

Symmetry reduction, gauge reduction, backreaction and consistent higher order perturbation theory

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April 30, 2024

Abstract

For interacting classical field theories such as general relativity exact solutions typically can only be found by imposing physically motivated (Killing) *symmetry* assumptions. Such highly symmetric solutions are then often used as *backgrounds* in a *perturbative* approach to more general non-symmetric solutions.

If the theory is in addition a *gauge* theory such as general relativity, the issue arises how to consistently combine the perturbative expansion with the gauge reduction. For instance it is not granted that the corresponding constraints expanded to a given order still close under Poisson brackets with respect to the non-symmetric degrees of freedom up to higher order.

If one is interested in the problem of *backreaction* between symmetric and non-symmetric degrees of freedom, then one also must consider the symmetric degrees of freedom as dynamical variables which supply additional terms in Poisson brackets with respect to the symmetric degrees of freedom and the just mentioned consistency problem becomes even more complicated.

In this paper we show for a general theory how to consistently combine all of these notions. The idea is to *first* perform the *exact* gauge reduction on the *full* phase space which results in the reduced phase space of observables and physical Hamiltonian respectively and *secondly* expand that physical Hamiltonian perturbatively. Surprisingly, this strategy is not only practically feasible but also avoids the above mentioned tensions.

There is also a variant of this strategy that employs only a *partial* gauge reduction with respect to some of the non-symmetric degrees of freedom on the *full* phase space. We show that in perturbation theory the left over constraints close up to higher orders but not exactly, unless there is only one of them such as in cosmology. Since such *classically anomalous* constraints are problematic to quantise, the *full* gauge reduction for which these issues are absent is preferred in this case.

1 Introduction

In interacting field theories (such as general relativity (GR)) to find the general, exact solution of the field equations is not feasible. However, exact solutions can often be found when high amounts of (Killing) symmetries are imposed because this effectively reduces the number of dimensions and simplifies the associated PDE system. An extreme case are the cosmological solutions by asking for homogeneous spacetimes which reduces the Einstein equations to a system of ODE's. Other well known examples are spherically symmetric or axi-symmetric spacetimes describing black holes of Schwarzschild or Kerr type respectively. See [1] for an almost complete list of known exact solutions of GR with and without matter.

To find more general solutions one can use perturbative methods. One uses an exact symmetric solution as *background* and the non-symmetric deviations of the field from that symmetric background as a *perturbation*. The field equations can then be expanded order by order with respect to these perturbations and one can attempt to find solutions to any desired accuracy with respect to the perturbative order.

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This simple idea gets complicated when the field theory under consideration is a gauge theory such as GR which is subject to the spacetime diffeomorphism gauge group. We will work in the Hamiltonian setting with an eye towards canonical quantisation and discuss here only gauge symmetries generated by constraints of first class type in Dirac's classification [2] and only the case of a totally constrained system for which the Hamiltonian of the theory is a linear combination of constraints. Every gauge system can be reduced to that form by getting rid of the second class constraints replacing the Poisson bracket by the Dirac bracket and by parametrising a possibly present physical Hamiltonian.

In the presence of such gauge symmetries, the exact field equations split into two sets, one of them presenting constraints on the initial data and the other one presenting dynamical equations. The dynamical equations in turn can be obtained from the Hamiltonian in terms of Poisson brackets on the full phase space. For GR the constraints are known as spatial diffeomorphism and Hamiltonian constraints which are of first class. Systems of first class constraints by definition are in involution under the Poisson bracket on the full phase space and generate gauge motions on it. The constraint surface in the phase space is the set of points where the constraints vanish and the reduced phase space is the set of gauge orbits of the constraint surface which comes equipped with its own Poisson bracket. Functions on the reduced phase space are by construction gauge invariant and present so called Dirac observables.

When it comes to perturbations around symmetric backgrounds, we split the phase space coordinates into two sets, one of them presenting the symmetric background, the other one the non-symmetric perturbations. One expands the constraints in powers of these perturbations and may call the constraints truncated to n -th order in those perturbations constraints of n -th order. At this point one has to make a decision whether one wants to take *backreaction* into account or not. If not, one treats the background variables as prescribed external functions and just considers the phase space described by the non-symmetric perturbations. If yes, the background variables are still dynamical, we still consider the full phase space but use coordinates adapted to the (Killing) symmetry under investigation. In either case, it is not at all clear whether the n -th order constraints are in involution, at least up to higher than n -th order. Without backreaction this is known to be the case for $n \leq 2$ (see e.g. [4]) for a general theory explaining the success of cosmological, Schwarzschild and Kerr perturbation theory resulting in the well known Mukhanov-Sasaki, Wheeler-Zerilli and Teukolsky equations respectively [8, 9, 10]. With backreaction this is known not to be the case in examples but there is a procedure for how to correct this within perturbation theory and with backreaction for the case of cosmology and for $n = 2$ [5]. Beyond $n = 2$, to the best knowledge of the author, there is no commonly accepted procedure for how to reconcile perturbation theory with gauge symmetry (with or without backreaction), see e.g. [6, 7] and references therein for two concrete proposals within the Lagrangian and Hamiltonian formulation respectively which are not obviously equivalent. This poses a severe problem because without a consistent notion of gauge invariance, the observables of the theory cannot be extracted and the connection with phenomenology becomes veiled. Furthermore, on the practical side, within the current proposals the gauge invariant variables have to be recalculated every time one increases the perturbative order. It would be more convenient to disentangle gauge invariance from perturbation theory.

A possible avenue has been suggested in [11] where one passed to the exact reduced phase space before performing perturbation theory. This solves the tension because the gauge symmetry has now been taken care of to all orders. One can then extract the physical Hamiltonian and observables using deparametrisation and perform perturbation theory in the usual way that is familiar from unconstrained theories, directly in terms of fully gauge invariant observables and including backreaction. However, in [11] this could only be achieved by adding artificial dust matter to GR. While the effects of the dust were shown to be negligible in the late universe for small dust energy tensor, it would be desirable to be able to follow the strategy of [11] also without dust matter.

In this paper we consider the more difficult but physically more interesting case of including backreactions. In principle this is nothing but the full theory, however, written in field coordinates adapted to the symmetry of interest. We show, for a general first class theory subject to mild structural conditions that are motivated by the perturbative structure of the constraints of GR when using Killing symmetry reductions, that the machinery of deparametrisation of gauge systems [3] can be consistently combined with perturbation theory. This can be done in two versions. Either one performs a full reduction of all constraints or only a partial reduction corresponding to constraints that are naturally associated with some of the non-symmetric degrees of freedom. The exact full reduction immediately leads to a fully gauge invariant physical Hamiltonian and is analogous to [11]

while the exact partial reduction is analogous to [5] and keeps some left over constraints which are in involution. Surprisingly, these exact expressions, which are in general known only implicitly, can be accessed perturbatively as we show in this paper. The corresponding perturbative techniques do not require more than standard Taylor expansions of the constraints and for GR these have been worked out to some extent also to higher than second order for several symmetric backgrounds. However, the consistency between gauge reduction and perturbation theory imposes that the bits and pieces of these expressions be assembled in a novel way.

At second order, the resulting expressions reproduce the results of [5] for second order cosmological perturbation theory with backreaction. Since our method is not confined to $n = 2$, it embeds the method of [5] in a wider context. Our method can also be applied to the case of more than one unreduced constraint. In that case, the unreduced, perturbed constraints do close up to higher orders (trivially, in the case of just one unreduced constraint, they close exactly at any order) but not exactly. Therefore, as quantising constraints which are already classically anomalous are problematic in the quantum theory, the partial reduction version appears to be disfavoured in this case (e.g. black hole perturbation theory). As an alternative, one may follow the theory developed in [12] precisely for such “only approximately” first class constraints which is designed to deal with this problem, roughly by considering the closure violation as rendering the approximate constraints second class and applying the quantisation methods developed for second class constraints [3].

The architecture of this paper is as follows:

In section two we explain the general research question and motivate the structure of the canonical gauge system with respect to the symmetry reduction using the Killing reductions that one uses in GR. We pin point the problems that arise when one tries to combine standard Taylor expansions of constraints with gauge reduction.

In section three we review the reduced phase space approach to first class gauge systems, in particular the notion of relational Dirac observables subordinate to a choice of gauge fixing conditions or “clock” functions and corresponding physical Hamiltonian. Equivalently one may use the gauge fixing approach leading to the so-called “true degrees of freedom” subordinate to such a choice of gauge fixing condition and corresponding “reduced” Hamiltonian.

In section four we combine sections two and three which leads to a split of the canonical coordinates into four groups: symmetric or non-symmetric gauge degrees of freedom and symmetric or non-symmetric true degrees of freedom. Likewise, the constraints split into two groups corresponding to symmetric or non-symmetric smearing functions. In abuse of notation we call them symmetric or non-symmetric but note that in general they neither close among themselves nor just generate gauge transformations just on the symmetric or non-symmetric degrees of freedom. We then solve the non-perturbative constraints for the gauge degrees of freedom exactly, subordinate to a choice of gauge fixings. The split described suggests to adapt the gauge fixings to that split and thus to reduce the symmetric or non-symmetric constraints with respect to some of the symmetric or non-symmetric gauge degrees of freedom respectively. The result of that step is a reduced Hamiltonian which just depends on the true degrees of freedom, both symmetric and non-symmetric.

For sufficiently complicated systems, this exact reduced Hamiltonian will be known only implicitly involving inversions of functions etc. which makes it of little practical use. Surprisingly, it is still possible to derive a practically useful perturbation theory. This comes in two versions, the fully reduced and the partially reduced version described above and we outline the full version in the same section. We will see that this involves nothing but standard Taylor expansions of the constraints but assembled in a novel fashion in order to meet the consistency with gauge invariance. Hence standard unreduced perturbation theory is still valid, but our approach assembles its ingredients directly and unambiguously into objects that have a physical (gauge invariant) meaning.

In section five we lay out the reduction theory for the partially reduced version, also called “reduction in stages”. The motivation for such an approach could be to perform a classical gauge reduction with respect to some of the non-symmetric degrees of freedom eliminating just the non-symmetric constraints and then to quantise the resulting remaining symmetric constraints. A prominent example for this is the hybrid approach to quantum cosmology [13]. Again, this is practically useful only when applying perturbation theory to the resulting constraints. The problem is that those perturbed resulting constraints do not close exactly but only up to higher order in perturbation theory which poses a challenge for quantisation, unless there is only one of them, which is

the case in cosmology which is why [13] is successful. We show that the “in stages” approach for systems with only one symmetric constraint reproduces the framework of [5] obtained for 2nd order cosmological perturbation theory with backreaction and thus embeds this framework into our perturbation theory that is also valid at higher orders.

