ij}(w_i\partial_j\phi) - [(\Phi - \psi)\psi^{ij} + \psi^i{}_k\psi^{jk}] (\partial_i\phi)(\partial_j\phi) \\ &\quad - \frac{1}{2}[(\Phi - \psi)^2 + w^2] \left[\tilde{V}(\phi_0 + \phi, a) + \frac{1}{2}{}^0\gamma^{ij}(\partial_i\phi)(\partial_j\phi) \right] , \end{aligned} \quad (51)$$

where

$$\tilde{V}(\phi, a) \equiv a^2 V(\phi) . \quad (52)$$

We have not linearized the scalar field; ϕ can be arbitrarily large. We have only dropped terms higher than quadratic in the metric perturbations. The terms in the first bracket give the Lagrangian for a spatially homogeneous scalar field $\phi_0(t)$. The second bracket gives contributions that are independent of the metric perturbations. The second and third lines give terms that are first order in the metric perturbations; the remaining lines give terms that are second order. The zeroth-order Lagrangian gives the equation of motion

$$\ddot{\phi}_0 + 2\eta\dot{\phi}_0 + \frac{\partial\tilde{V}}{\partial\phi_0} = 0 \quad (53)$$

and

$$a^2\rho_0 = \frac{1}{2}\dot{\phi}_0^2 + \tilde{V}(\phi_0, a) = 6(\eta^2 + K) , \quad (54a)$$

$$a^2 p_0 = \frac{1}{2}\dot{\phi}_0^2 - \tilde{V}(\phi_0, a) = -2(2\dot{\eta} + \eta^2 + K) . \quad (54b)$$

Together these imply

$$\frac{1}{4}\dot{\phi}_0^2 = \eta^2 - \dot{\eta} + K . \quad (55)$$

Now we linearize the scalar field by treating ϕ as a first-order quantity, similarly to the metric perturbations. The first-order scalar-field Lagrangian is

$$\frac{{}^1\mathcal{L}_M}{a^2\sqrt{{}^0\gamma}} = (\Phi - \psi) \left[\frac{1}{2}\dot{\phi}_0^2 - \tilde{V}(\phi_0, a) \right] + \dot{\phi}_0\dot{\phi} - \frac{\partial\tilde{V}}{\partial\phi_0}\phi - \dot{\phi}_0^2\Phi . \quad (56)$$

Varying this with respect to ϕ_0 reproduces equation (53). Varying it with respect to the metric perturbations and comparing with equations (46) and (47) reproduces equations (54a) and (54b). As with the gravitational action, the first-order matter action yields nothing new. We have to go to second order in the perturbations to see the dynamics of the perturbations.

The second-order scalar-field Lagrangian is

$$\begin{aligned} \frac{{}^2\mathcal{L}_M}{a^2\sqrt{{}^0\gamma}} &= \frac{1}{2} \left[\dot{\phi}^2 - {}^0\gamma^{ij}(\partial_i\phi)(\partial_j\phi) - \frac{\partial^2\tilde{V}}{\partial\phi_0^2}\phi^2 \right] - [(\Phi + \psi)\dot{\phi} + w^i\partial_i\phi] \dot{\phi}_0 \\ &+ \frac{1}{4} [(\Phi + \psi)^2 - w^2] \dot{\phi}_0^2 - \frac{1}{2} [(\Phi - \psi)^2 + w^2] \tilde{V}(\phi_0, a) - (\Phi - \psi) \frac{\partial\tilde{V}}{\partial\phi_0}\phi . \end{aligned} \quad (57)$$

Differentiating it gives

$$\begin{aligned} -\frac{1}{a^2\sqrt{0}\gamma}\frac{\delta(^2S_M)}{\delta\Phi} &= a^2\rho_0(\Phi - \psi) + \dot{\phi}_0\dot{\phi} + \frac{\partial\tilde{V}}{\partial\phi_0}\phi - \Phi\dot{\phi}_0^2 \\ &\equiv a^2[\rho_0(\Phi - \psi) + \delta\rho] , \end{aligned} \quad (58a)$$

$$-\frac{1}{a^2\sqrt{0}\gamma}\frac{\delta(^2S_M)}{\delta w_i} = a^2\rho_0 w^i + \dot{\phi}_0(^0\gamma^{ij})\partial_j\phi \equiv a^2[\rho_0 w^i - (\rho_0 + p_0)v^i] , \quad (58b)$$

$$\begin{aligned} -\frac{1}{a^2\sqrt{0}\gamma}\frac{\delta(^2S_M)}{\delta\psi_{ij}} &= \left[a^2 p_0(\Phi - \psi) + \dot{\phi}_0\dot{\phi} - \frac{\partial\tilde{V}}{\partial\phi_0}\phi - \Phi\dot{\phi}_0^2 \right] ^0\gamma^{ij} \\ &\equiv a^2[p_0(\Phi - \psi) + \delta p] ^0\gamma^{ij} . \end{aligned} \quad (58c)$$

As expected, the terms proportional to $a^2\rho_0$ and a^2p_0 cancel the last terms in equations (49) when the matter and gravitational actions are combined. The perturbations of energy density, velocity, and pressure are $\delta\rho$, v^i , and δp .

5.1 Hamiltonian Formulation

Before proceeding further with the ADM Lagrangian in a perturbed Robertson-Walker spacetime, we first compute the Hamiltonian for the scalar field, using the second-order Lagrangian. The canonical momentum of the scalar field is $\pi_\phi \equiv \partial(^2\mathcal{L}_M)/\partial\dot{\phi}$, which gives

$$\frac{\pi_\phi}{a^2\sqrt{0}\gamma} = \dot{\phi} - (\Phi + \psi)\dot{\phi}_0 . \quad (59)$$

Performing the Legendre transformation, we get

$$\begin{aligned} \frac{\mathcal{H}_M}{a^2\sqrt{0}\gamma} &= \frac{1}{2} \left[\frac{\pi_\phi^2}{(a^2\sqrt{0}\gamma)^2} + ^0\gamma^{ij}(\partial_i\phi)(\partial_j\phi) + \frac{\partial^2\tilde{V}}{\partial\phi_0^2}\phi^2 \right] + \frac{\pi_\phi}{a^2\sqrt{0}\gamma}(\Phi + \psi)\dot{\phi}_0 + \dot{\phi}_0 w^i \partial_i\phi \\ &\quad + \Phi\psi\dot{\phi}_0^2 + (\Phi - \psi)\frac{\partial\tilde{V}}{\partial\phi_0}\phi + \frac{1}{2} \left[\frac{1}{2}\dot{\phi}_0^2 + \tilde{V}(\phi_0, a) \right] [(\Phi - \psi)^2 + w^2] . \end{aligned} \quad (60)$$

With $a = 1$, the first set of terms (in square brackets) gives the Hamiltonian density of a scalar field in flat spacetime. The other terms give gravitational couplings.

Next we compute the ADM Hamiltonian by Legendre transformation of equation (48). The momentum conjugate to ψ_{ij} is $\pi^{ij} \equiv \partial^2\mathcal{L}_{\text{ADM}}/\partial\dot{\psi}_{ij}$, which gives

$$\frac{\pi^{ij}}{2a^2\sqrt{0}\gamma} = \dot{\psi}^{ij} + ^0\nabla^{(i}w^{j)} - ^0\gamma^{ij} \left[\dot{\psi} + 2\eta(\Phi + \psi) + ^0\nabla_k w^k \right] . \quad (61)$$

The ADM Hamiltonian density is given (up to irrelevant boundary terms) by

$$\begin{aligned} \frac{\mathcal{H}_{\text{ADM}}}{a^2\sqrt{0}\gamma} &= \dot{\Phi}\pi_\Phi + \dot{w}_i\pi^i + \frac{\pi_{ij}\pi^{ij} - \frac{1}{2}(\pi^k_k)^2}{4(a^2\sqrt{0}\gamma)^2} - \frac{\pi^{ij}}{a^2\sqrt{0}\gamma} [{}^0\nabla_{(i}w_{j)} + \eta(\Phi + \psi)^0\gamma_{ij}] \\ &\quad + 4\eta w^i\partial_i\psi - 12\eta^2\Phi\psi - 4K\psi_{ij}\psi^{ij} - 2(\Phi - \psi) [({}^0\nabla^2 + 2K)\psi - {}^0\nabla_i{}^0\nabla_j\psi^{ij}] \\ &\quad + ({}^0\nabla_i\psi)({}^0\nabla^i\psi) + ({}^0\nabla_k\psi^{ij})({}^1\gamma_{ij}^k) - 3(\eta^2 + K) [(\Phi - \psi)^2 + w^2] . \end{aligned} \quad (62)$$

The last term cancels the last term of equation (60).

The net Hamiltonian for the fields is given by adding equations (60) and (62):

$$\begin{aligned} H[\Phi, \pi_\Phi, w_i, \pi^i, \phi, \pi_\phi, \psi_{ij}, \pi^{ij}] &= \int (\mathcal{H}_{\text{ADM}} + \mathcal{H}_{\text{M}}) d^3x \\ &= \int (\mathcal{H}_\phi + \mathcal{H}_\psi + \mathcal{H}_{\text{int}} + \Phi\mathcal{H}_\Phi + w_i\mathcal{H}^i) d^3x , \end{aligned} \quad (63)$$

where

$$\mathcal{H}_\phi = \frac{a^2\sqrt{0}\gamma}{2} \left[\frac{\pi_\phi^2}{(a^2\sqrt{0}\gamma)^2} + {}^0\gamma^{ij}(\partial_i\phi)(\partial_j\phi) + \frac{\partial^2\tilde{V}}{\partial\phi_0^2}\phi^2 \right] , \quad (64a)$$

$$\begin{aligned} \mathcal{H}_\psi &= \frac{\pi_{ij}\pi^{ij} - \frac{1}{2}(\pi^k_k)^2}{4a^2\sqrt{0}\gamma} - \eta\psi\pi^k_k + a^2\sqrt{0}\gamma ({}^0\nabla_k\psi^{ij}) [{}^0\nabla^k\psi_{ij} - 2{}^0\nabla_{(i}\psi^k_{j)}] \\ &\quad - a^2\sqrt{0}\gamma ({}^0\nabla^i\psi) [{}^0\nabla_i\psi - 2{}^0\nabla^j\psi_{ij}] + 4K(\psi^2 - \psi_{ij}\psi^{ij})a^2\sqrt{0}\gamma , \end{aligned} \quad (64b)$$

$$\mathcal{H}_{\text{int}} = \left(\dot{\phi}_0\pi_\phi - a^2\sqrt{0}\gamma \frac{d\tilde{V}}{d\phi_0}\phi \right) \psi , \quad (64c)$$

$$\mathcal{H}_\Phi = \dot{\phi}_0\pi_\phi - \eta\pi^k_k + a^2\sqrt{0}\gamma \left[-2({}^0\nabla^2 + 2\eta + 4\eta^2)\psi + 2{}^0\nabla_i{}^0\nabla_j\psi^{ij} + \frac{\partial\tilde{V}}{\partial\phi_0}\phi \right] , \quad (64d)$$

$$\begin{aligned} \mathcal{H}^i &= \partial_j\pi^{ij} + {}^0\gamma^i_{jk}\pi^{jk} + a^2\sqrt{0}\gamma (\dot{\phi}_0\partial_j\phi + 4\eta\partial_j\psi)^0\gamma^{ij} \\ &= a^2\sqrt{0}\gamma \left[{}^0\nabla_j \left(\frac{\pi^{ij}}{a^2\sqrt{0}\gamma} \right) + (\dot{\phi}_0\partial_j\phi + 4\eta\partial_j\psi)^0\gamma^{ij} \right] . \end{aligned} \quad (64e)$$

We have ignored the Lagrange multiplier terms $\dot{\Phi}\pi_\Phi$ and $\dot{w}_i\pi^i$ since they play no role in the dynamics; Φ and w_i will follow from the equations of motion combined with gauge constraints. In equations (64), \mathcal{H}_ϕ depends only on ϕ and its conjugate momentum, \mathcal{H}_ψ depends only on ψ_{ij} and its conjugate momentum, and \mathcal{H}_{int} is a coupling between ϕ and ψ_{ij} . Because the Hamiltonian is independent of Φ and w_i , the corresponding momenta vanish weakly: $\pi_\Phi \approx 0$ and $\pi^i \approx 0$. As we will see, \mathcal{H}_Φ and \mathcal{H}^i are constraints on the dynamical fields ϕ and ψ_{ij} and their momenta.

The fundamental Poisson brackets are

$$\{\Phi(\mathbf{x}), \pi_\Phi(\mathbf{y})\} = \delta^3(\mathbf{x} - \mathbf{y}) , \quad (65a)$$

$$\{w_j(\mathbf{x}), \pi^i(\mathbf{y})\} = \delta^i_j \delta^3(\mathbf{x} - \mathbf{y}) , \quad (65b)$$

$$\{\phi(\mathbf{x}), \pi_\phi(\mathbf{y})\} = \delta^3(\mathbf{x} - \mathbf{y}) , \quad (65c)$$

$$\{\psi_{kl}(\mathbf{x}), \pi^{ij}(\mathbf{y})\} = \delta^i_{(k} \delta^j_{l)} \delta^3(\mathbf{x} - \mathbf{y}) . \quad (65d)$$

Using them, we obtain the classical time evolution of the canonical variables:

$$\dot{\phi} = \{\phi, H\} = \frac{\pi_\phi}{a^2 \sqrt{{}^0\gamma}} + (\Phi + \psi)\dot{\phi}_0 , \quad (66a)$$

$$\dot{\psi}_{ij} = \{\psi_{ij}, H\} = \frac{\pi_{ij} - \frac{1}{2}(\pi^k_k)^0 \gamma_{ij}}{2a^2 \sqrt{{}^0\gamma}} - {}^0\nabla_{(i} w_{j)} - \eta(\Phi + \psi)^0 \gamma_{ij} , \quad (66b)$$

$$\dot{\pi}_\Phi = \{\pi_\Phi, H\} = -\mathcal{H}_\Phi(\phi, \pi_\phi, \psi_{ij}, \pi^{ij}) \approx 0 , \quad (66c)$$

$$\dot{\pi}^i = \{\pi^i, H\} = -\mathcal{H}^i(\phi, \psi_{ij}, \pi^{ij}) \approx 0 , \quad (66d)$$

$$\dot{\pi}_\phi = \{\pi_\phi, H\} = a^2 \sqrt{{}^0\gamma} \left[{}^0\nabla^2 \phi - \frac{\partial^2 \tilde{V}}{\partial \phi_0^2} \phi - \frac{\partial \tilde{V}}{\partial \phi_0} (\Phi - \psi) + \dot{\phi}_0 ({}^0\nabla_i w^i) \right] , \quad (66e)$$

$$\begin{aligned} \frac{\dot{\pi}^{ij}}{a^2 \sqrt{{}^0\gamma}} &= \frac{\eta \pi^k_k {}^0 \gamma^{ij}}{a^2 \sqrt{{}^0\gamma}} + 2({}^0\nabla^2 - 2K)\psi^{ij} - 2({}^0\nabla^i {}^0\nabla^j - {}^0\gamma^{ij} {}^0\nabla^2)(\Phi - \psi) \\ &\quad + 2[2(\dot{\eta} + 2\eta^2)\Phi - 2K\psi + {}^0\nabla_k {}^0\nabla_l \psi^{kl} + 2\eta({}^0\nabla_k w^k)] {}^0\gamma^{ij} \\ &\quad - 4 {}^0\nabla^{(i} \nabla_k \psi^{j)k} + \left(\frac{d\tilde{V}}{d\phi_0} \phi - \frac{\dot{\phi}_0 \pi_\phi}{a^2 \sqrt{{}^0\gamma}} \right) {}^0\gamma^{ij} . \end{aligned} \quad (66f)$$

A superscript 0 has been neglected on the ∇_k on the third line of equation (66f) for notational clarity. Equations (66a) and (66b) reproduce equations (59) and (61), respectively. Equations (66c) and (66d) are secondary constraints which enforce the primary constraints $\pi_\Phi \approx 0$ and $\pi^i \approx 0$. They are equivalent to equations (49a) and (49b) combined with equations (58a) and (58b).

The last two equations, (66e) and (66f), contain the actual dynamics of the scalar and gravitational field. Combining equations (66a) and (66e) gives the equation of motion for the scalar field:

$$\ddot{\phi} + 2\eta\dot{\phi} - {}^0\nabla^2 \phi + \frac{\partial^2 \tilde{V}}{\partial \phi_0^2} \phi = -2 \frac{\partial \tilde{V}}{\partial \phi_0} \Phi + \dot{\phi}_0 (\dot{\Phi} + \dot{\psi}) + \dot{\phi}_0 ({}^0\nabla_i w^i) . \quad (67)$$

Combining equations (66b) and (66f) yields the equation of motion for ψ_{ij} . They are simplest when separated into the trace and trace-free parts. We write

$$\psi_{ij} = \Psi {}^0\gamma_{ij} - s_{ij} , \quad {}^0\gamma^{ij} s_{ij} = 0 . \quad (68)$$

Note that $\psi = 3\Psi$ where Ψ is the usual notation for the gauge-invariant spatial curvature perturbation. By combining the Hamilton equations (66), we get

$$\begin{aligned}
& \ddot{\Psi} + \eta(2\dot{\Psi} + \dot{\Phi}) + \frac{1}{3} {}^0\nabla^2(\Phi - \Psi) - K\Psi + (2\dot{\eta} + \eta^2)\Phi \\
&= \frac{1}{4} \left(\dot{\phi}_0 \dot{\phi} - \frac{\partial \tilde{V}}{\partial \phi_0} \phi - \Phi \dot{\phi}_0^2 \right) - \frac{1}{3a^2} \partial_t [a^2 ({}^0\nabla_k w^k)] + \frac{1}{6} {}^0\nabla_i {}^0\nabla_j s^{ij} , \\
&= 4\pi G a^2 \delta p - \frac{1}{3a^2} \partial_t [a^2 ({}^0\nabla_k w^k)] + \frac{1}{6} {}^0\nabla_i {}^0\nabla_j s^{ij} .
\end{aligned} \tag{69}$$

The traceless parts of equations (66b) and (66f) give

$$\begin{aligned}
& (\partial_t^2 + 2\eta\partial_t - {}^0\nabla^2 + 2K)s_{ij} - (\partial_t + 2\eta) {}^0\nabla_{(i} w_{j)} + \left({}^0\nabla_i {}^0\nabla_j - \frac{1}{3} {}^0\gamma^{ij} {}^0\nabla^2 \right) (\Psi - \Phi) \\
&= -\frac{1}{2} {}^0\gamma_{ij} (\partial_t + 2\eta) ({}^0\nabla_k w^k) - 2 {}^0\nabla_{(i} \nabla^k s_{j)k} .
\end{aligned} \tag{70}$$

Equations (69) and (70) simplify when we impose the transverse gauge conditions

$$\chi_0 \equiv {}^0\nabla_k w^k \approx 0 , \quad \chi^j \equiv {}^0\nabla_k s^{jk} = {}^0\nabla_k \left(\frac{1}{3} \psi {}^0\gamma^{jk} - \psi^{jk} \right) \approx 0 . \tag{71}$$

We have introduced the symbols χ_0 and χ^j for gauge constraints to be used later.

For the remainder of this subsection we assume these gauge conditions hold and explore the classical equations of motion. Then the right-hand side of equation (70) vanishes. Using the scalar-vector-tensor decomposition, the left-hand side separates into parts that are doubly transverse (s_{ij}), semi-transverse [${}^0\nabla_{(i} w_{j)}$], and doubly longitudinal ($\Phi - \psi$). All three parts must vanish separately, yielding

$$(\partial_t^2 + 2\eta\partial_t - {}^0\nabla^2 + K)s_{ij} = 0 , \tag{72a}$$

$$(\partial_t + 2\eta) {}^0\nabla_{(i} w_{j)} = 0 , \tag{72b}$$

$$\left({}^0\nabla_i {}^0\nabla_j - \frac{1}{3} {}^0\gamma^{ij} {}^0\nabla^2 \right) (\Psi - \Phi) = 0 . \tag{72c}$$

The first of these is the evolution equation for gravitational waves. The second equation implies $w_i = 0$: in linear theory, a scalar field cannot generate a vector mode. The third equation implies that $\Psi - \Phi$ is spatially homogeneous. Any time-varying contribution to this contribution may be gauged away by modifying that background curvature and hence is unmeasurable. We may therefore conclude that $\Phi = \Psi$.

Next we examine the secondary constraints. Using equations (59), (61), and (64d), $\mathcal{H}_\Phi = 0$ gives

$$\begin{aligned}
({}^0\nabla^2 + 3K)\Psi - 3\eta(\dot{\Psi} + \eta\Phi) &= \frac{1}{4} \left(\dot{\phi}_0 \dot{\phi} + \frac{\partial \tilde{V}}{\partial \phi_0} \phi - \Phi \dot{\phi}_0^2 \right) + \eta ({}^0\nabla_k w^k) - \frac{1}{2} {}^0\nabla_i {}^0\nabla_j s^{ij} \\
&= 4\pi G a^2 \delta \rho + \eta ({}^0\nabla_k w^k) - \frac{1}{2} {}^0\nabla_i {}^0\nabla_j s^{ij} .
\end{aligned} \tag{73}$$

From equations (49a) and (58a), this is equivalent to $\delta(^2S)/\delta\Phi = 0$. Similarly, using equations (61) and (64e), $\mathcal{H}^i = 0$ implies

$$\begin{aligned} \frac{1}{4}(^0\nabla^2 + 2K)w_i - ^0\nabla_i(\dot{\Psi} + \eta\Phi) &= -\frac{1}{4}^0\nabla_i(\dot{\phi}_0\phi) + \frac{1}{4}^0\nabla_i(^0\nabla_k w^k) + \frac{1}{2}^0\nabla_k \dot{s}^k{}_i \\ &= 4\pi G a^2(\rho_0 + p_0)v_i + \frac{1}{4}^0\nabla_i(^0\nabla_k w^k) + \frac{1}{2}^0\nabla_k \dot{s}^k{}_i. \end{aligned} \quad (74)$$

From equations (49b) and (58b), this is equivalent to $\delta(^2S)/\delta w_i = 0$. With the gauge conditions (71) imposed, equations (73) and (74) reduce to the standard equations for gauge-invariant perturbations. They are initial-value constraints; their time derivatives combined with equation (67) are redundant with equations (69) and (70).

Combining the equations of motion yields a single second-order equation for Ψ :

$$\ddot{\Psi} + 3(1 + c_w^2)\eta\dot{\Psi} + 3(c_w^2 - w)\eta^2\Psi - (5 + 3w)K\Psi - \nabla^2\Psi = 0, \quad (75)$$

where

$$w \equiv \frac{p_0}{\rho_0} = \frac{2(\eta^2 - \dot{\eta} + K)}{3(\eta^2 + K)} - 1, \quad c_w^2 \equiv \frac{dp_0}{d\rho_0} = w - \frac{1}{3} \frac{d \ln(1+w)}{d \ln a} = 1 + \frac{2}{3\eta\phi_0} \frac{\partial \tilde{V}}{\partial \phi_0}. \quad (76)$$

This equation is to be solved subject to appropriate initial conditions. Once Ψ is given, the scalar field follows from the longitudinal part of equation (74) (or equivalently from energy conservation),

$$\phi = \frac{4}{\phi_0}(\dot{\Psi} + \eta\Phi). \quad (77)$$

In the transverse gauge, the complete classical solution of the linear perturbation problem is given by the solutions of equations (72a) and (75) followed by (77), with $\Phi = \Psi$ and $w_i = 0$.

5.2 Reducing the Hamiltonian

The Hamiltonian of equation (63) is not ready for quantization because several of the fields are constrained. We need to eliminate the constrained degrees of freedom. As we will see, this involves two stages. In the first stage, we remove $g_{0\mu}$ leaving us with a Hamiltonian for ϕ and ψ_{ij} and their momenta. In the second stage, we reduce ψ_{ij} further to only its transverse-traceless part. These reductions will be performed using the method of Dirac brackets [2, 3, 4]. From now on, we drop the subscript 0 from the spatial metric, connection, and gradient. All fields are defined on the background Robertson-Walker space.

5.2.1 Eliminating $g_{0\mu}$

As we will see, the $p_{0\mu}$ parts of the metric perturbations are algebraically constrained in terms of ψ_{ij} and can be eliminated from the Hamiltonian system once we impose the appropriate constraints. We consider the following constraints: $\pi_\Phi \approx 0$ and $\pi^i \approx 0$ (primary); $\mathcal{H}_\Phi \approx 0$ and $\mathcal{H}^i \approx 0$ (secondary); and $\chi_0 \approx 0$ and $\chi_i \approx 0$ (gauge). We can reduce the Hamiltonian only if the Poisson brackets of all pairs of constraints vanish weakly. Such constraints are said to be first class.

The first step is therefore to evaluate the matrix of Poisson brackets of all pairs of constraints. Considering only the primary and secondary constraints, it is easy to see that they all vanish weakly except, possibly, $\{\mathcal{H}_\Phi(\vec{x}), \mathcal{H}^i(\vec{y})\}$. To evaluate this Poisson bracket, multiply $\mathcal{H}_\Phi(\vec{x})$ and $\mathcal{H}^i(\vec{y})$ by $A(\vec{x})B(\vec{y})$, where A and B are any functions whose Poisson brackets with all fields vanish. To handle the gradients appearing in the constraints, integrate the Poisson bracket over volume (either d^3x or d^3y). The following identity is useful:

$$\mathcal{L}^{jk}\gamma_{jk}^i = \nabla_j R^{ij} - R^{jk}\gamma_{jk}^i, \quad \mathcal{L}^{jk} \equiv R^{jk} + \gamma^{jmk}(\partial_l \partial_m - \gamma_{lm}^n \partial_n) - 2\gamma^{nlm(j} \gamma_{lm}^{k)} \partial_n + \gamma^{nlmo} \gamma_{lm}^j \gamma_{no}^k, \quad (78)$$

where $\gamma^{jmk} = \gamma^{jk}\gamma^{lm} - \gamma^{jl}\gamma^{km}$. The differential operator is defined so that $\mathcal{L}^{jk}\psi_{jk} = \nabla^2\psi - \nabla^j\nabla^k\psi_{jk}$. After some effort, using this identity one can show $\{\mathcal{H}_\Phi(\vec{x}), \mathcal{H}^i(\vec{y})\} = 0$. Thus, the Poisson brackets of the primary and secondary constraints vanish making them first-class constraints.

When gauge constraints are added, some of the Poisson brackets no longer vanish. We find

$$\{\chi_0(\mathbf{x}), \pi^i(\mathbf{y})\} = \left[\gamma^{ij}(\mathbf{x}) \frac{\partial}{\partial x^j} - \gamma^{jk}(\mathbf{x}) \gamma_{jk}^i(\mathbf{x}) \right] \delta^3(\mathbf{x} - \mathbf{y}), \quad (79a)$$

$$\begin{aligned} \{\chi_i(\mathbf{x}), \mathcal{H}_\Phi(\mathbf{y})\} &= -\eta \gamma^{jk}(\mathbf{x}) \left[\gamma_{ij}(\mathbf{y}) \frac{\partial}{\partial x^k} - \gamma_{il}(\mathbf{y}) \gamma_{jk}^l(\mathbf{x}) \right] \delta^3(\mathbf{x} - \mathbf{y}) \\ &+ \frac{1}{3} \eta \gamma^{jk}(\mathbf{x}) \left[\gamma_{jk}(\mathbf{y}) \frac{\partial}{\partial x^i} + \gamma_{kl}(\mathbf{y}) \gamma_{ij}^l(\mathbf{x}) \right] \delta^3(\mathbf{x} - \mathbf{y}), \end{aligned} \quad (79b)$$

$$\begin{aligned} \{\chi_j(\mathbf{x}), \mathcal{H}^i(\mathbf{y})\} &= -\frac{1}{2} \delta^i_j \gamma^{kl}(\mathbf{x}) \left[\frac{\partial^2}{\partial x^k \partial y^l} - \gamma_{kl}^m(\mathbf{x}) \frac{\partial}{\partial y^m} \right] \delta^3(\mathbf{x} - \mathbf{y}) \\ &- \frac{1}{2} \left[\gamma^{ik}(\mathbf{x}) \frac{\partial}{\partial x^k} - \gamma^{kl}(\mathbf{x}) \gamma_{kl}^i(\mathbf{x}) \right] \frac{\partial}{\partial y^j} \delta^3(\mathbf{x} - \mathbf{y}) \\ &+ \frac{1}{6} \left[2\gamma^{il}(\mathbf{x}) \frac{\partial}{\partial x^j} + \gamma^{ik}(\mathbf{x}) \gamma_{jk}^l(\mathbf{x}) + \gamma^{kl}(\mathbf{x}) \gamma_{jk}^i(\mathbf{x}) \right] \frac{\partial}{\partial y^l} \delta^3(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (79c)$$

Given four gauge constraints and eight original constraints, we expect a total of $8 - 4 = 4$ first-class constraints. Clearly π_Φ remains first class. Where are the other three first-class constraints?

By integrating the Poisson brackets over volume, one finds that $\{\chi_i(\mathbf{x}), \mathcal{H}_\Phi(\mathbf{y})\} \approx 0$, so that \mathcal{H}_Φ remains first class. The other two first-class constraints are found in the decomposition of $\pi^i(\mathbf{x})$ into longitudinal and transverse parts. To facilitate this decomposition in a curved space, first we define the divergence and curl of the tensor density $\pi^i(\mathbf{x})$,

$$\vec{\nabla} \cdot \vec{\pi} \equiv \partial_i \pi^i, \quad (\vec{\nabla} \times \vec{\pi})^k \equiv \epsilon^{ijk} \partial_i \left(\frac{\gamma_{jl} \pi^l}{\sqrt{\gamma}} \right). \quad (80)$$

Here, ϵ^{ijk} is the Levi-Civita tensor density, and the divergence and curl of tensor densities so defined are also tensor densities. Now we decompose $\pi^i(\mathbf{x})$:

$$\pi^i(\mathbf{x}) = \pi_{\parallel}^i + \pi_{\perp}^i, \quad \vec{\nabla} \cdot \vec{\pi}_{\perp} = 0, \quad \vec{\nabla} \times \vec{\pi}_{\parallel} = 0. \quad (81)$$

Substituting into equation (79a), we find $\{\chi_0(\mathbf{x}), \vec{\nabla} \times \vec{\pi}(\mathbf{y})\} \approx 0$ implying that the two independent components of $\vec{\pi}_{\perp}$ commute with all other constraints. Thus, of the original 8 first-class constraints, 4 ($\pi_{\Phi}, \mathcal{H}_{\Phi}, \pi_{\perp}^i$) remain first class, while the remaining 4 ($\pi_{\parallel}^i, \mathcal{H}^i$) become second-class. The new constraints (χ_0, χ_i) are also second-class. We now implement Dirac's method to convert the second-class constraints to first-class.