In section six we detail the perturbation theory for the remaining constraints of a partially reduced system including backreaction. The formulae we write can directly be applied to higher order cosmological perturbation theory with backreaction and thus can be applied for instance in the study of cosmological non Gaussianities. We supply these formulae for general orders in terms of an iteration scheme and solve the scheme explicitly for *third order*.

In section seven we conclude and give an outlook into the many future applications of the present work, such as quantum black hole perturbation theory which we have treated by the methods presented in the present paper in [14].

2 Symmetry reduction, gauge reduction, backreaction and perturbation theory

In the first subsection we motivate the general structure of the gauge systems for which we intend to develop perturbation theory around symmetric configurations using the example of general relativity (GR) where it is physically motivated to consider Killing reductions. In the second subsection we abstract from the example of GR and summarise the structure that we found in the first subsection. This structure is crucial for the constructions that follow in the subsequent sections.

2.1 Killing reductions in GR and mode decompositions

We consider a group G which acts via diffeomorphisms φ_g , $g \in G$ on tensor fields T on the spacetime manifold M . We have $\varphi_g \circ \varphi_{g'} = \varphi_{gg'}$ and $\varphi_{1_G} = 1_{\text{Diff}(M)}$. If the set of tensor fields under consideration includes a metric then it is sufficient to consider purely co-variant tensor fields so that the action is just by pull-back $T \mapsto \varphi^*T$ otherwise we also have to consider push-forwards for mixed tensors carrying also contra-variant structure. For the purpose of this motivation we confine ourselves to theories with metric fields, the additional details needed for the general case are easy to supply.

A tensor field is called symmetric with respect to G iff $\varphi_g^*T = T$ for all $g \in G$, otherwise non-symmetric. We also call a symmetric tensor a *zero mode* for reasons that become clear shortly. The group G acts of course also on M via φ_g and M has invariant submanifolds $N = \varphi_g(N)$ for all $g \in G$. We assume that the manifold M has the product structure $M = M_1 \times M_2$ with corresponding coordinates (ρ, θ) such that ρ labels the invariant submanifolds $N = N_\rho$, $\rho = \text{const.}$ and θ are “angular” coordinates on the N_ρ . In particular, the functions ρ are invariant scalars on M and φ_g acts non-trivially only on the coordinates θ . In other words, M is foliated by the leaves N_ρ diffeomorphic to M_2 with foliation parameters ρ .

This warped structure motivates to perform harmonic analysis on M_2 : We note that a (pseudo-) tensor t on M_2 has both a “spin” transformation of its indices and an “orbital” transformation of its arguments. The spin part can be considered as a finite dimensional representation π_s of G and the orbital part as an infinite dimensional one $\pi_o \equiv \phi$. and thus the tensor transforms in the infinite dimensional tensor product representation $\pi_s \otimes \pi_o$ as

$$[\varphi_g^*t](\theta) = \pi_s(g) \cdot t(\varphi_g(\theta)) \quad (2.1)$$

Suppose that such a representation can be decomposed into irreducibles π . An *irreducible tensor harmonic* t_π on M_2 of type π where π is an irreducible representation of G corresponds precisely to such a decomposition.

A distinguished role in what follows is played by an invariant metric field Ω on M_2 of Euclidian signature i.e. $\varphi_g^*\Omega = \Omega$, $g \in G$ which we assume to exist. It is a tensor harmonic of degree two with respect to the trivial representation. It follows that $d\mu(\theta) = |\det(\Omega)(\theta)|^{1/2} d\theta$ is an invariant measure on M_2 , that is

$$\int_{M_2} d\mu(\theta) f(\varphi_g(\theta)) = \int_{M_2} d\mu(\theta) f(\theta) =: \mu(f) \quad (2.2)$$

for all measurable functions f on M_2 . We assume that G and therefore M_2 is compact and μ or Ω can therefore be normalised such that $\mu(1) = 1$. Here $d\theta$ is the Lebesgue measure on M_2 . In the non-compact case one usually compactifies M_2 (e.g. toroidally) and considers a decompactification limit at the end of the quantisation process (thermodynamic limit).

Using Ω we can define an inner product on the space L_2^d of square integrable tensors on M_2 of degree d

$$\langle t, t' \rangle := \int_{M_2} d\mu(\theta) \overline{t(\theta)} \cdot [\otimes^d \Omega^{-1}(\theta)] \cdot t'(\theta) \quad (2.3)$$

where $\cdot$ denotes the only possible contraction of indices of the tensors involved with the inverse metric Ω^{-1} which grants that the inner product is positive. The complex conjugation in (2.3) can of course be dropped when the tensors are real valued but often it is convenient to consider complex valued tensors. We note that G acts unitarily on L_2^d .

To become more concrete, we consider first degree $d = 0$, i.e. scalars. Then $\mathcal{H} = L_2(M_2, d\mu)$ can be decomposed into invariant subspaces $\mathcal{H}_\pi$ corresponding to irreducible representations π . We pick an ONB L_k^π , $k = 1, \dots, \dim(\pi)$ wrt (2.3) in $\mathcal{H}_\pi$ and consider the map $I_{\pi', \pi}; \mathcal{H}_\pi \rightarrow \mathcal{H}_{\pi'}$ defined by $I_{\pi, \pi'} \cdot v := \sum_{k'} L_{k'}^{\pi'} \langle L_k^\pi, v \rangle_{\mathcal{H}}$. Using unitarity we see that $I_{\pi, \pi'}$ is an intertwiner. By definition of irreducible representations, the intertwiner must be trivial, i.e. the identity when the representations are equivalent and zero when they are not (Schur's lemma). It follows that the L_k^π form an orthonormal system of $\mathcal{H}$ and we assume that it is in fact an orthonormal basis i.e. that Plancherel's theorem holds. This decomposition denotes the "orbital" part $\pi_o = \pi$ of the decomposition. Now tensors of degree $d > 0$ can be obtained by combinations of multiple actions of the Ω compatible torsion free covariant differential D on scalars together with contractions by Ω and η where η is the totally skew pseudo-tensor on M_2 . A tensor is called polar and axial respectively if the number of η factors used is even and odd respectively so that the tensor itself is a tensor and pseudo tensor respectively. Given a basis of (pseudo-) tensors of degree d so obtained from scalars, we can decompose them into orthogonal subspaces with respect to the fibre metric $\otimes^d \Omega^{-1}$. These spaces are also invariant under G because they are built from covariant tensor operations. This decomposition denotes the "spin" part π_s of the decomposition. Now given a tensor of a certain spin type we can restrict the scalars on which the invariant tensor operations act to the orbital space labelled by π_s . This completes the concrete description of irreducible tensor harmonics of type $\pi_s \otimes \pi_o$.

The relevance of this with regard to perturbation theory is now as follows: Given a tensor field T on $M = M_1 \times M_2$, for fixed ρ we can consider it as a collection of tensor fields on M_2 . To do this we split the coordinates x^μ , $\mu = 0, \dots, m = m_1 + m_2 - 1$ into ρ^α , $\alpha = 0, \dots, m_1 - 1$ and θ^A , $A = 1, \dots, m_2$ and accordingly each tensor T on M of total degree d can be considered as a collection of tensors of degree $d_2 = 0, 1, \dots, d$ on M_2 with fixed $d_1 = d, d - 1, \dots, 0$ indices taking values in the set of values of α and the remaining the values of A . Each tensor in this collection transforms in some finite dimensional representation of G . This is because for G compact, its irreducible representations are completely classified, they are all finite dimensional and every representation decomposes into irreducibles [15]. Therefore, all tensor fields T on M can be uniquely decomposed into irreducible tensor harmonics. The expansion coefficients in that decomposition are tensors on M_1 i.e. we have a neat decomposition of any T on M into a linear combination of tensor products $t_1^\pi \otimes t_\pi$ where t_π is an irreducible tensor harmonic of type π on M_2 , called a *mode* and t_1^π is some tensor on M_1 . The perturbative structure is now defined by distinguishing between the tensors t_1^π corresponding to the trivial representation, i.e. the zero modes or symmetric tensors, and the tensors t_1^π corresponding to non-trivial representation, i.e. the non-zero modes or non-symmetric tensors. The zero modes are declared as background degrees of freedom while the non zero-modes are declared as perturbations.

So far we have used spacetime language. In the canonical approach one considers globally hyperbolic space-times (M, g) whose underlying manifold is diffeomorphic to a Cartesian product $\mathbb{R} \times \sigma$ for some $m - 1$ manifold σ [16]. We will assume that the φ_g preserve the time axis and therefore all that we have said applies also to $\sigma = \sigma_1 \times M_2$ with $M_1 = \mathbb{R} \times \sigma_1$. Next to the tensor fields themselves in the canonical formulation now one also needs their first time derivatives on the Cauchy surface σ or equivalently their conjugate momenta which are tensor densities of weight one of dual type (i.e. purely contra-variant if the tensor fields are purely co-variant). Thus for each tensor mode t_1^π we have a momentum p_1^π . These are automatically canonically conjugate. To see

this, we consider the symplectic structure at fixed t

$$\Theta = \int_{\sigma} d^{m-1}x P \cdot [\delta T] \quad (2.4)$$

where P is conjugate to T and both P, T have not yet been decomposed into tensor harmonics. Using coordinates such that $d^{m-1}x = d\rho d\mu$, we now expand both P, T into tensor harmonics $P^{\pi} \otimes t_{\pi}, T^{\pi} \otimes t_{\pi}$ and see that the mixed terms drop out because (2.4) is of the form of the inner product (2.3), specifically

$$\Theta = \sum_{\pi} \int_{\sigma_1} d\rho_1 P^{\pi} \cdot [\delta T^{\pi}] \quad (2.5)$$

where $\rho = (t, \rho_1)$ was used.

Next we come to the constraints. By construction, the constraints $C = C(T, P)$ are themselves tensor fields on σ of density weight one constructed from the canonical fields T, P while their smearing functions f are dual tensors of density weight zero. We decompose f into tensor harmonics $f^{\pi} \otimes t_{\pi}$, do the same with P, T and integrate out M_2 resulting in

$$C(F) = \int_{\sigma} d^{m-1}x f \cdot C = \sum_{\pi} \int_{\sigma_1} d\rho_1 f^{\pi} \cdot \langle t_{\pi}, C \rangle =: \sum_{\pi} \int_{\sigma_1} d\rho_1 f^{\pi} \cdot C_{\pi} \quad (2.6)$$

Note that C_{π} can depend non-trivially on all degrees of freedom $T^{\pi'}, P^{\pi'}$.

Perturbation theory now consists in singling out the symmetric degrees of freedom $Q_B = T^{\pi_t}, P_B = P^{\pi_t}$ with trivial representation π_t as background variables and to keep those $Q_{\pi} = T^{\pi}, P_{\pi} = P^{\pi}$ for non trivial representation $\pi \neq \pi_t$ as first order perturbation. Note that for each π we can have several “species” that may result from additional matter content or because there are several ways to couple spin and orbital dependence into the same π or because of the remaining tensor structure on M_1 . We suppress a corresponding species index in order not to clutter the notation. We can perform a Taylor expansion of the C_{π} in terms of the $Q_{\pi'}, P_{\pi'}$ with coefficients that depend only on the Q_B, P_B . Let $C_{\pi, (n)}$ be the n -th order perturbation of C_{π} i.e. a homogenous polynomial in the $Q_{\pi'}, P_{\pi'}$ of degree n . Then an important observation is that $C_{\pi, (0)} = 0$ if $\pi \neq \pi_t$ and $C_{\pi, (1)} = 0$ for $\pi = \pi_t$ because of the orthogonality properties of (2.3).

Finally it will be convenient to assume that the tensorial type with respect to M_2 of the smearing functions f of the constraints also appears among the list of canonical tensor fields or their canonical momenta, possibly after performing a canonical transformation. In GR these tensorial types are scalar and vectorial and the assumption just made is always met when decomposing the spatial metric with respect to the tensor type on M_2 .

We close this subsection by mentioning how the above general theory fits with the well known examples relevant for cosmology and black holes in four spacetime dimensions:

- i.
For cosmology we assume that σ is compact, say a 3-torus (choosing the torus sufficiently large we cannot observationally distinguish it from $\mathbb{R}^3$) whence $G = \text{SO}(2)^3$ is the translation group of the torus. The tensor harmonics are then just the Fourier modes of the torus labelled by a vector $\pi \in \mathbb{Z}^3$ and the manifold σ_1 is zero dimensional so that the integral over ρ_1 in (2.6) is discarded. The zero modes with $\pi = 0$ in this case are just homogeneous metric and matter degrees of freedom.
- ii.
For spherically symmetric Schwarzschild black holes the relevant group is $G = \text{SO}(3)$ and the tensor harmonics are the well known spherical tensor harmonics [17] which are labelled by indices $\pi = (I, l, m)$ where I is a discrete index depending on the tensor degree and l, m are the usual quantum numbers labelling the scalar harmonics $Y_{l, m}$ familiar from the theory of angular momentum. The zero modes are functions that depend only on the radial variable $\rho_1 = r$.
- iii.
For axi-symmetric Schwarzschild black holes the relevant group is $G = \text{SO}(2)$ and the tensor harmonics are again just the Fourier modes of the 1-torus labelled by $\pi \in \mathbb{Z}$. The zero modes are functions that depend only on the radial and axial variable $\rho_1 = (r, z)$.

Finally notice that while we have here only treated the case of bosonic tensor fields, an extension of tensor harmonics to spin harmonics i.e. fermionic fields is easily possible by passing to the covering group of the above groups which is still compact and otherwise performing the same decomposition into irreducibles, see e.g. [18].

2.2 Summary of the symmetry, gauge and perturbative structure and notation

We consider a phase space with canonically conjugate coordinates k^A, i_A where in field theory A takes values in a countably infinite index set (the mode labels π , the species labels and if σ_1 is not zero dimensional further labels e.g. corresponding to an orthonormal basis of $L_2(\sigma_1, d\rho_1)$) but in what follows that range could also be finite. Likewise we have non-perturbative constraints C_μ where again μ has countably infinite range in field theory but we can also consider finite range in what follows. We invoke the information about the symmetry structure of the background by splitting μ into pairs $\mu = (a, j)$ where a labels the zero (symmetric) modes of the smearing function f^μ and j the non-zero (non-symmetric) modes. Accordingly we have symmetric and non-symmetric constraints C_a, C_j respectively as coefficients of f^a, f^j respectively.

As motivated at the end of the previous subsection we can perform a corresponding split also among the canonical coordinates. But unless the theory is topological there will be additional degrees of freedom. Accordingly we split

$$(k^A, i_A) = ((q^a, p_a), (x^j, y_j), (Q^A, P_A), (X^J, Y_J)) \quad (2.7)$$

where the meaning is as follows: Both pairs (q, p) and (Q, P) correspond to zero modes, i.e. they are symmetric degrees of freedom. Both pairs (x, y) and (X, Y) correspond to non-zero modes, i.e. they are non-symmetric degrees of freedom. This emphasises their grouping with respect to the symmetry and perturbative structure, that is, one will expand with respect to x, y, X, Y around q, p, Q, P . On the other hand we can group them with respect to the gauge structure: The index picture suggests to consider the pairs (p, q) and (x, y) as pure gauge degrees of freedom while the pairs (P, Q) and (X, Y) are considered as true degrees of freedom.

In other words we have a twisting of four sectors corresponding to the symmetry and gauge aspect: There are both symmetric and non-symmetric observables $(P, Q), (X, Y)$ and both symmetric and non-symmetric gauge variables $(p, q), (x, y)$. The fact that these four pairs of variables are conjugate within the respective pair and have vanishing Poisson brackets between variables of different pairs was motivated in (2.5) above.

We can now develop perturbation theory on the unreduced phase space coordinatised by (2.7), that is, we perform a Taylor expansion of the constraints

$$C_a((p, q), (P, Q), (x, y), (X, Y)), C_j((p, q), (P, Q), (x, y), (X, Y)) \quad (2.8)$$

with respect to x, y, X, Y at fixed p, q, P, Q . We denote by $C_{a(n)}$ the n -th order contribution to C_a in that expansion which is a homogeneous polynomial of degree n in x, y, X, Y with coefficients which may depend non-polynomially on p, q, P, Q . The meaning of $C_{j(n)}$ is similar. On the other hand the expansion of the constraints to n -th order is denoted as

$$C_a^{(n)} = \sum_{k=0}^n C_{a(k)}, C_j^{(n)} = \sum_{k=0}^n C_{j(k)} \quad (2.9)$$

and we write $O(n)$ for any function on phase space whose perturbative expansion contains homogeneous orders of degree n or higher.

The observation made towards the end of the previous subsection translates into the statement that

$$C_{a(1)} = 0, C_{j(0)} = 0 \quad (2.10)$$

By assumption, the non-perturbative constraints are in involution, that is there are structure functions κ on the full phase space such that

$$\begin{aligned} \{C_a, C_b\} &= \kappa_{ab}^c C_c + \kappa_{ab}^j C_j \\ \{C_a, C_j\} &= \kappa_{aj}^b C_b + \kappa_{aj}^k C_k \\ \{C_j, C_k\} &= \kappa_{jk}^a C_a + \kappa_{jk}^l C_l \end{aligned} \quad (2.11)$$

where the Poisson brackets $\{.,.\}$ are with respect to all phase space coordinates and the indices $a, b, c, \dots$ and $j, k, l, \dots$ have the same range respectively, summation over repeated indices being implied.

We introduce a corresponding perturbative notation $\kappa_{**}^{*(n)}$, $\kappa_{**}^{*(n)}$ for the structure functions and introduce the following symmetric and non-symmetric Poisson bracket respectively

$$\{F, G\}_S := \{F, q^a\} \{p_a, G\} + \{F, Q^A\} \{P_A, G\} - \{G, q^a\} \{p_a, F\} - \{G, Q^A\} \{P_A, F\}, \quad \{F, G\}_{\bar{S}} := \{F, G\} - \{F, G\}_S \quad (2.12)$$

which just takes derivatives with respect to the symmetric and non-symmetric degrees of freedom respectively. It follows that $\{O(m), O(n)\}_S = O(m+n)$ and $\{O(m), O(n)\}_{\bar{S}} = O(m+n-2)$ which has the advantage that we can better keep track of the perturbative order. We can use this and matching of perturbative order to derive the infinite hierarchy of exact relations for $N = 0, 1, \dots$

$$\sum_{m+n=N; m, n \geq 0} \{C_{(m)}, C_{(n)}\}_S + \sum_{m+n=N+2; m, n \geq 1} \{C_{(m)}, C_{(n)}\}_{\bar{S}} = \sum_{m+n=N; m, n \geq 0} \kappa_{(m)} C_{(n)} \quad (2.13)$$

where we have suppressed the indices a, b, c, j, k, l which are the same as in (2.11).

The system (2.13) together with (2.10) contains important information, we only state more explicitly the first few of them relevant for perturbation theory up to $n = 2$:

$N = 0$:

i.

Since $\{C_a(0), .\}_{\bar{S}} = 0 = C_{a(1)}$

$$\{C_{a(0)}, C_{b(0)}\} = \kappa_{ab(0)}^c C_{c(0)} \quad (2.14)$$

i.e. the $C_{a(0)}$ are in involution with respect to the full Poisson bracket.

ii.

Since $C_{j(0)} = 0$

$$\{C_{j(1)}, C_{k(1)}\}_{\bar{S}} = \kappa_{jk(0)}^a C_{a(0)} \quad (2.15)$$

i.e. the $C_{j(1)}$ close modulo $C_{a(0)}$ but only with respect to the non-symmetric bracket.

iii.

Since $C_{a(1)} = C_{j(0)} = 0$

$$\kappa_{aj(0)}^b = 0 \quad (2.16)$$

$N = 1$:

i.

Using $C_{a(1)} = 0$

$$0 = \kappa_{ab(1)}^k C_{c(0)} + \kappa_{ab(0)}^j C_{j(1)} \quad (2.17)$$

ii.