In general, the set of all second-class constraints χ_m forms a matrix of Poisson brackets $C_{mn}(\mathbf{x}, \mathbf{y}) \equiv \{\chi_m(\mathbf{x}), \chi_n(\mathbf{y})\}$ whose inverse $C_{mn}^{-1}(\mathbf{x}, \mathbf{y}) = \{\chi_m(\mathbf{x}), \chi_n(\mathbf{y})\}^{-1} = -C_{nm}^{-1}(\mathbf{y}, \mathbf{x})$ is defined by the relations

$$\begin{aligned} \sum_k \int d^3 x' C_{mk}^{-1}(\mathbf{x}, \mathbf{x}') C_{kn}(\mathbf{x}', \mathbf{y}) &= \delta_{mn} \delta^3(\mathbf{x} - \mathbf{y}), \\ \sum_k \int d^3 x' C_{mk}(\mathbf{x}, \mathbf{x}') C_{kn}^{-1}(\mathbf{x}', \mathbf{y}) &= \delta_{mn} \delta^3(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (82)$$

The inverse matrix is used to define a new set of brackets, the Dirac brackets:

$$\begin{aligned} &\{U(\mathbf{x}), V(\mathbf{y})\}_{\text{D}} - \{U(\mathbf{x}), V(\mathbf{y})\} \\ &= - \sum_{k,l} \int d^3 x' \int d^3 y' \{U(\mathbf{x}), \chi_k(\mathbf{x}')\} C_{kl}^{-1}(\mathbf{x}', \mathbf{y}') \{\chi_l(\mathbf{y}'), V(\mathbf{y})\}. \end{aligned} \quad (83)$$

Here, U and V are any fields while the sum over (k, l) is taken over only the second-class constraints. It follows at once that the second-class constraints have vanishing Dirac brackets with all fields, so that all constraints become first-class. The key to reducing the Hamiltonian, a preliminary to canonical quantization, is to find the Dirac brackets.

In the present case it will prove useful to replace π_{\parallel}^i by a scalar potential:

$$\pi^i = -\sqrt{\gamma} \gamma^{ij} \partial_j \omega. \quad (84)$$

Equation (79a) can now be replaced by a Poisson bracket with $\omega(\mathbf{y})$:

$$\{\chi_0(\mathbf{x}), \pi^i(\mathbf{y})\} = -\sqrt{\gamma(\mathbf{y})} \gamma^{ij}(\mathbf{y}) \frac{\partial}{\partial y^j} \frac{\delta^3(\mathbf{x} - \mathbf{y})}{\sqrt{\gamma(\mathbf{x})}}. \quad (85)$$

In flat coordinates this change is trivial, but in a curved geometry one needs to integrate the Poisson brackets over volume with test function $A(\mathbf{x})B(\mathbf{y})$ to demonstrate the equivalence of equations (79a) and (85). Comparing equations (84) and (85), we obtain

$$\{\chi_0(\mathbf{x}), \omega(\mathbf{y})\} = \frac{\delta^3(\mathbf{x} - \mathbf{y})}{\sqrt{\gamma(\mathbf{x})}}. \quad (86)$$

The second-class constraints decouple into pairs (χ_0, ω) and (χ_j, \mathcal{H}^i) . The inverse constraint matrix element for the first pair are is

$$\{\chi_0(\mathbf{x}), \omega(\mathbf{y})\}^{-1} = -\{\omega(\mathbf{y}), \chi_0(\mathbf{x})\}^{-1} = -\sqrt{\gamma(\mathbf{x})} \delta^3(\mathbf{x} - \mathbf{y}). \quad (87)$$

It follows that the Dirac bracket of the vector gravitational potential and its canonical momentum vanishes:

$$\{w_j(\mathbf{x}), \pi^i(\mathbf{y})\}_D = 0. \quad (88)$$

At first this result is surprising because it implies that the field and canonical momentum do not obey canonical bracket relations. The resolution is that w_j and π^i vanish identically (both classically and quantum mechanically) because they are constrained rather than dynamical degrees of freedom. Physically, scalar mode linear density fluctuations cannot generate a vector mode.

The constraint matrix for the second pair of constraints is given by equation (79c). Inverting this is accomplished most easily with a mode expansion in the eigenfunctions of the spatial Laplace operator. To simplify the expressions we temporarily assume a flat Robertson-Walker background with Cartesian coordinates, obtaining the following Fourier representation: ***** (NO: USE P^i_j !! No need to use Fourier) *****

$$\{\chi_i(\mathbf{x}), \mathcal{H}^j(\mathbf{y})\}^{-1} = -\{\mathcal{H}^j(\mathbf{x}), \chi_i(\mathbf{y})\}^{-1} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}}{k^2} \left(\delta^i_j - \frac{1}{4} n^i n_j \right), \quad (89)$$

where $n^i \equiv k^i/k$. Because \mathcal{H}^i depends not only on π^{ij} but also on ϕ and ψ , the Dirac brackets couple π^{ij} to several fields. Using equation (83), one finds the complete set of

nonzero Dirac brackets to be

$$\{\Phi(\mathbf{x}), \pi_\Phi(\mathbf{y})\}_D = \delta^3(\mathbf{x} - \mathbf{y}) , \quad (90a)$$

$$\{\phi(\mathbf{x}), \pi_\phi(\mathbf{y})\}_D = \delta^3(\mathbf{x} - \mathbf{y}) , \quad (90b)$$

$$\{\psi_{kl}(\mathbf{x}), \pi^{ij}(\mathbf{y})\}_D = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \left[P_k^{(i} P_l^{j)} + \frac{1}{2} n_k n_l P^{ij} \right] , \quad (90c)$$

$$\{\pi_\phi(\mathbf{x}), \pi^{ij}(\mathbf{y})\}_D = \frac{3}{2} a^2 \dot{\phi}_0 \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \left(n^i n^j - \frac{1}{3} \delta^{ij} \right) , \quad (90d)$$

$$\{\pi^{ij}(\mathbf{x}), \pi^{kl}(\mathbf{y})\}_D = 6a^2 \eta \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} (\delta^{ij} n^k n^l - n^i n^j \delta^{kl}) , \quad (90e)$$

where

$$P^{ij} \equiv \gamma^{ij} - \nabla^i \nabla^j \nabla^{-2} \quad (91)$$

projects out the longitudinal parts of a vector and leaves a transverse vector unchanged. In flat spacetime, $P^{ij} = \gamma^{ij} - n^i n^j$ may be regarded as the (inverse) metric for the two-space orthogonal to the wavevector. Equation (91) generalizes this to arbitrary Robertson-Walker spaces with the understanding that $\nabla^{-2} f = g$ is equivalent to $\nabla^2 g = f$.

To proceed further we must decompose ψ_{ij} and π^{ij} into longitudinal and transverse parts. Symmetric two-index tensors may be decomposed into longitudinal and transverse parts as follows:

$$\psi_{ij}(\mathbf{x}) = \psi_{ij}^{(0)}(\mathbf{x}) + \psi_{ij}^{(1)}(\mathbf{x}) + \psi_{ij}^{(2)}(\mathbf{x}) , \quad (92)$$

and similarly for π^{ij} , where there exists a scalar field f and a transverse vector ψ_i^\perp such that

$$\psi_{ij}^{(0)} = \nabla_i \nabla_j f , \quad \psi_{ij}^{(1)} = \nabla_{(i} \psi_{j)}^\perp \quad \text{where} \quad \nabla^i \psi_i^\perp = 0 , \quad \nabla^i \psi_{ij}^{(2)} = 0 . \quad (93)$$

We are now assuming arbitrary Robertson-Walker background. The gauge conditions $\chi_0 = 0$ and $\chi_i = 0$ imply that we can write

$$\psi_{ij} = \nabla_i \nabla_j \nabla^{-2} \Psi + \psi_{ij}^{(2)} , \quad \Psi = \frac{1}{2} \gamma^{ij} \psi_{ij}^{(2)} = \frac{1}{3} \psi , \quad (94)$$

where $\psi_{ij}^{(2)}$ is doubly transverse (but not traceless). Similarly, the secondary constraint $\mathcal{H}^i = 0$ allows us to write

$$\frac{\pi^{ij}}{a^2 \sqrt{\gamma}} = -\nabla^i \nabla^j \nabla^{-2} \left(\dot{\phi}_0 \phi + 12\eta \Psi \right) + \frac{\pi_{(2)}^{ij}}{a^2 \sqrt{\gamma}} , \quad (95)$$

where $\pi_{(2)}^{ij}$ is doubly transverse (but not traceless).

Substituting equations (94) and (95) into (90c)–(90e), we get

$$\left\{ \psi_{kl}^{(2)}(\mathbf{x}), \pi_{(2)}^{ij}(\mathbf{y}) \right\}_{\text{D}} = P^i_k P^j_l \delta^3(\mathbf{x} - \mathbf{y}) , \quad (96a)$$

$$\left\{ \pi_\phi(\mathbf{x}), \pi_{(2)}^{ij}(\mathbf{y}) \right\}_{\text{D}} = -\frac{1}{2} a^2 \dot{\phi}_0 P^{ij} \delta^2(\mathbf{x} - \mathbf{y}) , \quad (96b)$$

$$\left\{ \pi_{(2)}^{ij}(\mathbf{x}), \pi_{(2)}^{kl}(\mathbf{y}) \right\}_{\text{D}} = 0 . \quad (96c)$$

We see that if we define new fields

$$\tilde{\psi}_{ij} \equiv \psi_{ij}^{(2)} , \quad \tilde{\pi}^{ij} \equiv \pi_{(2)}^{ij} - \frac{1}{2} a^2 \sqrt{\gamma} \dot{\phi}_0 P^{ij} \phi , \quad (97)$$

all Dirac brackets vanish except

$$\left\{ \phi(\mathbf{x}), \pi_\phi(\mathbf{y}) \right\}_{\text{D}} = \delta^3(\mathbf{x} - \mathbf{y}) , \quad \left\{ \tilde{\psi}_{kl}(\mathbf{x}), \tilde{\pi}^{kl}(\mathbf{y}) \right\}_{\text{D}} = P^i_k P^j_l \delta^3(\mathbf{x} - \mathbf{y}) . \quad (98)$$

Thus, $\tilde{\pi}^{ij}$ is the conjugate momentum to $\tilde{\psi}_{ij}$. Although we have nominally assumed a flat background, equations (98) are valid for an arbitrary Robertson-Walker background.

The construction of Dirac brackets is equivalent to a canonical transformation [3]. In the present case, the transformation from $(\phi, \psi_{ij}, \pi_\phi, \pi^{ij})$ to $(\hat{\phi}, \hat{\psi}_{ij}, \hat{\pi}_\phi, \hat{\pi}^{ij})$ is given by a type 3 generating functional,

$$\begin{aligned} F_3[\pi_\phi, \pi^{ij}, \hat{\phi}, \hat{\psi}_{ij}] &= - \int (\pi_\phi \hat{\phi} + \pi^{ij} \hat{\psi}_{ij}) d^3x \\ &+ \int \left[-6\eta \hat{\psi}_\parallel^2 + \frac{1}{2} \dot{\phi}_0 \hat{\phi} \left(\gamma^{ij} \hat{\psi}_{ij} - 3\hat{\psi}_\parallel \right) \right] a^2 \sqrt{\gamma} d^3x , \end{aligned} \quad (99)$$

where $\hat{\psi}_\parallel \equiv \nabla^i \nabla^j \nabla^{-2} \hat{\psi}_{ij}$ is the longitudinal part of $\hat{\psi}_{ij}$. The old and new fields are related by

$$\phi = -\frac{\delta F_3}{\delta \pi_\phi} , \quad \psi_{ij} = -\frac{\delta F_3}{\delta \pi^{ij}} , \quad \hat{\pi}_\phi = -\frac{\delta F_3}{\delta \hat{\phi}} , \quad \hat{\pi}^{ij} = -\frac{\delta F_3}{\delta \hat{\psi}_{ij}} . \quad (100)$$

Evaluating these equations gives $\hat{\phi} = \phi$, $\hat{\pi}_\phi = \pi_\phi$, and

$$\hat{\psi}_{ij} = \psi_{ij} = \tilde{\psi}_{ij} + \nabla_i \nabla_j \nabla^{-2} \hat{\psi}_\parallel , \quad (101a)$$

$$\frac{\hat{\pi}^{ij}}{a^2 \sqrt{\gamma}} = \frac{\tilde{\pi}^{ij}}{a^2 \sqrt{\gamma}} = \frac{\pi^{ij}}{a^2 \sqrt{\gamma}} + \nabla^i \nabla^j \nabla^{-2} (12\eta \hat{\psi}_\parallel + \dot{\phi}_0 \hat{\phi}) - \frac{1}{2} \dot{\phi}_0 P^{ij} \hat{\phi} , \quad (101b)$$

in agreement with equations (94), (95) and (97). The carets (but not the tildes) may be dropped from the right-hand side of these equations, with $\psi_\parallel = \hat{\psi}_\parallel = \Psi$.

The canonical transformation preserves the Poisson brackets. By restricting consideration to only the transverse degrees of freedom, one arrives at the Poisson brackets of

equation (98). Having shown that these are simply the Poisson brackets of transformed fields, we may drop the subscript D. The longitudinal degrees of freedom in the original fields ψ_{ij} and π^{ij} follow as a result of our gauge conditions from the transverse fields through equations (101). After replacing the Poisson brackets with Dirac brackets, all constraints are now first class. The constraints and equations of motion yield

$$\Phi = \Psi = \psi_{\parallel} = \frac{1}{2}\gamma^{ij}\tilde{\psi}_{ij}, \quad w_i = 0. \quad (102)$$

Like the primary, secondary, and gauge constraints, these are now strong equations (in quantum mechanics, operator equations). The constrained variables can now be eliminated from the Hamiltonian. We have reduced the dynamics to the four fields present in ϕ and $\tilde{\psi}_{ij}$.¹

Under a canonical transformation the Hamiltonian changes:

$$H \rightarrow H + \frac{\partial F_3}{\partial t}, \quad \frac{\partial F_3}{\partial t} = -6(\dot{\eta} + 2\eta^2) \int \psi_{\parallel}^2 a^2 \sqrt{\gamma} d^3x. \quad (103)$$

The new Hamiltonian is a functional of the fields $(\phi, \tilde{\psi}_{ij}, \pi_{\phi}, \tilde{\pi}^{ij})$. It is obtained by substituting equations (102) into the original Hamiltonian equation (63) and adding the correction term of equation (103). The new Hamiltonian may be written $H' = \int \mathcal{H}' d^3x$, where

$$\begin{aligned} \mathcal{H}' &= \frac{a^2 \sqrt{\gamma}}{2} \left[\frac{\pi_{\phi}^2}{(a^2 \sqrt{\gamma})^2} + (\nabla \phi)^2 + \frac{\partial^2 \tilde{V}}{\partial \phi_0^2} \phi^2 + \frac{3}{4} \dot{\phi}_0^2 \phi^2 \right] \\ &+ \frac{\tilde{\pi}_{ij} \tilde{\pi}^{ij} - \frac{1}{2} (\tilde{\pi}^k_k)^2}{4a^2 \sqrt{\gamma}} - \eta \psi_{\parallel} \tilde{\pi}^k_k + a^2 \sqrt{\gamma} \left(\nabla_k \tilde{\psi}_{ij} \right)^2 \\ &+ 2K a^2 \sqrt{\gamma} \left(\tilde{\psi}_{ij} \right)^2 + 2a^2 \sqrt{\gamma} (15\eta^2 - 9\dot{\eta} + 10K) \psi_{\parallel}^2 \\ &+ 4\dot{\phi}_0 \psi_{\parallel} \pi_{\phi} + \frac{1}{4} \dot{\phi}_0 \phi \tilde{\pi}^k_k + 2a^2 \sqrt{\gamma} \left(3\eta \dot{\phi}_0 - \frac{\partial \tilde{V}}{\partial \phi_0} \right) \phi \psi_{\parallel}, \end{aligned} \quad (104)$$

where $(\nabla \phi)^2 \equiv \gamma^{ij}(\partial_i \phi)(\partial_j \phi)$. It is straightforward to verify that this Hamiltonian (plus the now first-class constraint $\mathcal{H}_{\Phi} = 0$) reproduces the classical equations of motion obtained from the Lagrangian. In particular, equations (98) and (104) are valid for any curved Robertson-Walker background despite our temporary use of Cartesian coordinates in equations (89) and (90).