Using $C_{a(1)} = C_{j(0)} = 0$

$$\{C_{a(0)}, C_{j(1)}\}_S + \{C_{a(2)}, C_{j(1)}\}_{\bar{S}} = \kappa_{aj(0)}^k C_{k(1)} + \kappa_{aj(1)}^b C_{b(0)} \quad (2.18)$$

$N = 2$:

Using $C_{a(1)} = 0 = C_{j(0)}$

$$\{C_{a(0)}, C_{b(2)}\}_S + \{C_{a(2)}, C_{b(0)}\}_S + \{C_{a(2)}, C_{b(2)}\}_{\bar{S}} = \kappa_{ab(0)}^c C_{c(2)} + \kappa_{ab(0)}^j C_{j(2)} + \kappa_{ab(1)}^j C_{j(1)} + \kappa_{ab(2)}^c C_{c(0)} \quad (2.19)$$

We may now apply the following logic: As we consider the non-symmetric degrees of freedom as perturbations and since in GR the smearing functions also are dynamical degrees of freedom (lapse and shift functions, they are variables conjugate to the primary constraints of GR) in the expansion of the Hamiltonian

$$H(f, g) = f^a C_a + g^j C_j \quad (2.20)$$

we should consider also f^a as of zeroth order and g^j of first order. This argument is substantiated by another one which considers the gauge transformation $\delta F = \{H(f, g), F\}$ generated by (2.20). For a symmetric degree of

freedom $F \in \{q, p, Q, P\}$ which is of zeroth order we have $\Delta F = \{H(f, g), F\}_S$ while for a non-symmetric degree of freedom $F \in \{x, y, X, Y\}$ which is of first order we have $\Delta F = \{H(f, g), F\}_{\bar{S}}$. Since $C_a = C_{a(0)} + O(2)$ while $C_j = C_{j(1)} + O(2)$ the zeroth order character of F is preserved by δF iff f is considered as zeroth order and the first order character of F is preserved by δF iff g is considered as first order.

Following this logic the N -th order truncation of H is given by

$$H^{(N)}(f, g) = f^a C_a^{(N)} + g^j C_j^{(N-1)} \quad (2.21)$$

and we may ask whether the N -th order truncations $f^a C_a^{(N)}, g^j C_j^{(N-1)}$ are in involution for various values of N , either exactly or up to $O(N+1)$ terms at least. Due to $C_{a(1)} = C_{j(0)} = 0$ we have $H^{(0)}(f) = f^a C_{a(0)}$ which is in involution as demonstrated by (2.14) both with respect to the full bracket and the symmetric bracket only. This says that symmetry reduction excluding perturbations produces a consistent gauge system.

For $N = 2$ we find

$$H^{(2)}(f) = f^a [C_{a(0)} + C_{a(2)}] + g^j C_{j(1)} =: C^{(2)}(f) + C^{(1)}(g) \quad (2.22)$$

The analysis of the closure of the constraints now depends on whether one wants to incorporate backreaction or not. With backreaction, the system should close with respect to the full bracket $\{.,.\}$, without it, it should close with respect to the non-symmetric bracket $\{.,.\}_{\bar{S}}$.

I. No backreaction.

From (2.15) we have directly

$$\{C^{(1)}(g), C^{(1)}(g')\}_{\bar{S}} = g^j (g')^k \kappa_{jk(0)}^a C_{a(0)} = g^j (g')^k \kappa_{jk(0)}^a C_a^{(2)} - \{g^j (g')^k \kappa_{jk(0)}^a C_{a(2)}\} \quad (2.23)$$

We can close the algebra of the $C^{(1)}(g)$ exactly if we impose on p, q, P, Q that $C_{a(0)} = 0$ which without backreaction is possible as the background variables are considered as an external structure. This is what is usually done [19] and (2.23) it is then in fact Abelian. Otherwise it closes up to a term $C^{(2)}(f)$ modulo an $O(4)$ correction displayed as the curly bracket term in (2.23) if g, g' count as first order each. Next from (2.18)

$$\{C^{(1)}(g), C^{(2)}(f)\}_{\bar{S}} = \{C^{(1)}(g), C_{(2)}(f)\}_{\bar{S}} = g^j f^a [\kappa_{ja(0)}^k C_{k(1)} + \kappa_{ja(1)}^b C_{b(0)} - \{C_{j(1)}, C_{a(0)}\}_S] \quad (2.24)$$

where we used that $C_{a(0)}$ has vanishing $\{.,.\}_{\bar{S}}$ brackets. We can close (2.24) exactly if again we impose on p, q, P, Q that $C_{a(0)} = 0$ there and that it is a common critical point of the $C_{a(0)}$ i.e. their Hamiltonian vector fields vanish there so that the subtracted term in (2.24) vanishes. Together with the fact that $C_{a(1)} = 0$ this means that the Hamiltonian vector field of the non-perturbative C_a vanishes in the full phase space at the chosen p, q, P, Q and at $x = y = X = Y = 0$ which then is a point on the full constraint surface. When a takes only one value (cosmology) this is again standard [19]. Since the subtracted term in (2.24) is $O(2)$ this is in fact the only option. Finally from (2.19)

$$\begin{aligned} \{C^{(2)}(f), C^{(2)}(f')\}_{\bar{S}} &= \{C_{(2)}(f), C_{(2)}(f')\}_{\bar{S}} \\ &= f^a (f')^b [\kappa_{ab(0)}^c C_{c(2)} + \kappa_{ab(0)}^j C_{j(2)} + \kappa_{ab(1)}^j C_{j(1)} + \kappa_{ab(2)}^c C_{c(0)}] - \{C_{a(0)}, C_{b(2)}\}_S - \{C_{a(2)}, C_{b(0)}\}_S \\ &= f^a (f')^b [\kappa_{ab(0)}^b C_c^{(2)} + \kappa_{ab(0)}^j C_{j(2)} + \kappa_{ab(1)}^j C_{j(1)} + (\kappa_{ab(2)}^c - \kappa_{ab(0)}^c) C_{c(0)}] \\ &\quad - \{C_{a(0)}, C_{b(2)}\}_S - \{C_{a(2)}, C_{b(0)}\}_S \end{aligned} \quad (2.25)$$

which closes exactly if $C_{a(0)}$ and its Hamiltonian vector field vanishes at q, p, Q, P and if in addition $\kappa_{ab(0)}^j = 0$ there. From (2.16) which holds everywhere in the full phase space, this is indeed the case as the $C_{j(1)}$ are linearly independent.

II. Including backreaction.

Using the above results we find the full and exact Poisson bracket relations

$$\begin{aligned}
\{C^{(1)}(g), C^{(1)}(g')\} &= \{C^{(1)}(g), C^{(1)}(g')\}_{\bar{S}} + \{C^{(1)}(g), C^{(1)}(g')\}_S = g^j(g')^k \kappa_{jk(0)} {}^a C_{a(0)} + \{C^{(1)}(g), C^{(1)}(g')\}_S \\
&= g^j(g')^k \kappa_{jk(0)} {}^a C_{a(2)} + \{\{C^{(1)}(g), C^{(1)}(g')\}_S - g^j(g')^k \kappa_{jk(0)} {}^a C_{a(2)}\} \\
\{C^{(1)}(g), C^{(2)}(f)\} &= \{C^{(1)}(g), C^{(2)}(f)\}_{\bar{S}} + \{C^{(1)}(g), C^{(2)}(f)\}_S \\
&= \{C_{(1)}(g), C_{(2)}(f)\}_{\bar{S}} + \{C_{(1)}(g), C_{(0)}(f)\}_S + \{C_{(1)}(g), C_{(2)}(f)\}_S \\
&= g^j f^a [\kappa_{ja(0)} {}^k C_{k(1)} + \kappa_{ja(1)} {}^b C_{b(0)}] + \{C_{(1)}(g), C_{(2)}(f)\}_S \\
&= g^j f^a [\kappa_{ja(0)} {}^k C_{k(1)} + \kappa_{ja(1)} {}^b C_{b(2)}] + \{\{C_{(1)}(g), C_{(2)}(f)\}_S - g^j f^a \kappa_{ja(1)} {}^b C_{b(2)}\} \\
\{C^{(2)}(f), C^{(2)}(f')\} &= \{C^{(2)}(f), C^{(2)}(f')\}_{\bar{S}} + \{C^{(2)}(f), C^{(2)}(f')\}_S = \{C_{(2)}(f), C_{(2)}(f')\}_{\bar{S}} + \{C^{(2)}(f), C^{(2)}(f')\}_S \\
&= [\{C_{(2)}(f), C_{(2)}(f')\}_{\bar{S}} + \{C_{(0)}(f), C_{(2)}(f')\}_S + \{C_{(2)}(f), C_{(0)}(f')\}_S] + \{C_{(0)}(f), C_{(0)}(f')\}_S + \{C_{(2)}(f), C_{(2)}(f')\}_S \\
&= f^a(f')^b [\kappa_{ab(0)} {}^c C_{c(2)} + \kappa_{ab(0)} {}^j C_{j(2)} + \kappa_{ab(1)} {}^j C_{j(1)} \kappa_{ab(2)} {}^c C_{c(0)} + \kappa_{ab(0)} {}^c C_{c(0)}] + \{C_{(2)}(f), C_{(2)}(f')\}_S \\
&= f^a(f')^b [\kappa_{ab(0)} {}^c C_{c(2)} + \kappa_{ab(0)} {}^j C_{j(2)} + \kappa_{ab(1)} {}^j C_{j(1)} \kappa_{ab(2)} {}^c C_{c(0)}] + \{C_{(2)}(f), C_{(2)}(f')\}_S \\
&= f^a(f')^b [(\kappa_{ab(0)} {}^c + \kappa_{ab(2)} {}^c) C_{c(2)} + \kappa_{ab(0)} {}^j C_{j(2)} + \kappa_{ab(1)} {}^j C_{j(1)}] + \{\{C_{(2)}(f), C_{(2)}(f')\}_S - \kappa_{ab(2)} {}^c C_{c(2)}\} \quad (2.26)
\end{aligned}$$

where we used several times that $C_{a(0)}$ has vanishing $\{\cdot, \cdot\}_{\bar{S}}$ brackets. If we consider g, g' as first order objects, then the curly bracket term in the above relations is $O(4)$ and can be ignored in 2nd order perturbation theory. Then all three equations close up to the last equation to second order provided that in addition $\kappa_{ab(0)} {}^j = 0$ everywhere. In view of (2.16) which holds everywhere in phase space and the linear independence of $C_{a(0)}, C_{j(1)}$ this may actually hold but it is not entirely conclusive, so we must impose this as an extra condition if we are to follow this approach. It holds trivially if a takes only one value (cosmology).

If on the other hand we want (2.26) to close exactly and not only up to higher order, then as it stands the system is inconsistent. This explains why considerable effort must be invested to achieve closure in cosmology [5]. The motivation to have exact closure is that while in the classical theory one may be able to control errors when working with approximate equations, in the quantum theory it is vital to have exact relations because the quantum constraints determine the size of the physical Hilbert space. Anomalous, i.e. not exactly closing constraints, over-constrain the system and yield a physical Hilbert space which is too small to allow for the correct classical limit. The way that closure of (2.26) is achieved in [5] is by a clever combination of i. the exact relation (2.15) combined with ii. canonical transformations on the full phase correct up to second order and iii. absorption of higher order terms into smearing the functions f^a .

However, it is clear that the method of [5] repairs the system (2.26) only if a takes only one value (cosmology) and for $N = 2$ only. In fact, one can easily generalise (2.26) to higher orders but obtaining exact closure fails more and more severely the higher the order. Also closure up to higher order only occurs if one considers g, g' as of first order and one may feel uneasy with that viewpoint. The methods of this paper extend the results of [5] to a general gauge system subject to the assumptions spelled out in section 2.1 for an arbitrary range of a and for arbitrary N . We follow a route very different from the route chosen in [5]. Yet, for $N = 2$ and a taking only one value, we agree with [5].

3 Gauge reduction, gauge conditions, relational Dirac observables, physical Hamiltonian

This section is for the benefit of the reader not familiar with gauge reduction and the relational formalism. We explain here just the bare bones of this theory, see [3] for all the details and [20] for an exposition closer in notation to the present section. Familiar readers may immediately jump to the next section.

In this section we ignore the split with respect to the symmetric and non-symmetric variables and we ignore perturbation theory altogether and just assume that the phase space is coordinatised by canonical pairs (r^α, s_α) and (u^μ, v_μ) respectively where (r, s) plays the role of $(Q, P), (X, Y)$ and (u, v) the role of $((q, p), (x, y))$. The system is subject to first class constraints C_μ . The above split of the phase space variables is assumed to be

judiciously chosen in such a way that one may solve the constraints $C_\mu(r, s, u, v) = 0$ (locally) in terms of the momenta v_μ , that is we pass to equivalent constraints

$$\hat{C}_\mu(r, s, u, v) = v_\mu + h_\mu(r, s, u) \quad (3.1)$$

The dependence of the C_μ on the v_ν is usually polynomial and if the polynomial degree is higher than one then the functions h_μ are not unique but depend on finitely many “branches”. We assume that some physical motivation (e.g. positivity of energy) has been given to select one of those branches and consider henceforth the corresponding sector of the phase space that contains the constraint surface defined by (3.1).

Since the $\hat{C}_\mu$ are just linear combinations of the C_μ (with complicated phase space dependent coefficients) as $C = 0 \Leftrightarrow \hat{C} = 0$ on the sector considered, and the C_μ are first class, so must be the $\hat{C}_\mu$ i.e. there are structure functions $\hat{\kappa}$ such that

$$\{\hat{C}_\mu, \hat{C}_\nu\} = \hat{\kappa}_{\mu\nu}{}^\rho \hat{C}_\rho \quad (3.2)$$

Since the $\hat{C}$ contains v linearly, the l.h.s. of (3.2) is independent of v . Thus for any (r, s, u) we may evaluate the l.h.s. by setting $v = -h(r, s, u)$ on the r.h.s. As this vanishes identically, we conclude that the constraints $\hat{C}_\mu$ are *Abelian* on the full phase space $\{\hat{C}_\mu, \hat{C}_\nu\} = 0$. This fact will be very handy in what follows.

We split the following exposition in the “gauge invariance” and the “reduction” viewpoint. Both are equivalent descriptions of the reduced phase space. The gauge invariance viewpoint explicitly constructs the relational Dirac observables as functions on the full phase space. Here “relational” refers to the fact that one must select a set of gauge fixing conditions that enter explicitly into the construction: One can “project” any phase space function into a Dirac observable relative to these gauge fixing conditions, but neither the constraints nor the gauge fixing conditions are installed. By contrast, the reduction viewpoint explicitly installs both the constraints and the gauge fixing conditions. The degrees left over are called “true degrees of freedom”. The two viewpoints are equivalent in the sense that the relational Dirac observables and the true degrees of freedom subordinate to the same gauge fixing conditions are Poisson isomorphic and the corresponding physical respectively reduced Hamiltonians generate isomorphic equations of motion on the reduced phase space.

3.1 Gauge invariance viewpoint

Let τ^μ be any parameters (“multi-fingered time”), let $G^\mu := \tau^\mu - u^\mu$ be *gauge fixing conditions* for the “clock” variables u and let $F = F(r, s, u, v)$ be any function of the full phase. Define the “relational observable”

$$O_F(\tau) := F + \sum_{n=1}^{\infty} \frac{1}{n!} G^{\mu_1} \dots G^{\mu_n} [X_{\mu_1} \dots X_{\mu_n} \cdot F] \quad (3.3)$$

where $X_\mu \cdot F := \{\hat{C}_\mu, F\}$ is the Hamiltonian vector field of $\hat{C}_\mu$. Then the functions (3.3) share the following properties:

1. They are Dirac observables $X_\mu \cdot O_F(\tau) = 0$ for all μ, τ .
2. Linearity $O_F(\tau) + O_{F'}(\tau) = O_{F+F'}(\tau)$.
3. Compatibility with the pointwise product $O_F(\tau) O_{F'}(\tau) = O_{F \cdot F'}(\tau)$
4. Compatibility with complex conjugation $\overline{O_F(\tau)} = O_{\bar{F}}(\tau)$ if the G, C are real valued.
5. Dirac bracket homomorphism

$$\{O_F(\tau), O_{F'}(\tau)\} = \{O_F(\tau), O_{F'}(\tau)\}^* = O_{\{F, F'\}^*}(\tau) \quad (3.4)$$

where the Dirac bracket is defined by (note that in our convention $\{\hat{C}_\mu, G^\nu\} = -\delta_\mu^\nu$)

$$\{F, F'\}^* = \{F, F'\} - [\{F, \hat{C}_\mu\} \{G^\mu, F'\} - \{F', \hat{C}_\mu\} \{G^\mu, F\}] \quad (3.5)$$

6. Let $t \mapsto \tau(t)$ be a 1-parameter curve, F a function depending only on r, s and $O_F(t) := O_F(\tau(t))$. Then

$$\frac{d}{dt} O_F(t) = \{H(t), O_F(t)\}, \quad H(t) = O_{\dot{\tau}^\mu(t) h_\mu}(\tau(t)) \quad (3.6)$$

i.e. $H(t)$ defines the generator of time evolution defined by the one parameter curve in clock space.

Due to property 3. above, it is not necessary that one is able to compute the series involved in (3.3): Given a function $F = F(r, s, u, v)$ we may rewrite it as $\hat{F}(r, s, u, \hat{C})$ and find setting $R^\alpha(t) := O_{r^\alpha}(t)$, $S_\alpha(t) := O_{s_\alpha}(t)$ that $O_F(t) = \hat{F}(R(t), S(t), \tau(t), \hat{C})$. Thus functions depending non-trivially on u, v are of no interest when we pass to the constraint surface $\hat{C} = 0$ which is preseved by definition of first class constraints. Therefore we are interested only the algebra of Dirac observables which are functions of R, S only. In particular

$$H(t) = \dot{\tau}^\mu(t) h_\mu(R(t), S(t), \tau(t)) \quad (3.7)$$

which is in general explicitly time dependent through the dependence of h_μ on u .

We note that the functions R, S stay conjugate variables

$$\{S_\alpha(t), R^\beta(t)\} = \delta_\alpha^\beta, \quad \{S_\alpha(t), S_\beta(t)\} = \{R^\alpha(t), R^\beta(t)\} = 0 \quad (3.8)$$

3.2 Reduction viewpoint

A Poisson algebraically equivalent description can be given as follows: We identify v as the constrained momenta, u as the pure gauge degrees of freedom and r, s as the true degrees of freedom coordinatising the reduced phase space. Indeed the gauge cut $G = 0$ through the constraint surface $\hat{C} = 0$ is in one to one correspondence with the gauge orbits of points on $\hat{C}$ if i. the gauge $G = 0$ can always be installed and ii. every gauge orbit is intersected precisely once (admissible gauge choice). In order that the gauge conditions $G^\mu = \tau^\mu(t) - u^\mu$ be preserved under gauge transformations we must have $\dot{\tau}^\mu = \{\hat{f}^\nu \hat{C}_\nu, u^\mu\}$ that is $\dot{f}^\mu = \dot{\tau}^\mu =: \hat{f}_*^\mu$. The reduced Hamiltonian is then defined as the effective Hamiltonian on the reduced phase space whose action coincides with that of the original constrained Hamiltonian at the gauge cut. Thus let $F = F(r, s)$ just depend on the true degrees of freedom r, s . Then by definition $H = H(r, s; t)$ is the function obeying

$$\{H(t), F\} = \{C(f), F\}_{\hat{C}=0, G=0, f=f_*} \quad (3.9)$$

or by rewriting the constraints $C(f) = \hat{C}(\hat{f})$ in terms of new Lagrange multipliers (which then depend on phase space but this immaterial as long as the linear map between $\hat{C}$ and C is non-singular as both $f, \hat{f}$ become fixed as definite phase space functions by stability)

$$\{H(t), F\} = \{\hat{C}(\hat{f}), F\}_{\hat{C}=0, G=0, \hat{f}=\hat{f}_*} \quad (3.10)$$

which is solved by

$$H(t) = \dot{\tau}^\mu(t) h_\mu(r, s, \tau(t)) \quad (3.11)$$

and thus coincides with (3.7) under the Poisson bracket isomorphism $(r, s) \mapsto R, S$.

Thus, given the extra structure provided by the gauge fixing conditions, one may arrive at a reduced phase space description equivalently in terms of manifestly gauge invariant Dirac observables or the true degrees of freedom and given a one parameter family of gauge fixings one recovers a physical (i.e. observable) notion of dynamics even for totally constrained systems.

We will apply the true degrees of freedom description to our gauge system combined with perturbation theory with respect to *non-symmetric observables*.