¹Note that the transverse field is *not* traceless so it has three degrees of freedom instead of two. We will find later that the trace part can also be eliminated from the Hamiltonian.

5.2.2 Eliminating the Trace

The Hamiltonian simplifies if we decompose the transverse gravitational fields into trace and trace-free parts,

$$\tilde{\psi}_{ij} = P_{ij}\psi_{\parallel} + \psi_{ij}^{\text{TT}}, \quad \tilde{\pi}^{ij} = \frac{1}{2}P^{ij}\tilde{\pi}^k{}_k + \pi_{\text{TT}}^{ij}, \quad (105)$$

where $\psi_{ij}^{\text{TT}} = -s_{ij}$ and $P^{ij}\psi_{ij}^{\text{TT}} = P_{ij}\pi_{\text{TT}}^{ij} = 0$. Equation (104) gives

$$H' = H'_0 + H_{\text{TT}}, \quad (106)$$

where $H'_0 = \int \mathcal{H}'_0 d^3x$ with

$$\begin{aligned} \mathcal{H}'_0 &= \frac{a^2\sqrt{\gamma}}{2} \left[\frac{\pi_\phi^2}{(a^2\sqrt{\gamma})^2} + (\nabla\phi)^2 + \frac{\partial^2\tilde{V}}{\partial\phi_0^2}\phi^2 + \frac{3}{4}\dot{\phi}_0^2\phi^2 \right] \\ &+ 4\dot{\phi}_0\psi_{\parallel}\pi_\phi + \frac{1}{4}\dot{\phi}_0\phi\tilde{\pi}^k{}_k - \eta\psi_{\parallel}\tilde{\pi}^k{}_k + 2a^2\sqrt{\gamma} \left(3\eta\dot{\phi}_0 - \frac{\partial\tilde{V}}{\partial\phi_0} \right) \phi\psi_{\parallel} \\ &+ 2a^2\sqrt{\gamma}(\nabla\psi_{\parallel})^2 + 6a^2\sqrt{\gamma}(\dot{\phi}_0^2 + \eta^2 + \dot{\eta})\psi_{\parallel}^2, \end{aligned} \quad (107)$$

and

$$H_{\text{TT}} = \int \left[\frac{\pi_{ij}^{\text{TT}}\pi_{\text{TT}}^{ij}}{4a^2\sqrt{\gamma}} + a^2\sqrt{\gamma}(\nabla_k\psi_{ij}^{\text{TT}})^2 + 2Ka^2\sqrt{\gamma}(\psi_{ij}^{\text{TT}})^2 \right] d^3x. \quad (108)$$

The nonzero Poisson brackets of these new variables are

$$\{\psi_{\parallel}(\mathbf{x}), \tilde{\pi}^k{}_k(\mathbf{y})\} = \delta^3(\mathbf{x} - \mathbf{y}), \quad \{\psi_{kl}^{\text{TT}}(\mathbf{x}), \pi_{\text{TT}}^{ij}(\mathbf{y})\} = \left[P^{(i}P^{j)} - \frac{1}{2}P_{kl}P^{ij} \right] \delta^3(\mathbf{x} - \mathbf{y}). \quad (109)$$

The transverse-traceless degrees of freedom are ready for quantization. For completeness, we give the classical equations of motion arising from H_{TT} :

$$(\partial_t^2 + 2\eta\partial_t - \nabla^2 + 2K)\psi_{ij}^{\text{TT}} = 0, \quad (110)$$

in agreement with equation (72a).

The scalar degrees of freedom, on the other hand, are not ready for quantization. The Hamiltonian H'_0 lacks a canonical kinetic term proportional to $(\tilde{\pi}^k{}_k)^2$, implying that the equation of motion for ψ_{\parallel} does not involve $\tilde{\pi}^k{}_k$. Consequently, the initial value of $\tilde{\pi}^k{}_k$ cannot be determined from initial values for ψ_{\parallel} and $\dot{\psi}_{\parallel}$. Instead, one must impose the initial value constraint $\mathcal{H}_\Phi = 0$. Equations (64d) and (101) give

$$\chi_1 \equiv -\frac{\mathcal{H}_\Phi}{a^2\sqrt{\gamma}} = \frac{\eta\tilde{\pi}^k{}_k}{a^2\sqrt{\gamma}} - \frac{\dot{\phi}_0\pi_\phi}{a^2\sqrt{\gamma}} - \frac{\partial\tilde{V}}{\partial\phi_0}\phi + 4(\nabla^2 + 3\dot{\eta} + 3\eta^2)\psi_{\parallel} \approx 0. \quad (111)$$

Taking the time derivative of this constraint and using the equations of motion gives another constraint on ψ_{\parallel} and $\tilde{\pi}^k_k$,

$$\chi_2 \equiv \frac{\dot{\chi}_1}{\dot{\eta} - \eta^2} = \frac{\tilde{\pi}^k_k}{a^2 \sqrt{\gamma}} + 3\dot{\phi}_0 \phi + 24\eta\psi_{\parallel} \approx 0 . \quad (112)$$

Taking the time derivative again yields $\dot{\chi}_2 = \chi_1 - 2\eta\chi_2$, so (χ_1, χ_2) form a closed algebra under time evolution. These constraints will allow us to reduce the phase space $(\phi, \pi_{\phi}, \psi_{\parallel}, \tilde{\pi}^k_k)$ by two dimensions. They are weak equations because they are second-class constraints until we apply the method of Dirac brackets (or equivalently find a canonical transformation that makes them canonical fields) to make them first-class.

The Poisson bracket of the constraints is

$$C_{12}(\mathbf{x}, \mathbf{y}) \equiv \{\chi_1(\mathbf{x}), \chi_2(\mathbf{y})\} = \frac{4}{a^2 \sqrt{\gamma(\mathbf{y})}} (\nabla_x^2 + 3K) \delta^3(\mathbf{x} - \mathbf{y}) , \quad (113)$$

and its inverse is given by

$$C_{21}^{-1}(\mathbf{x}, \mathbf{y}) = \frac{1}{4} a^2 \sqrt{\gamma(\mathbf{x})} g(\mathbf{x}, \mathbf{y}) = \frac{1}{4} a^2 \sqrt{\gamma(\mathbf{y})} g(\mathbf{y}, \mathbf{x}) , \quad (114)$$

where $g(\mathbf{x}, \mathbf{y})$ is defined as the bounded solution of

$$(\nabla_x^2 + 3K) g(\mathbf{x}, \mathbf{y}) = \delta^3(\mathbf{x} - \mathbf{y}) = (\nabla_y^2 + 3K) g(\mathbf{y}, \mathbf{x}) . \quad (115)$$

The other elements of $C_{mn}^{-1}(\mathbf{x}, \mathbf{y})$ with $(m, n) \in \{1, 2\}$ follow from the relations

$$C_{mn}^{-1}(\mathbf{x}, \mathbf{y}) = C_{nm}^{-1}(\mathbf{y}, \mathbf{x}) = -C_{nm}^{-1}(\mathbf{x}, \mathbf{y}) = -C_{mn}^{-1}(\mathbf{y}, \mathbf{x}) . \quad (116)$$

Substituting equations (113) and (114) into (83), we find the following nonzero Dirac brackets:

$$\{\phi(\mathbf{x}), \pi_{\phi}(\mathbf{y})\}_{\text{D}} = \delta^3(\mathbf{x} - \mathbf{y}) - \frac{3}{4} \dot{\phi}_0^2 g(\mathbf{x}, \mathbf{y}) , \quad (117a)$$

$$\{\phi(\mathbf{x}), \psi_{\parallel}(\mathbf{y})\}_{\text{D}} = \frac{\dot{\phi}_0 g(\mathbf{x}, \mathbf{y})}{4a^2 \sqrt{\gamma(\mathbf{y})}} = \frac{\dot{\phi}_0 g(\mathbf{y}, \mathbf{x})}{4a^2 \sqrt{\gamma(\mathbf{x})}} , \quad (117b)$$

$$\{\phi(\mathbf{x}), \tilde{\pi}^k_k(\mathbf{y})\}_{\text{D}} = -6\eta \dot{\phi}_0 g(\mathbf{x}, \mathbf{y}) , \quad (117c)$$

$$\{\psi_{\parallel}(\mathbf{x}), \pi_{\phi}(\mathbf{y})\}_{\text{D}} = \frac{1}{4} \left(\frac{\partial \tilde{V}}{\partial \phi_0} + 3\eta \dot{\phi}_0 \right) g(\mathbf{x}, \mathbf{y}) , \quad (117d)$$

$$\begin{aligned} \frac{\{\pi_{\phi}(\mathbf{x}), \tilde{\pi}^k_k(\mathbf{y})\}_{\text{D}}}{a^2 \sqrt{\gamma(\mathbf{y})}} &= 3\dot{\phi}_0 \left[\delta^3(\mathbf{x} - \mathbf{y}) - \frac{3}{4} \dot{\phi}_0^2 g(\mathbf{y}, \mathbf{x}) \right] \\ &\quad + 6\eta \left(\frac{\partial \tilde{V}}{\partial \phi_0} + 3\eta \dot{\phi}_0 \right) g(\mathbf{y}, \mathbf{x}) , \end{aligned} \quad (117e)$$

$$\{\psi_{\parallel}(\mathbf{x}), \tilde{\pi}^k_k(\mathbf{y})\}_{\text{D}} = \frac{3}{4} \dot{\phi}_0^2 g(\mathbf{x}, \mathbf{y}) . \quad (117f)$$

These relations ensure that χ_1 and χ_2 have vanishing Dirac brackets with all canonical variables $(\phi, \pi_\phi, \psi_\parallel, \tilde{\pi}^k_k)$. Consequently, χ_1 and χ_2 are first-class constraints with respect to the Dirac brackets and we may use $\chi_1 = \chi_2 = 0$ to eliminate two degrees of freedom. The retained degrees of freedom are

$$\hat{\phi} \equiv \phi, \quad \hat{\pi} \equiv \pi_\phi - \frac{\dot{\phi}_0}{8\eta} \tilde{\pi}^k_k. \quad (118)$$

The Dirac bracket of these fields is simply

$$\left\{ \hat{\phi}(\mathbf{x}), \hat{\pi}(\mathbf{y}) \right\}_D = \delta^3(\mathbf{x} - \mathbf{y}). \quad (119)$$

Equations (118) and (119), together with the now first-class constraints (111) and (112), imply equations (117).

As noted previously, the construction of Dirac brackets is equivalent to a canonical transformation. The transformation from $(\phi, \psi_\parallel, \pi_\phi, \tilde{\pi}^k_k)$ to $(\hat{\phi}, \chi_2, \hat{\pi}, \chi_1)$ is

$$F_3[\pi_\phi, \tilde{\pi}^k_k, \hat{\phi}, \chi_2, t] = - \int \pi_\phi \hat{\phi} d^3x + \frac{1}{48\eta} \int \tilde{\pi}^k_k \left(\frac{\tilde{\pi}^k_k}{a^2 \sqrt{\gamma}} + 6\dot{\phi}_0 \hat{\phi} \right) d^3x. \quad (120)$$

The transformation is independent of χ_2 because of the first-class constraint $\chi_1 = 0$. Only the scalar field and its (new) conjugate momentum enter the dynamics. The functional derivatives of the generating function with respect to the fields reproduces the constraints $\chi_1 = \chi_2 = 0$ and equations (118).

The reduced Hamiltonian for the scalar degrees of freedom is $H_0 = H'_0 + \partial F_3 / \partial t$. Dropping the carets on ϕ and π , the Hamiltonian is $H_0[\phi, \pi, t] = \int \mathcal{H}_0 d^3x$ with

$$\begin{aligned} \mathcal{H}_0 = & \frac{a^2 \sqrt{\gamma}}{2} \left[\frac{\pi^2}{(a^2 \sqrt{\gamma})^2} + (\nabla \phi)^2 + \frac{\partial^2 \tilde{V}}{\partial \phi_0^2} \phi^2 + \frac{3\dot{\phi}_0}{4\eta} \frac{\partial \tilde{V}}{\partial \phi_0} \phi^2 + \frac{3\dot{\phi}_0^2}{16\eta^2} (3\eta^2 - \dot{\eta} + 3K) \phi^2 \right] \\ & - \frac{3}{16} \frac{\dot{\phi}_0^2}{\eta} (\phi \pi + \pi \phi) + 2a^2 \sqrt{\gamma} \Psi (\Delta + 3K) \Psi + 2a^2 \partial_i (\sqrt{\gamma} \Psi \gamma^{ij} \partial_j \Psi), \end{aligned} \quad (121)$$

where $\Psi \equiv \psi_\parallel$ is the solution of the first-class constraint

$$4(\Delta + 3K)\Psi = \frac{\dot{\phi}_0 \pi}{a^2 \sqrt{\gamma}} + \left[\frac{\partial \tilde{V}}{\partial \phi_0} + \frac{3\dot{\phi}_0}{2\eta} (\eta^2 + \dot{\eta} - K) \right] \phi. \quad (122)$$

The last term in equation (121) is a surface term and may be dropped.

We have succeeded in reducing the Hamiltonian and may now drop the subscript D on the Poisson brackets. As a check on the reduction procedure, we evaluate the classical

equations of motion,

$$\dot{\phi} = \{\phi, H_0\} = \frac{\pi}{a^2\sqrt{\gamma}} - \frac{3\dot{\phi}_0^2}{8\eta}\phi + \dot{\phi}_0\Psi, \quad (123a)$$

$$\begin{aligned} \dot{\pi} = \{\pi, H_0\} = & \frac{3\dot{\phi}_0^2}{8\eta}\pi + a^2\sqrt{\gamma} \left[\Delta - \frac{\partial^2\tilde{V}}{\partial\phi_0^2} - \frac{3\dot{\phi}_0}{4\eta} \frac{\partial\tilde{V}}{\partial\phi_0} - \frac{3\dot{\phi}_0^2}{8\eta} \left(\frac{\dot{\eta}}{\eta} + \frac{3\dot{\phi}_0^2}{8\eta} \right) \right] \phi \\ & - a^2\sqrt{\gamma} \left(\frac{\partial\tilde{V}}{\partial\phi_0} + 3\eta\dot{\phi}_0 - \frac{3\dot{\phi}_0^3}{8\eta} \right) \Psi. \end{aligned} \quad (123b)$$

Taking the time derivative of equation (122) and using equations (123), we get

$$\frac{1}{4}\dot{\phi}_0\phi = \dot{\Psi} + \eta\Psi, \quad (124)$$

in agreement with equation (77). We also get the classical equation of motion for ϕ ,

$$\ddot{\phi} + 2\eta\dot{\phi} - \Delta\phi + \frac{\partial^2\tilde{V}}{\partial\phi_0^2}\phi = -2\frac{\partial\tilde{V}}{\partial\phi_0}\Psi + 4\dot{\phi}_0\dot{\Psi} = \dot{\phi}_0^2\phi + 2\ddot{\phi}_0\Psi, \quad (125)$$

in agreement with equation (67). Gravitational effects lead to an effective negative mass-squared term $m_{\text{eff}}^2 = -16\pi G\dot{\phi}_0^2$ as well as a coupling between the acceleration of the background field and the gravitational potential.