3.3 Choice of gauge

What the above formalism does not tell is, which gauge fixing condition to choose. Although all admissible choices are by definition related by a gauge transformation and thus merely correspond to different but gauge equivalent sections of the constraint surface, thus providing an explicit coordinatisation of the reduced phase

space (space of gauge orbits), the choice has a strong impact on the form of the reduced Hamiltonian as it decides which degrees of freedom to freeze and which are to be evolved. As the variables that are prescribed define a reference frame (through the Lagrange multipliers that are fixed) it is clear that the physical Hamiltonian depends on that reference frame. Thus the selection of gauge requires physical input, e.g. one may require that the physical Hamiltonian acquires the form of the standard model Hamiltonian on Minkowski space in regions of the phase space that correspond to the flat Minkowski metric.

Another issue is the following: In the previous sections we have considered gauge conditions of the form $q^a = \tau^a(t)$, $x^j = \rho^j(t)$ which depend on a time parameter t and thus define a one parameter family of sections that gives rise to an evolution. Such an explicit time dependence of the gauge condition is a viable choice. However, one would like to minimise such freedom when physical principles are one's disposal that help to downsize the number of possibilities. In the context of perturbation theory it is motivated to consider $\rho^j \equiv 0$ as the x, y are "small" but as far as τ^a is concerned, this is not the case. When the index a has univalent range (cosmology) then the choice of the remaining function $\tau^a(t)$ is nothing but a reparametrisation of the time variable and thus essentially unique. However, when a takes more than one value, in particular an infinite number, the issue becomes more serious because an infinite number of arbitrary parameters cannot be fixed by any experiment (predictivity).

Fortunately, precisely in situations when a takes an infinite range there is another effect that in fact allows the time dependence of $\tau^a(t)$ to be trivial. Such gauge conditions are called "coordinate conditions" [22]. Typically this happens when our discrete description descends from a field theory rather than a finite dimensional Hamiltonian system. Note that even in this case and as mentioned at the beginning of section 2, a discrete description is still possible by expanding the fields in terms of a countable set of mode functions L_a (say Hermite functions if the non-compact part of the spatial topology consists of copies of $\mathbb{R}$).

The origin of the effect is that the continuum constraints depend on spatial derivatives and that there is a boundary [22]. In that case, the symplectic structure and the constraints are no longer automatically finite and functionally differentiable. In order to ensure this, one must specify boundary or decay conditions on the canonical variables and the test functions that smear the constraints as one approaches the boundary and the constraints can typically be made functionally differentiable if one adds a boundary term which is finite when the specified decay behaviour holds but whose variation is singular and cancels the singular variation of the constraint. Thus the Hamiltonian in its functionally differentiable form and in terms of the original constraints not solved for $v_\mu = -h_\mu$ is now given by

$$H(f) = C(f) + B(f) \quad (3.12)$$

where $B(f)$ is the boundary term. A gauge transformation is defined by those f for which $B(f) = 0$ and a symmetry transformation by those f for which $B(f) \neq 0$. In both cases f must obey the specified decay behaviour. The reduced phase space is still defined by coordinate conditions $G^\mu = u^\mu - \tau^\mu = 0$, $u^\mu = u_*^\mu := \tau^\mu$ with constant functions on the phase space τ^μ and by the solutions of the constraints $C_\mu = 0$. Since there are differential equations involved, while this system can be rewritten in the form $\hat{C}_\mu = v_\mu + h_\mu(r, s; u; V) = 0$, $v_\mu^* := -h_\mu(r, s; u = u_*; V)$ it depends on integration constants V_A . These can be considered as initial conditions on the boundary when solving the differential equations, thus the constraints on the boundary are identically satisfied for all values of V_A . Therefore the number of independent constraints is reduced by the number of those integration constants and we impose only as many gauge fixing conditions as there are independent constraints. We may without loss of generality pick V_A as the values of v_A on the boundary where A runs through some index set denoting boundary degrees of freedom, it is contained in the bulk index set with labels μ . We may then pick U^A as the values of u^A on the boundary and impose gauge fixing conditions only on u^μ where μ is not a boundary label and the gauge fixing condition is still a constant function τ^μ for those fixed u^μ on the phase space. This will be made more explicit below.

The smearing functions are specified by gauge stability

$$\{H(f), G^\mu\}_{u=u_*, v^*} = \{H(f), u^\mu\}_{u=u_*, v^*} = 0 \quad (3.13)$$

because τ^μ does not explicitly depend on time. However, because of the derivatives involved, which is why (3.13) is not imposed for all μ , namely not for $\mu = A$, this now does not imply $f = 0$ but yields a differential equation with non-trivial solutions $f^\mu = f_*^\mu(r, s; V, \lambda)$ which depends on yet other integrations constants λ^A . This f_*

obeys the decay behaviour specified but it generically corresponds to a symmetry transformation and not a gauge transformation. Now for any function $F = F(r, s; U, V)$ we define the reduced Hamiltonian as before

$$\{H, F\} = \{H(f), F\}_{w=w_*, f=f_*} \quad (3.14)$$

where $w = (u, v)$ but now it is less clear how to write H explicitly. Since the boundary term is linear in f we have (it does not depend on derivatives of f after integrating by parts)

$$B(f) = f^A j_A \quad (3.15)$$

where the index α runs through the boundary subset of the bulk index set to which μ belongs and the current j_A defines the smearing function independent part of the boundary function on the full phase space. That λ^A, U^A, V_A, f^A are all labelled by the same index set is no coincidence but again due to the fact that we can define initial conditions for the differential equations to be solved, equivalent to integration constants, at the boundary.

Let $j^* = j_{w=w_*}$ then

$$\begin{aligned} \{B(f)_{w=w_*}, F\}_{f=f_*} &= f_*^A \{j_A^*, F\} \\ &= \{H(f)_{w=w_*}, F\}_{f=f_*} \\ &= \{H(f), F\}_{w=w_*, f=f_*} + \{H(f), u^\mu\}_{w=w_*, f=f_*} \{v_\mu^*, F\} - \{H(f), v_\mu\}_{w=w_*, f=f_*} \{u_\mu^*, F\} \\ &= \{H, F\} \end{aligned} \quad (3.16)$$

where in the second step we used that $H = B$ on the constraint surface, in the third we expanded the Poisson bracket into explicit dependence of $H_{w_*}(f)$ on r, s and implicit one through w_* and in the last we noted that u_* is a constant on the phase space and (3.13), (3.14).

We see that a closed expression for H can be obtained provided that there exists a function $\chi(j)$ such that $f_*^A = [\partial\chi/\partial j_A]_{j=j_*}$. Then $H = \chi(j_*)$. One may use the freedom in the choice of the integration constants λ on which f^* depends in order to achieve that this condition holds because there will be typically as many integration constants, i.e. initial conditions on the boundary, as there are boundary indices α . The simplest case is that f_* is a constant on the phase space, then simply $H = f_*^A j_A^*$.

The above discussion follows closely [22] but deviates somewhat from the description in the previous section in that we have shifted the focus from the constraints $\hat{C}$ solved for the momenta to the original ones. We will therefore now describe an equivalent procedure which uses the $\hat{C}$ more directly and which offers a complementary point of view of how the integration constants U, V, λ come into play. We go back to the split description $\hat{C}_a, \hat{C}_j$ and for simplicity consider the case that the $\hat{C}_j$ have already been reduced by the gauge $x^j = 0$ which is possible as in the form $\hat{C}_a, \hat{C}_j$ the constraints are mutually commuting. The case of a joint treatment of q^a, x^j is similar.

Since spatial derivatives acting on the mode functions can be expressed as a finite linear combination of mode functions again, a derivative in the continuum description translates into a kind of difference (with respect to the label a) in the discrete description. This means that when computing Poisson brackets, one has to integrate (sum) by parts, leading to boundary contributions and bulk contributions of the bracket provided that there is a boundary as we will assume. To describe this more explicitly, we assume (a situation often encountered in practice) that we can split the label a into pairs (r, i) where partial integration (summing) is with respect to r at fixed i and w.l.g. r has range in $\mathbb{R}_0^+ (\mathbb{Z}_0^+)$. The boundary contribution depends on the values of the fields (q^a, p_a, R) , $R = (Q^A, P_A, X^J, Y_J)$ and the Lagrange multipliers f^a at $r = \infty$ while the bulk contribution depends in particular on derivatives $f^{a'}$ (differences) of the f^a .

Likewise, rewriting the constraints C_a in the form $\hat{C}_a = p_a + h_a(q, R)$ there is an issue: As derivatives (differences) of the momenta p_a are involved, to solve $C_a = 0$ for the p_a means solving a differential (difference) equation. As such equations require initial conditions or integration constants in order for a unique solution to exist, in this case we should rather write $h_a(q, R) = -S_a(c_0; q, R)$ where $c_0 = \{c_{r=0, i}\}$ is a collective notation for the integration constants. If we do not want to give c_0 the status of new degrees of freedom, we can solve the equation $p_{r=0, i} = S_{r=0, i}(c_0, q, R)$ for c_0 and insert the solution into $S_a(c_0, q, R)$ yielding $S_a(p_0, q, R)$ where now by construction $S_{r=0, i}(p_0, q, R) = p_{r=0, i}$. It follows that the constraints $\hat{C}_{0, i} := \hat{C}_{r=0, i} \equiv 0$ are identically

satisfied and thus we should in fact only impose gauge fixing conditions on $q^{r,i}$, $r > 0$. In this way the function h_a acquires the form $-S_a(p_0, q_0, \{q^b\}_{b>0}, R) =: \hat{h}_a(\{q^b\}_{b>0}, \hat{R})$ where we have augmented the true degrees of freedom R to $\hat{R}$ by the canonical pairs $(q^{0,i}, p_{0,i})$ and $b = (r, i) > 0 \Leftrightarrow r > 0$. The $q^{0,i}, p_{0,i}$ play the role of the U^A, V_A above and we have relabelled the indices A by i as here we are dealing with split form of the constraints and consider only the C_a and not all of the C_μ .

We can now rewrite the constraints C_a in terms of the $\hat{C}_a$ but since C_a depends on derivatives (differences) of p while in $\hat{C}_a$ no derivatives (differences) of p appear, this rewriting necessarily involves derivatives (differences) of the $\hat{C}_a$. In the case that C_a depends polynomially on the momenta p and its derivatives (differences) and if only first derivatives (differences) are involved, C_a can be written as a linear combination of $\hat{C}$ and its first derivatives $D\hat{C}$ (differences) with phase space dependent coefficients (simply by expanding $p_a = \hat{C}_a - \hat{h}_a$) say

$$C_a = \sum_{b \geq 0} \gamma_a^b \hat{C}_b + \delta_a^b (D\hat{C})_b \quad (3.17)$$

Since vanishing of constraints means vanishing of their derivatives (differences) the vanishing of $\hat{C}_a$ for all $a \geq 0$ implies the vanishing of C_a for all $a \geq 0$. Conversely the vanishing of C_a for all $a \geq 0$ implies a differential (difference) equation for the $\hat{C}_a$ which implies that $\hat{C}_a \propto \hat{C}_0 \equiv 0$. Thus the the sets of constraints are indeed equivalent. Next, integrating (summing) by parts

$$\sum_{a \geq 0} f^a C_a = \sum_i f^{\infty,i} \hat{C}_{\infty,i} - f^{0,i} \hat{C}_{0,i} + \sum_{a \geq 0} \hat{f}^a \hat{C}_a, \quad \hat{f}^a = \sum_{b \geq 0} \gamma_b^a f^b - D[\delta_b^a f^b] \quad (3.18)$$

where we have denoted a second boundary by the label ∞ . Imposing stability of $G^a = q^a - \tau^a = 0$, $a > 0$ under gauge transformations imposes $\hat{f}^a = 0$, $a > 0$ which is a *homogeneous, linear* differential (difference) equation for f^a which can be solved in the form $f^{r,i} = \lambda^j \tilde{f}_j^{r,i}$, $r \geq 0$ where λ^i are free parameters while the invertible propagator $\tilde{f}$ is uniquely determined by that differential equation and say the initial condition $\tilde{f}_i^{0,j} = \delta_i^j$. We can now compute the reduced Hamiltonian H that follows from these gauge fixing conditions acting on functions $F = F(\hat{R})$

$$\begin{aligned} \{H, F\} &:= \left\{ \sum_{a \geq 0} f^a C_a, F \right\}_{C=G=f-\lambda \cdot \tilde{f}=0} = \sum_i \{f^{\infty,i} \hat{C}_{\infty,i} - f^{0,i} \hat{C}_{0,i}, F\}_{C=G=f-\lambda \cdot \tilde{f}=0} \\ &= \sum_i [f^{\infty,i} \{\hat{C}_{\infty,i}, F\} - f^{0,i} \{\hat{C}_{0,i}, F\}]_{C=G=f-\lambda \cdot \tilde{f}=0} = \sum_{i,j} \lambda^j (\tilde{f}_j^{\infty,i})_{G=C=0} \{p_{\infty,i} + \hat{h}_{\infty,i}, F\}_{C=G=0} \\ &= \sum_{i,j} \lambda^j (\tilde{f}_j^{\infty,i})_{G=C=0} \{\hat{h}_{\infty,i}, F\}_{G=0} = \sum_{i,j} \lambda^j (\tilde{f}_j^{\infty,i})_{G=C=0} \{(\hat{h}_{\infty,i})_{G=0}, F\} \end{aligned} \quad (3.19)$$

where in the first step we used that the Poisson bracket must act on $\hat{C}$ in order not to vanish and that $\hat{f} = 0$ when $f = \lambda \cdot \tilde{f}$ so that only the boundary term in (3.18) survives, in the second step again that the Poisson bracket must involve $\hat{C}$, in the third that $\hat{C}_{0,i}$ vanishes identically, in the fourth that F does not depend on q^a , $a > 0$ and in particular not on $q^{\infty,i}$ and in the fifth that as F does not depend on p_a , $a > 0$ we can impose $G^a = 0$, $a > 0$ before computing the Poisson bracket.

Since (3.19) is supposed to be of the form $\{H, F\}$ and since $\tilde{f}_{G=C=0}^\infty$ is a non-trivial matrix valued function on phase space we are forced to choose λ to be of the form

$$\lambda^i := \left(\frac{d\chi(z)}{dz_i} \right)_{z=E} ([\tilde{f}_{G=C=0}^\infty]^{-1})_j^i; \quad E_i(\hat{R}) := \hat{h}_{\infty,i}(\{q^b = \tau^b\}_{b>0}, \hat{R}), \quad (3.20)$$

where χ is an arbitrary function which plays the same role as in the above version using the boundary term formulation while $E_i(\hat{R})$ is the analog of j_A^* . Note that λ correctly does not depend on q^a , $a > 0$. Then

$$H(\hat{R}) = \chi(E(\hat{R})) \quad (3.21)$$

is the physical Hamiltonian.

Thus the time independent gauge fixing which is possible when the constraints depend on derivatives (differences) of the momenta is similar to the case of the time dependent gauge fixing when the constraints just depend algebraically on the momenta: The fact that derivatives are involved releases a several parameter freedom in the gauge fixed Lagrange multipliers f^a parametrised by λ while in the case of just algebraic dependence at least one such parameter (called t) must be supplied in the gauge fixing condition itself. The final physical Hamiltonian in both cases can be written in terms of the solution $p_a = -\hat{h}_a$, $y_j = -\hat{h}_j$ of $C_a = C_j = 0$ restricted to $x^j = 0$, $q^a = \tau^a$. The difference is that in the time independent case $q^a = \tau^a$ only for $a > 0$ corresponding to the fact that there is “one constraint less” per index i , i.e. that $p_{0,i}$ cannot be solved for due to the presence of the derivatives (differences). Another difference is that while in the case of time dependent gauge fixings the function χ in (3.21) is linear in the h_a and involves all a , while in the time independent case it involves only $a = \infty$ and is not necessarily linear. The possible forms of χ will be determined by the condition that (3.20) yields an allowed smearing function, i.e. with the specified decay behaviour such that H is in fact well defined, i.e. both finite in value as functionally differentiable.

Remarks:

1.

The discussion unveils the origin of the additional observables p_0, q^0 (e.g. mass, charge, angular momentum plus conjugate configuration variables in case of black holes) which are not present in the case without derivatives of momenta (e.g. in cosmology).

2.

The presence of momentum derivatives offers the possibility to consider time independent gauge fixings thus freeing the physical Hamiltonian from any explicit time dependence, i.e. the reduced system is conservative.

3.

We note that in case that the constraints are not solvable algebraically for the momenta but rather involve a differential (difference) equation we can compute the solution $S_a(\{q^b\}_{b>0}, \hat{R})$ by the Picard-Lindelöf method [23] i.e. by transforming the differential (difference) equation into an integral (sum) equation

$$p_{r,i} = p_{0,i} + I_{r,i}(p, q, R), \quad I_{0,i}(p, q, R) = 0 \quad (3.22)$$

and iterating the right hand side. The perturbative scheme explained in the next section relies on the computation of a solution of (3.22) at zeroth order with respect to X, Y i.e. by solving it for $X = Y = 0$. This does not introduce any non-polynomial dependence of the solution $p_a(0)$ so obtained on X, Y but in general it will involve $\{q^a\}_{a>0}, p_0, Q^A, P_A$ non-polynomially which is also true in the case without momentum derivatives (differentials) (except that no dependence on p_0 is present). As the perturbative scheme of the next section only relies on the polynomial dependence of C_a, C_j with respect to x, y, X, Y , it also applies in presence of momentum differentials. See below for cases where non-polynomial dependence at least of Q, P can be avoided.

4.

As the physical Hamiltonian involves taking $r \rightarrow \infty$ in (3.22) it typically involves an integral (sum) over all r which therefore provides additional “smearing” of products of operator valued distributions upon quantisation of the fields Q, P, X, Y involved and thus improves the chance that the physical Hamiltonian itself be promotable to an operator. For the same reason, in the time dependent case one will choose $\tau^a(t) \neq 0$ for all a in order to have an integral (sum over a) involved.

5.

The perturbative algorithm of the next section directly computes h_a, h_j and thus $E_i = \sum_{n=0} E_{i,(n)}$ in (3.20) perturbatively and if χ in (3.21) is linear in E_i , this also directly computes H perturbatively. If χ is non-linear, an additional perturbative Taylor expansion of χ is required, schematically

$$H = \chi(E_{(0)}) + \sum_{k=0} \frac{1}{k!} \chi^{(k)}(E_{(0)}) \left[\sum_{l=1} E_{(l)} \right]^k = \chi(E_{(0)} + \chi^{(1)} E_{(1)} + \left[\frac{1}{2} \chi^{(2)} E_{(1)}^2 + \chi^{(1)} E_{(2)} \right] + \dots \quad (3.23)$$

which again constructs H perturbatively.

6.

If the perturbative algorithm of the next section involves solving differential (difference) equations then this can be

done using the Picard-Lindelöf method by reformulating the problem as an integral equation as sketched above. This involves in addition an expansion of the integrand around the integration constant p_0 thereby constructing $\hat{h}_\infty$ as an iterated integral over polynomial expressions now not only in X, Y but also in Q, P with possibly non-polynomial dependence on p_0, q^0 . This makes a quantisation of H conceivable even if Q, P, X, Y are fields rather than finitely many degrees of freedom. Moreover, since then the interaction terms of the symmetric background observables Q, P with the non-symmetric perturbation observables X, Y is such that Q, P appear only in integrated form e.g. in a mass term for X, Y there is a chance that the corresponding backreaction can be treated with the methods of space adiabatic perturbation theory even if Q, P are fields [29, 28] with Q, P playing the role of the “slow” variables and X, Y that of the “fast”. The intuition behind this adiabatic split of the observables is that the Q, P are by construction the *average* over the action of the symmetry group on all observables Q, P, X, Y which make them similar to the centre of mass mode (mass weighted *average*) in classical mechanics with the much larger total mass as compared to the individual ones. The challenge is that in the field theory case the Weyl quantisation scheme for Q, P on which SAPT relies has to be extended to infinitely many degrees of freedom (this is in contrast to cosmology where the phase space of the Q, P is finite dimensional). A possible regularisation consists in working with a mode cut-off on the Q, P degrees of freedom and thus to make the phase space of the Q, P finite dimensional. Then at the end one removes that cut-off using methods of renormalisation.

7.

In both the time dependent and time independent cases we have considered gauge fixing conditions of the form $G^a = q^a - \tau^a$, $G^j = x^j - \rho^j$ where τ, ρ are constant on the phase space. More general gauge fixing conditions of the form $G = \tilde{G} - \tau$ are possible where τ is again constant on phase space but $\tilde{G}$ is a non-constant function such that the matrix $\Delta := \{C, G\}$ is invertible. Then most of the statements of section (3.1) remain valid if one replaces $\hat{C}$ by $\Delta^{-1} \cdot C$ just that exact relations become weak (i.e. they hold modulo $C = 0$). However, in this case it is difficult to make concrete statements about the form of the reduced Hamiltonian. Moreover, if $\tilde{G}$ also involves the momenta p, y , then the perturbative scheme of the next section would break down because we could not disentangle the solution of the constraints in terms of p, y at fixed q, x from imposition of the gauge conditions. It is therefore important to stick to such “simple” gauge conditions that involve only the configuration degrees of freedom.