Taking the time derivative of equation (124) and using equations (122) and (123) gives

$$[\partial_t^2 + 3(1+c^2)\eta\partial_t + 3(c^2-w)\eta^2 - K(5+3w) - \Delta] \Psi = 0, \quad (126)$$

in agreement with equation (75). Here,

$$w \equiv \frac{p_0}{\rho_0} = \frac{\dot{\phi}_0^2 - 2\tilde{V}(\phi_0)}{\dot{\phi}_0^2 + 2\tilde{V}(\phi_0)}, \quad c^2 \equiv \frac{dp_0}{d\rho_0} = 1 + \frac{2}{3\eta\dot{\phi}_0} \frac{\partial\tilde{V}}{\partial\phi_0} = -\frac{1}{3} \left(1 + \frac{2\ddot{\phi}_0}{\eta\dot{\phi}_0} \right). \quad (127)$$

The Hamiltonian of equation (121) is not unique, even for the scalar field ϕ . It proves convenient to invoke one more canonical transformation:

$$F_3[\pi, \phi, t] = - \int \pi\phi d^3x + \frac{a^2\dot{\phi}_0^2}{8} \int \phi^2 \left[\frac{3}{2\eta} + \frac{\partial_t \ln(\dot{\phi}_0/a)}{\Delta + 3K + \frac{1}{4}\dot{\phi}_0^2} \right] \sqrt{\gamma} d^3x. \quad (128)$$

The new momentum variable will be denoted π_ϕ , and should not be confused with the variable of the same name appearing in equation (120) and preceding. Note also the notation in which the spatial Laplace operator is treated like a number. Its meaning is given only when a mode expansion is performed, where it is replaced by its eigenvalue.

For example, with a Fourier integral in flat space, $\Delta = -k^2$. After the canonical transformation (128), the Hamiltonian in the field ϕ (which is unchanged by the transformation) and its new momentum π_ϕ has become free of $\phi\pi_\phi$ cross-terms:

$$H[\phi, \pi_\phi, t] = \frac{1}{2} \int \left[\frac{(1 + \theta_\phi)\pi_\phi^2}{a^2\sqrt{\gamma}} - \frac{a^2\sqrt{\gamma}\phi^2}{1 + \theta_\phi}(\Delta - \mu_\phi^2) \right] d^3x, \quad (129)$$

where we have defined

$$\theta_\phi \equiv \frac{\dot{\phi}_0^2}{4(\Delta + 3K)}, \quad \mu_\phi^2 \equiv \frac{\partial^2 \tilde{V}}{\partial \phi_0^2} - \dot{\phi}_0^2 + [\partial_t \ln(\dot{\phi}_0/a)] \partial_t \ln(1 + \theta_\phi). \quad (130)$$

Note that θ_ϕ and μ_ϕ^2 depend on both time and wavenumber. The Newtonian gauge gravitational potential is given by the solution of

$$4(\Delta + 3K)\Psi = \frac{\dot{\phi}_0\pi_\phi}{a^2\sqrt{\gamma}} - \frac{\partial_t[\ln(\dot{\phi}_0/a)]\dot{\phi}_0\phi}{(1 + \theta_\phi)}. \quad (131)$$

The classical equation of motion for ϕ is given by

$$\frac{1 + \theta_\phi}{a^2} \frac{\partial}{\partial t} \left(\frac{a^2 \dot{\phi}}{1 + \theta_\phi} \right) = (\Delta - \mu_\phi^2)\phi. \quad (132)$$

The scalar field evolves like a damped harmonic oscillator whose effective mass μ_ϕ^2 and damping rate $\partial_t \ln[a^2/(1 + \theta_\phi)]$ depend on momentum through the k -dependence of θ_ϕ . For short wavelengths, $|\Delta + 3K| \gg \dot{\phi}_0^2/4$, $\theta_\phi \rightarrow 0$ and the field evolution reduces to that of a scalar field on an unperturbed Robertson-Walker background. However, for long wavelengths, $|\Delta + 3K| \ll \dot{\phi}_0^2/4$, the evolution is significantly modified by the self-gravity of the scalar field fluctuations. Neglecting the effect of metric perturbations leads to an error in the field evolution and therefore in the calculation of inflationary perturbations.

5.2.3 Alternative fields: Curvature and gravitational potential

Equations (121) and (129) use the scalar field perturbation ϕ as the fundamental field, with two different choices of canonical momentum. It is always possible to make a canonical transformation to different variables. There are two reasons for wanting to make such a transformation. First, the Hamiltonian and the equations of motion can be simplified — the new scalar field variable can have a different damping rate and effective mass. Second, the scalar field perturbation ϕ is only indirectly related to the curvature perturbations remaining after inflation. To avoid complicated dynamics, it would be better to choose a field more closely related to the geometry.

The ideal choice of field variable would be one that becomes constant when the wavelength is much greater than the Hubble distance (i.e. the field is massless), independently of the dynamics of the background expansion. When a single scalar field is the only form of matter, or the perturbations are isentropic, such a variable is the curvature perturbation κ (Bertschinger 2005). In the scalar field case,

$$\kappa \equiv \left(\frac{2\eta}{a\dot{\phi}_0} \right)^2 \frac{\partial}{\partial t} \left(\frac{a^2}{\eta} \Psi \right) . \quad (133)$$

We make a canonical transformation from (ϕ, π) to (κ, π_κ) as follows:

$$\begin{aligned} \phi &= \frac{z\kappa}{a} - \frac{(\eta - \dot{\eta}/\eta)\pi_\kappa}{az\sqrt{\gamma}(\Delta + 3K)} , \\ \pi &= -Aaz\sqrt{\gamma}\kappa + \frac{a\pi_\kappa}{z} + \frac{a(\eta - \dot{\eta}/\eta)A\pi_\kappa}{z(\Delta + 3K)} , \end{aligned} \quad (134)$$

where we have defined two functions of the background solution,

$$z \equiv \frac{a\dot{\phi}_0}{\eta} , \quad A \equiv \eta - \frac{3\dot{\phi}_0^2}{8\eta} - \frac{\ddot{\phi}_0}{\dot{\phi}_0} . \quad (135)$$

The Hamiltonian for the new canonical variables is

$$H[\kappa, \pi_\kappa, t] = \frac{1}{2} \int \left[\frac{(1 + \theta_\kappa)\pi_\kappa^2}{z^2\sqrt{\gamma}} - \frac{z^2\sqrt{\gamma}\kappa^2}{1 + \theta_\kappa} (\Delta - \mu_\kappa^2) \right] d^3x , \quad (136)$$

where

$$\theta_\kappa \equiv -\frac{3Kc^2}{\Delta + 3K} , \quad \mu_\kappa^2 \equiv -3K(1 - c^2) \quad (137)$$

and c^2 was defined in equation (127). Note that μ_κ in general depends on time but not wavenumber; θ_κ depends on both. The Newtonian gauge gravitational potential is given by the solution of

$$4(\Delta + 3K)\Psi = \frac{\eta\pi_\kappa}{a^2\sqrt{\gamma}} . \quad (138)$$

The classical equation of motion for κ is

$$\frac{1 + \theta_\kappa}{z^2} \frac{\partial}{\partial t} \left(\frac{z^2\dot{\kappa}}{1 + \theta_\kappa} \right) = (\Delta - \mu_\kappa^2)\kappa . \quad (139)$$

The Hamiltonian and equations of motion for (κ, π_κ) are similar to those for (ϕ, π_ϕ) , with the important difference that $\theta_\kappa = \mu_\kappa = 0$ if $K = 0$. More generally, we can approximate $\theta_\kappa = \mu_\kappa = 0$ for all length scales much smaller than the curvature distance,

$|\Delta| \gg |K|$. In this case the curvature perturbation evolves as a massless scalar field and therefore becomes constant for wavelengths much longer than the Hubble distance.

We have not succeeded in finding a canonical transformation that eliminates the mass term in a curved Robertson-Walker universe. Finding such a transformation is equivalent to reducing equation (139) to quadratures.

Long-wavelength curvature perturbations remain constant in a flat universe even when the composition of the universe changes at reheating as well as through any stages of adiabatic evolution (Bertschinger 2005). For matter with constant equation of state parameter $w = p/\rho$ (either a scalar field during power-law inflation or a fluid with no entropy perturbation), the curvature perturbation is related to the Newtonian gauge potential by

$$\kappa = \frac{5 + 3w}{3(1 + w)}\Psi \quad \text{if } |K| \ll |\Delta| \ll \eta^2 \quad \text{and } \dot{w} = 0. \quad (140)$$

During inflation and reheating, $\dot{w} \neq 0$ and Ψ changes with time even for long wavelengths when $K = 0$ because there is an entropy perturbation associated with the scalar field (Bertschinger 2005). However, κ remains constant. After reheating, when $w = \frac{1}{3}$, $\Psi = \frac{2}{3}\kappa$. The curvature perturbation κ is therefore the most convenient variable to use for calculating inflationary perturbations.

Given the transformation from (ϕ, π) to (κ, π_κ) , it is straightforward to express κ in terms of ϕ and $\dot{\phi}$:

$$\kappa = \frac{a\phi}{z} + \frac{\dot{\phi}_0(\eta - \dot{\eta}/\eta)}{z(1 + \theta_\phi)(\Delta + 3K)} \frac{\partial}{\partial t} \left(\frac{a\phi}{\dot{\phi}_0} \right). \quad (141)$$

Equation (141) allows one to compute the curvature perturbation (which is constant for long wavelengths) if one uses ϕ as the primary field variable.

One might guess that the Newtonian gauge gravitational potential Ψ also would be a good field to choose. The canonical transformation from (κ, π_κ) to (Ψ, π_Ψ) is given by the type 1 generating functional

$$F_1[\kappa, \Psi, t] = \int \left[yz\sqrt{\gamma}(\Delta + 3K)\kappa\Psi - \frac{1}{2}\sqrt{\gamma}(\Delta + 3K)\frac{y}{z}\frac{\partial}{\partial t}(yz)\Psi^2 \right] d^3x, \quad (142)$$

where we have defined

$$y \equiv \frac{4a}{\dot{\phi}_0}. \quad (143)$$

The generating gives the transformation via

$$\pi_\kappa = \frac{\delta F_1}{\delta \kappa}, \quad \pi_\Psi = -\frac{\delta F_1}{\delta \Psi}, \quad H[\Psi, \pi_\Psi, t] = H[\kappa, \pi_\kappa, t] + \frac{dF_1}{dt}. \quad (144)$$

Using this, the new Hamiltonian is

$$H[\Psi, \pi_\Psi, t] = \frac{1}{2} \int \left\{ -\frac{\pi_\Psi^2}{y^2\sqrt{\gamma}(\Delta + 3K)} + y^2\sqrt{\gamma}[(\Delta + 3K)\Psi][(\Delta - \mu_\Psi^2)\Psi] \right\} d^3x, \quad (145)$$

where

$$\mu_{\Psi}^2 \equiv \mu_{\kappa}^2 + \frac{z}{y} \frac{\partial}{\partial t} \left[\frac{1}{z^2} \frac{\partial}{\partial t} (yz) \right] . \quad (146)$$

The classical equation of motion for Ψ is

$$\frac{1}{y^2} \frac{\partial}{\partial t} (y^2 \dot{\Psi}) = (\Delta - \mu_{\Psi}^2) \Psi . \quad (147)$$

In general, $\mu_{\Psi}^2 \neq 0$ implying that the gravitational potential changes with time for long wavelengths. One exception is power-law inflation in a flat universe, for which $\mu_{\Psi}^2 = 0$. However, reheating leads invariably to a change in Ψ , so it is preferable to use the curvature perturbation κ to track the amplitude of inflationary perturbations.

Next we consider two other variables appearing in the literature, which simplify the equation of motion (but not its solution) by eliminating the damping terms.

5.2.4 Transformation to Mukhanov's variables

Mukhanov introduced a transformation to eliminate the damping in a flat universe, reducing the problem to a harmonic oscillator with time-dependent mass in flat space-time (Mukhanov, Feldman, & Brandenberger). We generalize his variable to a curved Robertson-Walker background:

$$\chi \equiv z_K \kappa \equiv \frac{z\kappa}{\sqrt{1+\theta_{\kappa}}} = \frac{a\phi + (1-4K/\dot{\phi}_0^2)z\Psi}{\sqrt{1+\theta_{\kappa}}} . \quad (148)$$

The canonical transformation from (κ, π_{κ}) to (χ, π_{χ}) is

$$\kappa = \frac{\chi}{z_K} , \quad \pi_{\kappa} = z_K \pi_{\chi} - \dot{z}_K \sqrt{\gamma} \chi , \quad (149)$$

resulting in the Hamiltonian

$$H[\chi, \pi_{\chi}, t] = \frac{1}{2} \int \left[\frac{\pi_{\chi}^2}{\sqrt{\gamma}} - \frac{\sqrt{\gamma} \chi^2}{2} (\Delta - \mu_{\chi}^2) \right] d^3x , \quad (150)$$

with

$$\mu_{\chi}^2 \equiv -\frac{\ddot{z}_K}{z_K} - 3K(1-c^2) . \quad (151)$$

The Hamiltonian reduces to that of a field in flat spacetime with time-dependent mass μ_{χ} . For a flat background, $z_K = z$ and $\mu_{\chi}^2 = -\ddot{z}/z$ depends on time but not wavenumber; for a curved background it depends on both. The classical equation of motion for χ is

$$\ddot{\chi} = (\Delta - \mu_{\chi}^2) \chi . \quad (152)$$

The damping term proportional to the first time derivative of the field has been eliminated. The mass term implies that χ changes with time for wavelengths longer than the Hubble length. However, the curvature perturbation $\kappa = \chi/z_K$ does become constant for long wavelengths as discussed in the previous subsection.

5.2.5 Transformation to Garriga's variables

On a curved Robertson-Walker background, the Hamiltonian takes a particularly simple form in the variables (q, p) given by Garriga et al. (Nucl. Phys. B 513, 343, 1998). The scalar field variable is related very simply to the Newtonian gauge gravitational potential:

$$q = \frac{4a}{\dot{\phi}_0} \Psi . \quad (153)$$

The canonical transformation from (κ, π_κ) to (q, p) is²

$$\begin{aligned} \kappa &= \frac{\dot{z}}{z^2} q - \frac{p}{z\sqrt{\gamma}(\Delta + 3K)} , \\ \pi_\kappa &= z\sqrt{\gamma}(\Delta + 3K)q , \end{aligned} \quad (154)$$

resulting in the Hamiltonian

$$H[q, p, t] = \frac{1}{2} \int \left\{ -\frac{p^2}{\sqrt{\gamma}(\Delta + 3K)} + \sqrt{\gamma}[(\Delta + 3K)q][(\Delta - \mu_q^2)q] \right\} d^3x , \quad (155)$$

where

$$\mu_q^2 \equiv \partial_t \left(\frac{\dot{z}}{z} \right) - \left(\frac{\dot{z}}{z} \right)^2 - 3K(1 - c^2) = \dot{\eta} - \eta^2 - 4K - \dot{\phi}_0 \partial_t^2 \left(\frac{1}{\dot{\phi}_0} \right) . \quad (156)$$

Garriga et al. have an overall sign error in the Lagrangian equivalent to equation (150); Gratton and Turok corrected the error (Phys. Rev. D60, 123507, 1999; astro-ph/9902265).

The classical equation of motion for q is

$$\ddot{q} = (\Delta - \mu_q^2)q . \quad (157)$$

As was the case with Mukhanov's variables, the damping terms have been eliminated. Now, however, μ_q^2 is independent of wavenumber in all cases. The presence of a mass term implies that q changes with time for wavelengths longer than the Hubble length. The curvature perturbation $\kappa = -\partial_t(q/z)$ does become constant for long wavelengths.

We have found five different choices for the field variable: ϕ , κ , Ψ , χ , and q . Any one of these may be used for computing inflationary fluctuations. It remains to be seen if they give identical results — this depends on the choice of the vacuum state.

6 Quantization

Canonical quantization proceeds by promoting the fields and their canonical momenta to Heisenberg operators and Poisson brackets to commutators, for example

$$\{A, B\} \rightarrow -i[A, B] . \quad (158)$$

²This requires a Type 1 or Type 4 generating function.

The fields and momenta obey the canonical commutation relations, illustrated here for the pair (p, q) ,

$$[q(\mathbf{x}, t), q(\mathbf{y}, t)] = [p(\mathbf{x}, t), p(\mathbf{y}, t)] = 0, \quad [q(\mathbf{x}, t), p(\mathbf{y}, t)] = i\delta^3(\mathbf{x} - \mathbf{y}) \quad (159)$$

and

$$\begin{aligned} [\psi_{ij}^{\text{TT}}(\mathbf{x}, \mathbf{t}), \psi_{kl}^{\text{TT}}(\mathbf{y}, t)] &= [\pi_{\text{TT}}^{ij}(\mathbf{x}, \mathbf{t}), \pi_{\text{TT}}^{kl}(\mathbf{y}, t)] = 0, \\ [\psi_{kl}^{\text{TT}}(\mathbf{x}, \mathbf{t}), \pi_{\text{TT}}^{ij}(\mathbf{y}, t)] &= i \left[P_k^{(i} P_l^{j)} - \frac{1}{2} P_{kl} P^{ij} \right] \delta^3(\mathbf{x} - \mathbf{y}). \end{aligned} \quad (160)$$

The time evolution of these operators is given by

$$\dot{q}(\mathbf{x}, t) = -i[q, H], \quad \dot{p}(\mathbf{x}, t) = -i[p, H], \quad \dot{\psi}_{ij}^{\text{TT}}(\mathbf{x}, \mathbf{t}) = -i[\psi_{ij}^{\text{TT}}, H], \quad \text{etc.} \quad (161)$$

One complication compared with quantum field theory in flat spacetime is that the Hamiltonian in a Robertson-Walker spacetime is in general time-dependent. This is only a technical complication; we will solve equations (161) for the time evolution of the operators.

We assume a flat background space, $K = 0$, with Cartesian coordinates.

6.1 Scalar Mode

We have a choice of Hamiltonians to quantize, having found a series of different canonical variables for the Hamiltonian system. These may be regarded simply as different choices of coordinates for the phase space of our Hamiltonian system and as such they all describe identical dynamics. From the viewpoint of fluctuations, the natural choice of variables is (κ, π_κ) because κ becomes constant for waves stretched beyond the Hubble length. However, we will have to calculate fluctuations assuming a vacuum state. It is unclear whether the vacuum is canonically invariant – we’ll have to check. If it is not, we would get different inflationary fluctuations depending on the choice of variables, a clearly unphysical situation. It seems likely the choice of vacuum matters, we should pick the vacuum defined by (ϕ, π) or ϕ, π_ϕ – hopefully they are the same!

This section should be rewritten to consider the general case, however for now it’s left in terms of the variables (q, p) .

6.1.1 Scalar Mode using (q, p)

We expand the fields p and q in Fourier space as follows:

$$q(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} (2k^3)^{-1/2} [e^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}, t) + \text{h.c.}] , \quad (162a)$$

$$p(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} \left(\frac{k}{2}\right)^{1/2} [e^{i\mathbf{k}\cdot\mathbf{x}} b(\mathbf{k}, t) + \text{h.c.}] . \quad (162b)$$

The operators $a(\mathbf{k}, t)$ and $b(\mathbf{k}, t)$ are Heisenberg operators obeying the evolution equations

$$\dot{a} = -i[a, H] , \quad \dot{b} = -i[b, H] . \quad (163)$$

We can not write $a(\mathbf{k}, t) = e^{-i\omega t}a(\mathbf{k}, 0)$ and $b(\mathbf{k}, t) = \dot{a}(\mathbf{k}, t)$ as in flat space, because the background spacetime curvature modifies the evolution of modes. Calculating the correct evolution requires the Hamiltonian. Substitution into equation (150) yields

$$H(t) = \int \frac{d^3k}{4k} \left[\mathcal{H}_0(\mathbf{k}, t) + \mathcal{H}_-(\mathbf{k}, t) + \mathcal{H}_-(\mathbf{k}, t)^\dagger \right] ,$$

$$\mathcal{H}_0 = \omega^2(aa^\dagger + a^\dagger a) + bb^\dagger + b^\dagger b , \quad \mathcal{H}_- = \omega^2 aa_- + bb_- , \quad (164)$$

where $\omega^2 \equiv k^2 + \mu^2(t)$, $a \equiv a(\mathbf{k}, t)$, $a_- \equiv a(-\mathbf{k}, t)$ and similarly for b and b_- . It is easy to see that in general one expects $[\mathcal{H}_0(\mathbf{k}_1, t), \mathcal{H}_-(\mathbf{k}_2, t)] \neq 0$ and $[\mathcal{H}_-(\mathbf{k}_1, t), \mathcal{H}_-(\mathbf{k}_2, t)^\dagger] \neq 0$. As a result, the eigenstates of $\mathcal{H}_0(\mathbf{k}, t)$ (the usual Fock states) are not eigenstates of the Hamiltonian. Moreover, eigenstates of the time-dependent Hamiltonian do not form a convenient basis because, in general, $[H(t_1), H(t_2)] \neq 0$.

These behaviors arise because the modes with wavevectors \mathbf{k} and $-\mathbf{k}$ are coupled. This is a generic feature of quantum field theory in curved spacetime.³ The usual procedure for dealing with this coupling is the Bogoliubov transformation. Equivalently, one must find a canonical transformation that separates the Hamiltonian. Here we proceed directly by solving the Heisenberg operator equations of motion, deriving the Bogoliubov transformation (and hence the canonical transformation that separates the Hamiltonian) as part of the solution.

Integrating the evolution equations (163) requires us to evaluate the equal-time commutation relations for the time-dependent operators a , b , a^\dagger and b^\dagger . These can be found using the fact that Hamiltonian evolution is unitary, with propagator

$$U(t, t_0) = \mathbb{T} e^{-i \int_{t_0}^t H(t') dt'} \equiv \lim_{\epsilon \rightarrow 0} e^{-i\epsilon H(t-\epsilon)} e^{-i\epsilon H(t-2\epsilon)} \dots e^{-i\epsilon H(t_0)} , \quad (165)$$

where \mathbb{T} denotes the time-ordered product. Given the operators at some initial time t_0 , $a(\mathbf{k}, t) = U^\dagger a(\mathbf{k}, t_0) U$. It follows that the commutators themselves evolve by the same unitary transformation.

In an inflationary universe the conformal time t is large and negative at early times (we take $t = 0$ to be the end of inflation). At the beginning of inflation, the modes of interest have wavelengths much shorter than the Hubble distance, i.e. $(kt)^2 \gg 1$, implying $\mu^2 \ll k^2$. In this case $\omega^2 \approx k^2$ and the mode evolution reduces to the limit of Minkowski spacetime. Thus at any sufficiently early time t_0 we may write

$$a(\mathbf{k}, t_0) = a_0(\mathbf{k}) e^{-ikt_0} , \quad b(\mathbf{k}, t_0) = -ika(\mathbf{k}, t_0) , \quad (166)$$

³A real classical field theory has half as many modes because $a(\mathbf{k}, t) = a^*(-\mathbf{k}, t)$. A quantum field has $a(\mathbf{k}, t) \neq a^\dagger(-\mathbf{k}, t)$. The evolution of the two distinct modes \mathbf{k} and $-\mathbf{k}$ is coupled by the \mathcal{H}_- terms in the Hamiltonian.

where a_0 obeys the usual commutation relations following from equations (159). These commutators are invariant under unitary transformations, yielding

$$\begin{aligned} [a(\mathbf{k}_1, t), a(\mathbf{k}_2, t)] &= [a(\mathbf{k}_1, t), b(\mathbf{k}_2, t)] = [b(\mathbf{k}_1, t), b(\mathbf{k}_2, t)] = 0, \\ [a(\mathbf{k}_1, t), a^\dagger(\mathbf{k}_2, t)] &= -\frac{i}{k_1} [a(\mathbf{k}_1, t), b^\dagger(\mathbf{k}_2, t)] = \frac{1}{k_1^2} [b(\mathbf{k}_1, t), b^\dagger(\mathbf{k}_2, t)] = \delta^3(\mathbf{k}_1 - \mathbf{k}_2). \end{aligned} \quad (167)$$

Equations (163), (164) and (167) now give

$$\begin{aligned} \dot{a} &= \frac{1}{2}(b + b_-^\dagger) - \frac{i\omega^2}{2k}(a + a_-^\dagger), \\ \dot{b} &= -\frac{\omega^2}{2}(a + a_-^\dagger) - \frac{ik}{2}(b + b_-^\dagger). \end{aligned} \quad (168)$$

The exact solution to these equations subject to the initial conditions (166) is

$$a(\mathbf{k}, t) = \frac{1}{2} \left(u + \frac{i}{k} \dot{u} \right) a_0(\mathbf{k}) + \frac{1}{2} \left(u^* + \frac{i}{k} \dot{u}^* \right) a_0^\dagger(-\mathbf{k}), \quad b = -ika, \quad (169)$$

where $u(k, t)$ is the solution to the ordinary differential equation

$$\ddot{u} = -\omega^2 u, \quad (170)$$

subject to initial condition $u \rightarrow e^{-ikt}$ as $kt \rightarrow -\infty$. The solution is normalized by the Wronskian

$$u\dot{u}^* - \dot{u}u^* = 2ik. \quad (171)$$

Equation (169) gives the desired Bogoliubov transformation. Equation (162b) may now be replaced by

$$p(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} \left(\frac{k^3}{2} \right)^{1/2} [-ie^{i\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}, t) + \text{h.c.}] . \quad (172)$$

In de Sitter space, $\mu^2 = 0$ and $u = e^{-ikt}$. In this case there is no mixing of modes.

Given the exact solution for $a(\mathbf{k}, t)$, we may rewrite the quantum fields in terms of the Schrödinger operators as follows:

$$q(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} q(\mathbf{k}, t), \quad q(\mathbf{k}, t) \equiv \frac{u a_0(\mathbf{k}) + u^* a_0^\dagger(-\mathbf{k})}{\sqrt{2k^3}}, \quad (173a)$$

$$p(\mathbf{x}, t) = \int \frac{d^3k}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} p(\mathbf{k}, t), \quad p(\mathbf{k}, t) \equiv \sqrt{\frac{k}{2}} \left[\dot{u} a_0(\mathbf{k}) + \dot{u}^* a_0^\dagger(-\mathbf{k}) \right]. \quad (173b)$$

We see that $q(\mathbf{k}) = q^\dagger(-\mathbf{k})$ and $p(\mathbf{k}) = p^\dagger(-\mathbf{k})$. These conditions are guaranteed by the requirement that $q(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ be Hermitian and they are analogous to the conditions on the Fourier transform of a real classical field. However, in the quantum case $a_0(\mathbf{k})$ and $a_0^\dagger(-\mathbf{k})$ are distinct operators (in particular, they do not commute).

6.1.2 Inflationary power spectrum

We assume that the universe begins inflation in the Bunch-Davies vacuum, corresponding to the Minkowski vacuum for modes whose wavelength is much smaller than the Hubble distance, so that

$$a_0(\mathbf{k})|0\rangle = 0, \quad \langle 0|a_0(\mathbf{k}_1)a_0^\dagger(\mathbf{k}_2)|0\rangle = \delta^3(\mathbf{k}_1 - \mathbf{k}_2). \quad (174)$$

Using equations (173), we obtain the two-point function of the q -field:

$$\langle 0|q(\mathbf{x}_1, t_1)q(\mathbf{x}_2, t_2)|0\rangle \equiv \int \frac{d^3k}{(2\pi)^3} \frac{u(k, t_1)u^*(k, t_2)}{2k^3} e^{i\mathbf{k}\cdot(\mathbf{x}_1 - \mathbf{x}_2)}, \quad (175)$$

giving an equal-time power spectrum $P_{qq}(k, t) = |u|^2/(2k^3)$. The factor $u_1u_2^*$ reduces to $e^{ik(t_2-t_1)}$ in Minkowski and de Sitter spacetimes as expected based on microcausality. Interestingly, equation (175) is unaffected by the mixing of modes: the same result would have followed if $a(\mathbf{k}, t) = u(k, t)a_0(\mathbf{k})$ in equation (162).

The power spectrum of the gravitational potential $\Phi = \dot{\phi}_0 q/4a$ is $P_\Phi = (\dot{\phi}_0/4a)^2 P_{qq}$ and the power per logarithmic wavenumber interval is

$$\delta_k^2 \equiv \frac{d\sigma_\Phi^2}{d \ln k} = \frac{k^3 P_\Phi(k, t)}{2\pi^2} = \left| \frac{\tilde{u}}{2\pi} \right|^2 = 4G^2(\rho_0 + p_0)|u|^2, \quad \tilde{u} \equiv \frac{4\pi G \dot{\phi}_0}{a} u(k, t), \quad (176)$$

where we have used $(\dot{\phi}_0/a)^2 = \rho_0 + p_0$ and have restored the units of G . Note that Φ is the quantity that directly induces the scalar microwave background and matter perturbations in the later universe. The variable \tilde{u} gives the time-dependence of the gravitational potential; it obeys equation (126).

Equation (176) appears initially to differ significantly from the canonical result $\delta_k \sim H^2/\dot{\phi}_0$ (where here the dot is a proper time derivative). If $|u| \sim 1$, the perturbation amplitude for the physical (conformal Newtonian gauge) gravitational potential is smaller than $H^2/\dot{\phi}_0$ by a factor approximately $(\rho_0 + p_0)/\rho_0 = 1 + w$. Since this factor is small during inflation, the correct amplitude of density perturbations is much smaller *during inflation* than is usually assumed. However, we must be careful here! The gravitational potential \tilde{u} is not constant even for $(kt)^2 \ll 1$. In this long-wavelength limit the solution to equation (126) is

$$\tilde{u} \propto \frac{\eta}{a^2} \int^t (1+w)a^2 dt. \quad (177)$$

The solution is independent of time only for $w = \text{constant}$. During inflation, $1+w$ slowly increases, and during reheating it increases rapidly to $\frac{4}{3}$. This will cause \tilde{u} to increase. Roughly speaking, we may expect \tilde{u} to increase by a factor $(1+w_i)^{-1}$ between the time a mode first crosses the Hubble length (when $w = w_i$) and the end of reheating. This will boost the CMB anisotropy up to the result of the standard calculation!

Specifically, we want to find $A(k, t)$ as $kt \rightarrow 0$, where

$$\frac{\dot{\phi}_0}{4a} u(k, t) = A(k, t) \frac{9\eta}{4a^2} \int_{t_0}^t \frac{\dot{\phi}_0^2 a^2}{6\eta^2} dt . \quad (178)$$

The amplitude $A(k, 0)$ is just the value of \tilde{u} after reheating. During the radiation-dominated era \tilde{u} does not evolve for $(kt)^2 \ll 1$, so $A(k, 0)$ is precisely the input to CMB anisotropy and structure formation models. The power spectrum is related to A by $\delta_k^2 = |A/2\pi|^2$.

We now integrate the scalar field and perturbation equations numerically to find $A(k)$. Using the time variable $\xi \equiv \ln a$, the background scalar field equation of motion becomes

$$\frac{d^2\phi_0}{d\xi^2} + \left[12 - \left(\frac{d\phi_0}{d\xi} \right)^2 \right] \left(\frac{1}{2} \frac{d \ln V}{d\phi_0} + \frac{1}{4} \frac{d\phi_0}{d\xi} \right) = 0 . \quad (179)$$

The equation of state is

$$1 + w = \frac{1}{6} \left(\frac{d\phi_0}{d\xi} \right)^2 . \quad (180)$$

For an exponential potential, $d \ln V / d\phi_0$ is constant and equation (179) can be integrated exactly. If $(d\phi_0/d\xi)^2 < 12$ the solutions are stable and approach the attractor $d\phi_0/d\xi = -2d \ln V / d\phi_0$ corresponding to power-law inflation. For a power-law potential, $V \propto \phi^n$, the equation of motion depends only on n and not on the mass scale. Provided that the initial slope $|d\phi_0/d\xi|$ is not too large in magnitude, slow-roll inflation will result during which $d\phi_0/d\xi \approx -2n/\phi_0$. The number of e-foldings is approximately $\phi_i^2/4n$ where ϕ_i is the starting value. Getting 60 e-foldings requires $\phi_i > 3\sqrt{n/2} M_{\text{P}}$ where $M_{\text{P}} = G^{-1/2}$ is the Planck mass.

The perturbation amplitude follows from $A \equiv u/B$ where the following equations need to be solved (given here for reference):

$$\begin{aligned} \frac{dB}{d\xi} + \left(1 + \frac{d^2\phi_0/d\xi^2}{d\phi_0/d\xi} \right) B &= \frac{3}{2} \left[\frac{12 - (d\phi_0/d\xi)^2}{2V(\phi_0)} \right]^{1/2} \frac{d\phi_0}{d\xi} , \\ \frac{d^2u}{d\xi^2} + \left[1 - \frac{1}{4} \left(\frac{d\phi_0}{d\xi} \right)^2 \right] \frac{du}{d\xi} + \left(\frac{k^2 + \mu^2}{\eta^2} \right) u &= 0 , \\ \frac{\mu^2}{\eta^2} &= -6 + \frac{1}{4} \left(\frac{d\phi_0}{d\xi} \right)^2 - \left(\frac{a}{\eta} \right)^2 \left(\frac{d^2V}{d\phi_0^2} + 8 \frac{dV/d\phi_0}{d\phi_0/d\xi} \right) - 2 \left(\frac{a}{\eta} \right)^4 \left(\frac{dV/d\phi_0}{d\phi_0/d\xi} \right)^2 \\ \left(\frac{a}{\eta} \right)^2 &= \frac{12 - (d\phi_0/d\xi)^2}{2V} . \end{aligned} \quad (181)$$

The mode function u must be integrated until $k^2 \ll \eta^2$ by which time $A = u/B$ should become independent of time.

The rest of this section isn't so useful now — we need to just integrate the Friedmann and scalar field equations, then integrate equation (177) with $1 + w = \dot{\phi}_0^2/(6\eta^2)$.

It is straightforward to numerically integrate the Friedmann and background scalar field equations and equation (170) to get $\tilde{u}(k, t)$. A simple exact solution exists for a flat universe when $p_0/\rho_0 = w$ is a constant (power-law inflation):

$$a(t) = (t/t_0)^\nu, \quad \phi_0(t) = \sqrt{\frac{\nu(\nu+1)}{4\pi G}} \log(t/t_0), \quad \nu \equiv \frac{2}{1+3w}. \quad (182)$$

Here, t_0 is a constant. The corresponding potential for $\nu \leq 1$ is

$$V(\phi_0) = \frac{\nu(2\nu-1)}{8\pi G t_0^2} e^{\phi_0 \sqrt{16\pi G(\nu+1)/\nu}}. \quad (183)$$

Inflation requires $-1 \leq w < -\frac{1}{3}$ so that $\nu \leq -1$, and $t_0 < 0$. The conformal time t is negative and increases towards zero as $a \rightarrow \infty$. The scalar mode function is

$$u(k, t) = k t h_\nu^{(2)}(kt), \quad h_\nu^{(2)}(x) \equiv \left(\frac{\pi}{2x}\right)^{1/2} [J_{\nu+1/2}(x) - iY_{\nu+1/2}(x)]. \quad (184)$$

Here $h_\nu^{(2)}$ is the spherical Bessel function of the third kind (i.e., a spherical Hankel function). It has the limiting behavior (for $\nu < -\frac{1}{2}$)

$$h_\nu^{(2)}(x) \sim \begin{cases} -\frac{i \exp[+i\pi(\nu+1/2)]}{2(2\nu+1)} \frac{\Gamma(1/2-\nu)}{\Gamma(3/2)} (x/2)^\nu & \text{as } x \rightarrow 0, \\ \frac{1}{x} \exp -i \left[x - (\nu+1)\frac{\pi}{2} \right] & \text{as } x \rightarrow \infty. \end{cases} \quad (185)$$

The power per logarithmic wavenumber interval is (restoring all the units)

$$\begin{aligned} \frac{k^3 P_\Phi(k)}{2\pi^2} &= \left[\frac{2\Gamma(1/2-\nu)}{(2\nu+1)\Gamma(3/2)} \right]^2 \frac{\hbar G \nu(\nu+1)}{4\pi c^5 t_0^2} \left| \frac{kt_0}{2} \right|^{2(\nu+1)} \\ &= \left[\frac{2\Gamma(1/2-\nu)}{(2\nu+1)\Gamma(3/2)} \right]^2 \left(\frac{\nu+1}{4\pi\nu} \right) \frac{\hbar G H^2}{c^5} \left| \frac{kt}{2} \right|^{2(\nu+1)}. \end{aligned} \quad (186)$$

Note that Φ has become independent of time for $(kt)^2 \ll 1$. For a single scalar field, $1 + \nu \leq 0$ so the scalar index $n_s \equiv 1 + 2(\nu+1) < 1$.

6.1.3 Quantum to Classical Transition

We can use our exact solution for the Heisenberg operator evolution to investigate the transition from quantum perturbations to classical random fields. The description is simplest in the Schrödinger picture, where the state vector is denoted $|\Psi(t)\rangle$. According to the standard rules of quantum mechanics, measurement of any observable \hat{O} leads to the collapse of the wavefunction to an eigenstate of \hat{O} with eigenvalue O drawn from the

probability distribution $|\langle O|\Psi(t)\rangle|^2$. We do not attempt here to describe how the wave function collapses. Instead, we show that unitary evolution leads to the perturbations evolving classically when they are stretched far beyond the Hubble distance. We then solve the Schrödinger equation and present the probability density functional of $q(\mathbf{x}, t)$ as a path integral. Finally, we investigate the phenomenon of squeezing using the Wigner function.

Using equation (175), we obtain the exact time structure function

$$\langle 0|[\Phi(\mathbf{x}, t_1) - \Phi(\mathbf{x}, t_2)]^2|0\rangle = \int \frac{d^3k}{(2\pi)^3} \frac{|\tilde{u}(k, t_1) - \tilde{u}(k, t_2)|^2}{2k^3}. \quad (187)$$

In the limit of small scales, $(kt)^2 \gg 1$, the power spectrum of $\Phi(\mathbf{x}, t_1) - \Phi(\mathbf{x}, t_2)$ equals $2[1 - \cos k(t_2 - t_1)]P_\Phi$ and the field fluctuates with time. However, on large scales $\tilde{u}(k, t)$ evolves much more slowly. In particular, if the equation of state is constant, $\tilde{u}(k, t)$ is independent of time for $(kt)^2 \ll 1$ and the long-wavelength gravitational potential perturbations become frozen in. If the equation of state changes, the structure function changes exactly according to the classical evolution of $\Phi(\mathbf{k}, t)$. In other words, the field values for a given \mathbf{k} at successive times are very highly correlated and the field evolves classically. Quantum fluctuations generated on scales comparable to or smaller than the Hubble distance become frozen and evolve classically when $(kt)^2 \ll 1$.

The next question is, what classical values do the long-wavelength components of the field take? This question can be answered by solving the Schrödinger equation for the time-dependent wavefunction. Defining the Schrödinger state vector at time t by

$$|\Psi(t)\rangle = U|0\rangle \quad (188)$$

where U is the time evolution operator, equation (174) implies

$$Ua_0(\mathbf{k})U^\dagger|\Psi(t)\rangle = 0 \quad \forall \mathbf{k}. \quad (189)$$

Now, $a(\mathbf{k}, t) = U^\dagger a_0(\mathbf{k})U$, and from equation (169) (suppressing the arguments where there is no ambiguity)

$$a_0 = UaU^\dagger = \frac{1}{2} \left(u^* - \frac{i}{k} \dot{u}^* \right) a - \frac{1}{2} \left(u^* + \frac{i}{k} \dot{u}^* \right) a_-^\dagger, \quad (190)$$

yielding

$$Ua_0U^\dagger = \frac{1}{2} \left(u^* - \frac{i}{k} \dot{u}^* \right) a_0 - \frac{1}{2} \left(u^* + \frac{i}{k} \dot{u}^* \right) a_{0-}^\dagger. \quad (191)$$

This last result is easily confirmed using $a_0 = U^\dagger(Ua_0U^\dagger)U$.

We define the following Schrödinger operators:

$$\begin{aligned} q_0(\mathbf{k}) &\equiv \frac{1}{\sqrt{2k^3}} \left[a_0(\mathbf{k}) + a_0^\dagger(\mathbf{k}) \right], \\ p_0(\mathbf{k}) &\equiv \sqrt{\frac{k^3}{2}} \left[-ia_0(\mathbf{k}) + ia_0^\dagger(\mathbf{k}) \right]. \end{aligned} \quad (192)$$

Their commutator is

$$[q_0(\mathbf{k}_1), p_0(\mathbf{k}_2)] = i\delta^3(\mathbf{k}_1 - \mathbf{k}_2) , \quad (193)$$

implying that in the coordinate representation we may write

$$p_0 = -i\delta^3(0)\frac{\partial}{\partial q_0} . \quad (194)$$

The Dirac delta function is necessary because of our continuum representation of the fields; with quantization in a periodic cube of length L , $\delta^3(0) \rightarrow (L/2\pi)^3$. It arises because we are considering only the two modes \mathbf{k} and $-\mathbf{k}$. When we compute correlators below, the delta functions will disappear.

We now apply equation (189) to the pair of modes $(\mathbf{k}, -\mathbf{k})$ with $q_1 \equiv q_0(\mathbf{k})$, $q_2 \equiv q_0(-\mathbf{k})$. The Schrödinger wavefunction $\Psi(q_1, q_2, t) = \langle q_1, q_2 | \Psi(t) \rangle$ is annihilated by the pair of operators

$$\begin{aligned} U(a_1 + a_2)U^\dagger &= -i\dot{u}^* \sqrt{\frac{k}{2}}(q_1 + q_2) + \frac{u^*\delta^3(0)}{\sqrt{2k^3}} \left(\frac{\partial}{\partial q_1} + \frac{\partial}{\partial q_2} \right) , \\ U(a_1 - a_2)U^\dagger &= u^* \sqrt{\frac{k^3}{2}}(q_1 - q_2) - \frac{i\dot{u}^*\delta^3(0)}{\sqrt{2k^5}} \left(\frac{\partial}{\partial q_1} - \frac{\partial}{\partial q_2} \right) . \end{aligned} \quad (195)$$

At a sufficiently early time t_0 when $(kt_0)^2 \gg 1$, the system is in the Bunch-Davies vacuum, $|\Psi(t_0)\rangle = |0\rangle$. Solving the time evolution given by equation (189) yields

$$\Psi(q_1, q_2, t) = N \exp \left[-\frac{k^3(1 + \theta^2)}{4\theta\delta^3(0)}(q_1^2 + q_2^2) + \frac{k^3(1 - \theta^2)}{2\theta\delta^3(0)}q_1q_2 \right] , \quad (196)$$

where N is a normalization constant and

$$\theta \equiv -\frac{i\dot{u}^*}{ku^*} , \quad \theta_r \equiv \frac{1}{2}(\theta + \theta^*) = \frac{1}{|u|^2} , \quad \theta_i \equiv \frac{i}{2}(\theta^* - \theta) = -\frac{1}{k} \frac{d \ln |u|}{dt} . \quad (197)$$

The probability density is

$$|\Psi|^2 = N^2 \exp \left[-\frac{(q_1^2 + q_2^2 - 2\rho q_1 q_2)}{2\sigma^2(1 - \rho^2)} \right] , \quad \sigma^2 \equiv \frac{|u|^2(1 + |\theta|^2)\delta^3(0)}{4k^3} , \quad \rho \equiv \frac{1 - |\theta|^2}{1 + |\theta|^2} , \quad (198)$$

from which we see $N^{-2} = 2\pi\sigma^2\sqrt{1 - \rho^2}$.

Here define q_\pm and diagonalize the wave function, then discuss expectation values of products of q . Write down the path integral form.

We can use equation (198) to check equation (175) for $\mathbf{x}_1 = \mathbf{x}_2 = 0$ and $t_1 = t_2 = t$ using the Schrödinger representation:

$$\langle \Psi(t) | q(0, t_0) q(0, t_0) | \Psi(t) \rangle = \int \frac{d^3 k_1}{(2\pi)^3} \int \frac{d^3 k_2}{(2\pi)^3} \langle \Psi(t) | q_0(\mathbf{k}_1) q_0(\mathbf{k}_2) | \Psi(t) \rangle . \quad (199)$$

Taking the expectation value using equation (198) gives

$$\langle \Psi(t) | q_0(\mathbf{k}_1) q_0(\mathbf{k}_2) | \Psi(t) \rangle = \sigma_1^2(k_1) \delta^3(\mathbf{k}_1 - \mathbf{k}_2) + \rho \sigma_1^2(k_1) \delta^3(\mathbf{k}_1 + \mathbf{k}_2) , \quad (200)$$

where

$$\sigma_1^2(k) \equiv \frac{|u|^2(1 + |\theta|^2)}{4k^3} . \quad (201)$$

Although $|\theta|^2$ can be much larger than 1, the net spectral density is $|u|^2/(2k^3)$ because of partial cancellation of the two terms in equation (200). When $|\theta|^2 \gg 1$, $\rho \rightarrow -1$ and $q_0(-\mathbf{k}) \approx -q_0(\mathbf{k})$ as we will see below.

The parameter θ determines the correlations between the modes \mathbf{k} and $-\mathbf{k}$, i.e. the squeezing. For $(kt)^2 \gg 1$, $\theta = 1$, $\rho = 0$ and there is no squeezing. When modes are stretched far beyond the Hubble length, $kt \rightarrow 0^-$, $\theta \rightarrow -i\infty$ and $\rho \rightarrow -1$.

6.1.4 Wigner Function

The Wigner function is a generalization of the Schrödinger probability distribution to include momentum — it gives a probability distribution on phase space. It is defined by

$$W(\mathbf{q}, \mathbf{p}, t) = \int \frac{d^2r}{(2\pi)^2} e^{-i\mathbf{p}\cdot\mathbf{r}} \Psi^*(\mathbf{q} - \frac{1}{2}\mathbf{r}, t) \Psi(\mathbf{q} + \frac{1}{2}\mathbf{r}, t) . \quad (202)$$

Here \mathbf{q} , \mathbf{p} , and \mathbf{r} are two-vectors with components $q_1 = q_0(\mathbf{k})$, $q_2 = q_0(-\mathbf{k})$ and so on. Carrying out the integral gives

$$W(\mathbf{q}, \mathbf{p}, t) = \frac{1}{\pi^2} e^{-S/2} , \quad S = \mathbf{q} \cdot \mathbf{M}^{-1} \cdot \mathbf{q} + 4(\mathbf{p} - \bar{\mathbf{p}}) \cdot \mathbf{M} \cdot (\mathbf{p} - \bar{\mathbf{p}}) , \quad (203)$$

where

$$\mathbf{M} = \sigma^2 \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} , \quad \bar{\mathbf{p}} = \beta(\rho q_1 - 2q_2, \rho q_2 - 2q_1) , \quad \beta = \frac{\theta_i}{4\sigma^2(1 - \rho^2)\theta_r} . \quad (204)$$

The Wigner function can be simplified with by applying two unitary transformations. First, we take the following linear combinations of mode variables,

$$q_{\pm} \equiv \frac{q_1 \pm q_2}{\sqrt{2}} , \quad p_{\pm} \equiv \frac{p_1 \pm p_2}{\sqrt{2}} , \quad (205)$$

yielding

$$S = S_+ + S_- , \quad S_{\pm} = \frac{q_{\pm}^2}{\sigma^2(1 \pm \rho)} + 4\sigma^2(1 \pm \rho)[p_{\pm} + \beta(\pm 2 - \rho)q_{\pm}]^2 . \quad (206)$$

Next, we reduce the variables to four independent standard normal deviates $(\xi_{\pm}, \eta_{\pm})^4$:

$$\begin{aligned}\frac{q_{\pm}}{\sqrt{\sigma^2(1 \pm \rho)}} &= \frac{\xi_{\pm} + \eta_{\pm} \sqrt{\lambda_{\pm}}}{\sqrt{1 + \lambda_{\pm}}}, \\ 2p_{\pm} \sqrt{\sigma^2(1 \pm \rho)} &= \frac{\xi_{\pm}}{\sqrt{\lambda_{\pm}(1 + \lambda_{\pm})}} - \frac{\eta_{\pm} \lambda_{\pm}}{\sqrt{1 + \lambda_{\pm}}}.\end{aligned}\quad (207)$$

We introduced the auxiliary variables λ_{\pm} defined by

$$\lambda_{\pm} \equiv 1 + \frac{1}{2}\gamma_{\pm}^2 + \frac{1}{2}\gamma_{\pm}\sqrt{4 + \gamma_{\pm}^2}, \quad \gamma_{\pm} \equiv \frac{(\pm 2 - \rho)\theta_i}{2(1 \mp \rho)\theta_r}.\quad (208)$$

The Wigner function is now fully decoupled: $S = \xi_+^2 + \xi_-^2 + \eta_+^2 + \eta_-^2$. All the correlations of field values q_{\pm} and momenta p_{\pm} for the modes \mathbf{k} and $-\mathbf{k}$ are encoded in equations (207).

At early times, $(kt)^2 \gg 1$, $\rho = \beta = \gamma_{\pm} = 0$ so that q_{\pm}/σ and $2\sigma p_{\pm}$ are independent standard normal deviates. The harmonic oscillator ground state corresponds for all modes to a minimum uncertainty wavepacket, $\sigma_q \sigma_p = \frac{1}{2}$.

At late times, $kt \rightarrow 0^-$, $1 + \rho \rightarrow 0^+$ and the Bunch-Davies vacuum is strongly squeezed. There are two effects apparent in equations (207). The factors of $\sqrt{1 \pm \rho}$ on the left hand side stretch or shrink the distributions of (q_{\pm}, p_{\pm}) as $\rho \rightarrow -1$. In addition, the field and momentum variables become strongly correlated when $\lambda \rightarrow 0$ or $\lambda \rightarrow \infty$.

To see these effects, consider first the $+$ mode with phase space variables (q_+, p_+) . For this mode, in the limit $\rho \rightarrow -1$,

$$\sigma^2(1 + \rho) = \frac{|u|^2 \delta^3(0)}{2k^3}.\quad (209)$$

The field value and its momentum are strongly correlated for this mode: as $\gamma_+ \approx (3\theta_i)/(4\theta_r) \rightarrow -\infty$,

$$\lambda_+ \rightarrow \gamma_+^{-2} \rightarrow 0.\quad (210)$$

In this limit the ξ_+ variates dominate q_+ and p_+ , leading to a strong correlation:

$$\frac{q_+}{\sqrt{\sigma^2(1 + \rho)}} \approx \frac{2\sqrt{\sigma^2(1 + \rho)}}{|\gamma_+|} p_+ \approx \xi_+.\quad (211)$$

For the other mode, the standard deviation of the field is larger by a factor $|\theta|$:

$$\sigma^2(1 - \rho) = \frac{|\theta|^2 |u|^2 \delta^3(0)}{2k^3}.\quad (212)$$

⁴Note, (ξ_{\pm}, η_{\pm}) are all real numbers

For this mode, $\gamma_- \approx -\theta_i^3/(4\theta_r) \rightarrow +\infty$ and

$$\lambda_- \rightarrow \gamma_-^2 \rightarrow \infty . \quad (213)$$

Again the field value and its momentum are strongly correlated, now with an opposite sign:

$$\frac{q_-}{\sqrt{\sigma^2(1-\rho)}} \approx -\frac{2\sqrt{\sigma^2(1-\rho)}}{|\gamma_-|} p_- \approx \eta_- . \quad (214)$$

From $\langle q_+^2 \rangle \ll \langle q_-^2 \rangle$, it follows that $|q_1 + q_2| \ll |q_1 - q_2|$ hence $q_2 \approx -q_1$ or $q_0(-\mathbf{k}) \approx -q_0(\mathbf{k})$ as anticipated after equation (200).

Explain, based on the momenta and squeezing, why the field behaves classically as found in equation (187).

Then: given a mode expansion for one set of canonical variables, are the $a_0(\mathbf{k})$ the same for all sets of canonical variables? Is the vacuum definite?

Then: what if have not a pure vacuum, but a thermal density matrix?

Todo: Show a figure of the Wigner function for the plus and minus modes. discuss how quantum fields may now be treated as random variables.

Todo: Check that the expectation values are canonical invariants, i.e. that one gets the same inflationary perturbations using κ , q , or χ . After eq. (127) do scalar field in unperturbed RW to show error. Fourier expansion p. 21. Restore $\kappa = 8\pi G$.

6.2 Tensor Mode

This section must be redone to get the correct time evolution by solving the operator equations of motion as done for the scalar

The tensor mode fields are expanded as follows:

$$\psi_{ij}^{\text{TT}}(\mathbf{x}, t) = \frac{1}{a(t)} \sum_{\sigma} \int \frac{d^3k}{(2\pi)^{3/2}} (2k)^{-1/2} [e^{i\mathbf{k}\cdot\mathbf{x}} g_-(k, t) e_{\sigma, ij}(\mathbf{k}) a_{\sigma}(\mathbf{k}) + \text{h.c.}] , \quad (215a)$$

$$\pi_{\text{TT}}^{ij}(\mathbf{x}, t) = a(t) \sum_{\sigma} \int \frac{d^3k}{(2\pi)^{3/2}} (2k)^{-1/2} [e^{i\mathbf{k}\cdot\mathbf{x}} u_-(k, t) e_{\sigma, ij}(\mathbf{k}) a_{\sigma}(\mathbf{k}) + \text{h.c.}] , \quad (215b)$$

where $u_{\pm} \equiv a\partial(a^{-1}g_{\pm})/\partial t$ and the sum is over the two gravitational wave polarizations or helicity states. We assume that the Fock states for each mode (σ, \mathbf{k}) provide a complete basis for Hilbert space. The polarization basis tensors obey the relations

$$e_{\sigma, ij}^*(\mathbf{k}) = e_{\sigma, ij}(-\mathbf{k}) , \quad e_{\sigma_1, ij}(\mathbf{k}) e_{\sigma_2}^{*ij}(\mathbf{k}) = \delta_{\sigma_1\sigma_2} , \quad \sum_{\sigma} e_{\sigma, kl}(\mathbf{k}) e_{\sigma}^{*ij}(\mathbf{k}) = P_k^{(i} P_l^{j)} - \frac{1}{2} P_{kl} P^{ij} . \quad (216)$$

The creation and annihilation operators obey the commutation relations

$$[a_{\sigma_1}(\mathbf{k}_1), a_{\sigma_2}(\mathbf{k}_2)] = 0, \quad [a_{\sigma_1}^\dagger(\mathbf{k}_1), a_{\sigma_2}^\dagger(\mathbf{k}_2)] = 0, \quad [a_{\sigma_1}(\mathbf{k}_1), a_{\sigma_2}^\dagger(\mathbf{k}_2)] = \delta_{\sigma_1\sigma_2} \delta^3(\mathbf{k}_1 - \mathbf{k}_2). \quad (217)$$

These plus the Wronskian $\dot{g}_+g_- - g_+\dot{g}_- = 2ik$ ensure that ψ_{ij}^{TT} and π_{TT}^{ij} obey the correct commutation relations. Moreover, the time evolution of $g_\pm(k, t)$ and $u_\pm(k, t) = \dot{g}_\pm - \eta g_\pm$ ensure the correct evolution of the fields in the Heisenberg representation.

Equations (215) differ from the mode expansion in flat spacetime because of the background spacetime curvature. This leads to a striking difference in the Hamiltonian when expressed as a sum over modes:

$$H_{\text{TT}} = \frac{1}{4} \sum_{\sigma} \int \frac{d^3k}{k} \left\{ (u_-^2 + k^2 g_-^2) a_{\sigma}(\mathbf{k}) a_{\sigma}(-\mathbf{k}) + (u_+^2 + k^2 g_+^2) a_{\sigma}^\dagger(\mathbf{k}) a_{\sigma}^\dagger(-\mathbf{k}) \right. \\ \left. + (u_- u_+ + k^2 g_- g_+) [a_{\sigma}(\mathbf{k}) a_{\sigma}^\dagger(\mathbf{k}) + a_{\sigma}^\dagger(\mathbf{k}) a_{\sigma}(\mathbf{k})] \right\}. \quad (218)$$

In flat spacetime, or in Robertson-Walker spacetime with $k^2 \rightarrow \infty$, $g_\pm \rightarrow \exp(\pm ikt)$ and $u_\pm \rightarrow \dot{g}_\pm$, so that only the terms multiplied by $u_- u_+ + k^2 g_- g_+ = 2k^2$ remain in the sum over modes. The result is the usual energy $(N + \frac{1}{2})\hbar\omega$ per mode, with $\omega = k$.

[Try Bogoliubov transformation to diagonalize H_{TT} :

$$a_{\sigma}(\mathbf{k}) = u_{\sigma}(\mathbf{k}) b_{\sigma}(\mathbf{k}) + v_{\sigma}(\mathbf{k}) b_{\sigma}^\dagger(-\mathbf{k}), \\ a_{\sigma}^\dagger(\mathbf{k}) = u_{\sigma}^*(\mathbf{k}) b_{\sigma}^\dagger(\mathbf{k}) + v_{\sigma}^*(\mathbf{k}) b_{\sigma}(-\mathbf{k}), \quad (219)$$

where $b_{\sigma}(\mathbf{k})$ and $b_{\sigma}^\dagger(\mathbf{k})$ obey the same commutation relations as $a_{\sigma}(\mathbf{k})$ and $a_{\sigma}^\dagger(\mathbf{k})$.]

The vacuum state is defined so that $a_{\sigma}(\mathbf{k})|0\rangle = 0$ for any (σ, \mathbf{k}) and is normalized so that $\langle 0|0\rangle = 1$, implying $\langle 0|a_{\sigma_1}(\mathbf{k}_1) a_{\sigma_2}^\dagger(\mathbf{k}_2)|0\rangle = \delta_{\sigma_1\sigma_2} \delta^3(\mathbf{k}_1 - \mathbf{k}_2)$. This gives equal-time correlator

$$\langle 0|\psi_{\text{TT}}^{ij}(\mathbf{x}, t) \psi_{\text{TT}}^{\text{TT}}(\mathbf{y}, t)|0\rangle = \left[P_k^{(i} P_l^{j)} - \frac{1}{2} P_{kl} P^{ij} \right] \int d^3k e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \left[\frac{g_+(k, t) g_-(k, t)}{4ka^2} \right]. \quad (220)$$

The term in square brackets in the integrand is the power spectrum $P_{\text{TT}}(k, t)$.⁵ For power-law inflation with $\lambda < -\frac{1}{2}$ and $a = |t/t_0|^\lambda$, (after restoring the correct units with a factor $16\pi G$) it becomes

$$P_{\text{TT}}(k, t) = \pi G \left(\frac{3}{1-2\lambda} \right)^2 \left[\frac{\Gamma(3/2 - \lambda)}{\Gamma(5/2)} \right]^2 \left| \frac{t_0}{2} \right|^{2\lambda} k^{2\lambda-1}. \quad (221)$$

For $w = -1$, $\lambda \rightarrow -1$ and we obtain the expected scale-invariant spectrum $4\pi k^3 P_{\text{TT}} = (4\pi)^2 G H^2$ where H is the Hubble constant during inflation.

Introduction: Almost the entire difficulty of Hamiltonian gravity lies in finding the correct Hamiltonian, or equivalently, eliminating the constrained degrees of freedom.

⁵The power spectrum is normalized so that the total power is $\int P_{\text{TT}} d^3k$ and not $\int P_{\text{TT}} d^3k / (2\pi)^3$.

7 Appendix: Mode Expansion in Open Robertson-Walker Spaces

7.1 Classical solutions

We consider an arbitrary Robertson-Walker background and we expand the spatial dependence in eigenfunctions of the (Laplace-Beltrami) operator ∇^2 :

$$\psi_{\parallel}(\mathbf{x}, t) = a^{-1} f_{\pm}(k, t) Q(\mathbf{x}; \mathbf{k}) , \quad s_{ij}(\mathbf{x}, t) = a^{-1} \epsilon_{ij} g_{\pm}(k, t) Q_{ij}(\mathbf{x}; \mathbf{k}) . \quad (222)$$

Here \mathbf{k} are a set of eigenvalues labeling the appropriate scalar or tensor spherical harmonics (e.g. k, l, m in spherical coordinates) and ϵ_{ij} is a polarization tensor. The scalar and tensor eigenfunctions obey⁶

$$\nabla^2 Q = (-k^2 + K)Q , \quad \nabla^2 Q_{ij} = (-k^2 + 3K)Q_{ij} . \quad (223)$$

References

- [1] R. Arnowitt, S. Deser, and C. W. Misner 1962.
- [2] P. A. M. Dirac 1959, Phys. Rev. 114, 924.
- [3] T. Maskawa and H. Nakajima 1976, Prog. Theor. Phys. 56, 1295.
- [4] S. Weinberg 1995, *The Quantum Theory of Fields* (Cambridge Univ. Press), section 7.6.
- [5] E. Bertschinger 1996, in *Cosmology and Large Scale Structure, proc. Les Houches Summer School, Session LX*, ed. R. Schaeffer, J. Silk, M. Spiro, and J. Zinn-Justin (Amsterdam: Elsevier Science).
- [6] B. S. DeWitt 1967, Phys. Rev. 160, 1113.
- [7] W. Hu, U. Seljak, M. White, and M. Zaldarriaga, Phys. Rev. D57, 3290 (1998).

⁶Our k corresponds to q of Ref. [7]. The spectrum of eigenvalues has $k \geq 0$.