4 Perturbation theory in terms of Dirac observables

In principle, given the theory provided in the previous section, the strategy is clear: We declare Q, P, X, Y as the true degrees of freedom and $q, x; p, y$ as the pure gauge and constrained degrees of freedom respectively, compute the reduced Hamiltonian $H(t) = H(Q, P, X, Y; t)$ using gauge fixing conditions $G^a = \tau^a - q^a$, $G^j = \rho^j - x^j$ and, e.g. for explicitly timed dependent gauge fixings, a one parameter curve $t \mapsto (\tau(t), \rho(t))$ therein and finally apply standard Hamiltonian perturbation theory to $H(t)$ with respect to the non-symmetric observables X, Y . This way the difficult question of how to perform perturbation theory on the unreduced phase space while keeping the first class property of the perturbed constraints is avoided altogether. The question that is left open is whether this is feasible. In this section we develop the reduction viewpoint which is technically more convenient.

We thus start again with the gauge system defined by (2.8), (2.10), (2.11). By (2.10), the leading order contribution to C_j is $C_{j(1)}$ which linear in the perturbations x, y, X, Y while the leading order contribution to C_a is $C_{a(0)}$ which is independent of the perturbations. We assume that we can solve C_j exactly for y_j in the form (modulo global issues in phase space, see the previous section)

$$C_j(p, q, x, y, P, Q, X, Y) = 0 \Leftrightarrow \tilde{C}_j = y_j + \tilde{h}_j(p, q, x; P, Q, X, Y) = 0 \quad (4.1)$$

We insert the solution $y_j = -\tilde{h}_j$ into C_a and assume that we can solve it exactly for p_a in the form

$$(C_a)_{y=-\tilde{h}} = 0 \Leftrightarrow \hat{C}_a = p_a + h_a(q, x; P, Q, X, Y) \quad (4.2)$$

Then we insert $p_a = -\hat{h}_a$ into $\tilde{C}_j$ and find

$$\hat{C}_j = y_j + h_j(q, x; P, Q, X, Y), \quad h_j = (\tilde{h}_j)_{p=-h} \quad (4.3)$$

By the theory provided in the previous section, the physical Hamiltonian is given by

$$H(t; P, Q, X, Y) = \dot{\tau}^a(t) h_a(\tau(t), \rho(t); P, Q, X, Y) + \dot{\rho}^j(t) h_j(\tau(t), \rho(t); P, Q, X, Y) \quad (4.4)$$

which can be Taylor expanded with respect to the observables X, Y to any desired order provided we can construct $H(t; P, Q, X, Y)$ sufficiently explicitly.

Whether this is the case depends critically on the form of the constraints. If C_a, C_j depend non-polynomially on the momenta p, y this will be impossible. Fortunately in physical applications this is not the case if the pair (C_a, C_j) results from the symmetric – non-symmetric split of constraints C_μ which depend polynomially on all momenta i_A . This will be the case if the underlying Lagrangian depends on finitely many time derivatives by the Ostrogradski method [21]. Since the symmetry split does not affect polynomiality, for these theories C_a, C_j depend polynomially on all momenta and in particular on p, y .

While not necessary for what follows, we note that the constraints that we encounter in GR are not polynomial in the configuration coordinates. However, they can in fact also be made polynomial with respect to all variables if we multiply them by phase space dependent factors that are classically non vanishing (certain powers of the determinant of the intrinsic metric). While this would make a significant difference in the Dirac approach to constrained systems in which one quantises the constraints on the unreduced phase space, this has *no influence* on the reduced Hamiltonian in the reduced phase space approach. The reason for this is that given constraints C_μ , a non-singular matrix $M_\mu{}^\nu$ and gauge fixing conditions G^μ such that $\Delta_\mu{}^\nu = \{C_\mu, G^\nu\}$ is non-singular, the smearing functions $f^\mu, \tilde{f}^\mu$ of $C_\mu, \tilde{C}_\mu := M_\mu{}^\nu C_\nu$ are determined as $\hat{f}, \hat{\tilde{f}}$ by fixing the gauge and respectively satisfy $\hat{f}^\nu \Delta_\nu{}^\mu = \dot{\tau}^\mu = \hat{\tilde{f}}^\nu \tilde{\Delta}_\nu{}^\mu$ where $\tilde{\Delta} = \Delta \cdot M$. Then the reduced Hamiltonian is computed from $\{H, F\} := \{f^\mu C_\mu, F\}_{C=G=f-\tilde{f}=0}$ and this coincides with $\{\tilde{H}, F\} := \{\tilde{f}^\mu \tilde{C}_\mu, F\}_{\tilde{C}=G=\tilde{f}-\hat{\tilde{f}}=0}$ thanks to invertibility of M . This has the following significance in perturbation theory: In the polynomial form, the perturbative expansion of the constraints is obviously a finite series while in the non-polynomial form that series is infinite with little control on the radius of convergence. Accordingly in the polynomial form the task to compute the perturbative expansion is itself *possible to all orders*, it is exactly available and as such is a *non-perturbative* expression. One just chooses to write the constraints in variables that are adapted to the symmetry under discussion, *without dropping terms*. For instance, in vacuum GR it is possible to write the constraints as polynomials of order ten. In this form one can carry out mode expansions and mode integrals discussed in section 2 in closed form, it just requires elementary methods from harmonic analysis on the symmetry group. Thus the shift of focus from the constraints to the reduced phase space leads to a *significant simplification and improvement* in the computational effort and the error control. Nevertheless, the perturbative expansion of the physical Hamiltonian involves an infinite series unless all momenta appear only linearly. This is because for higher polynomial degree one needs to take (square) roots and their perturbative expansion yields an infinite series. The algorithm of theorem 4 displayed below computes that series directly perturbatively. Note that only in fortunate cases the non-perturbative expression of the polynomial form of the constraint may in fact allow to take those (square) roots exactly so that a non-perturbative expression for the reduced Hamiltonian is available, on the other hand, the presence of square roots may complicate its quantisation.

Coming back to the task of solving the constraints for the momenta whether or not the constraints are polynomial also in the configuration variables, still the task of solving the system of polynomial equations (in the momenta) $C_a = C_j = 0$ for $p_a = -h_a, y_j = -h_j$ appears to be hopeless: Solving systems of polynomials defining algebraic varieties is the main task in the field of algebraic geometry [24] and already for a finite number of non-linear polynomials an extremely difficult task (unless the equations can be decoupled into polynomials in just one variable of degree at most four) and an active field of research in pure mathematics. Since in our field theoretic setting we are dealing with an *infinite* number of polynomials, we are even leaving the terrain of known mathematics when trying to solve the infinite, coupled system *exactly*. Even if we could do so, since typically an infinite number of non-linear equations are involved, there are an infinite number of sign choices to be made when selecting the various roots. What saves the day is that here we are interested in a *perturbative setting* and we will show that in this case one can find a unique solution perturbatively. That solution also delivers the perturbation theory for the physical Hamiltonian in *one stroke*.

Systems of polynomial equations are equivalent to larger systems of polynomial equations whose degree is at most two. For instance the cubic system $x^3 + 2x^2 + 3y = 0, xy^2 + 4xy + 5x = 0$ in two variables and two

equations is equivalent to the quadratic system $u = xy, v = x^2, xv + 2v + 3y = 0, yu + 4u + 5x = 0$ in four variables and four equations. Thus we may assume that C_a, C_j depend at most quadratically on the momenta p, y, P, Y . In GR this is even the case without enlarging the system. Accordingly we isolate the dependence of C_a, C_j on p, y using the following notation:

$$\begin{aligned} C_a &= U_a + K_a^b p_b + L_a^j y_j + A_a^{bc} p_b p_c + B_a^{jk} y_j y_k + C_a^{bj} p_b y_j \\ C_j &= V_j + M_j^a p_a + N_j^k y_k + D_j^{ab} p_a p_b + E_j^{kl} y_k y_l + F_j^{ak} p_a y_k \end{aligned} \quad (4.5)$$

where

$$\begin{aligned} U_a &= u_a + u_a^A P_A + u_a^J Y_J + u_a^{AB} P_A P_B + u_a^{JK} Y_J Y_K + u_a^{AJ} P_A Y_J \\ V_j &= v_j + v_j^A P_A + v_j^J Y_J + v_j^{AB} P_A P_B + v_j^{JK} Y_J Y_K + v_j^{AJ} P_A Y_J \\ K_a^b &= k_a^b + k_a^{bA} P_A + k_a^{bJ} Y_J \\ L_a^j &= l_a^j + l_a^{jA} P_A + l_a^{jJ} Y_J \\ M_j^a &= m_j^a + m_j^{aA} P_A + m_j^{aJ} Y_J \\ N_j^k &= n_j^k + n_j^{kA} P_A + n_j^{kJ} Y_J \end{aligned} \quad (4.6)$$

The notation is as follows: The coefficients U, V and K, L, M, N and A, B, C, D, E, F respectively displayed in (4.5) are second order and first order and zeroth order polynomials in P_A, Y_J respectively as displayed in (4.6) where the various coefficients u, v, k, l, m, n (which are functions of q, x, Q, X only) are known in terms of their Taylor expansion in terms of x, X using standard perturbation theory on the unreduced phase space. Without loss of generality A_a^{bc}, D_j^{ab} and B_a^{kl}, E_j^{kl} respectively are symmetric in b, c and k, l respectively.

As before, we will denote by $(\cdot)_{(n)}$ the n -th order monomial in the Taylor expansion of $(\cdot)$ wrt x, y, X, Y with coefficient functions that depend only on q, Q . Thus e.g.

$$U_{a(n)} = u_{a(n)} + u_{a(n)}^A P_A + u_{a(n-1)}^J Y_J + u_{a(n)}^{AB} P_A P_B + u_{a(n-2)}^{JK} Y_J Y_K + u_{a(n-1)}^{AJ} P_A Y_J \quad (4.7)$$

The motivated identities $C_{a(1)} = C_{j(0)} = 0$ (2.10) now translate into

$$\begin{aligned} C_{a(1)} &= U_{a(1)} + K_{a(1)}^b p_b + L_{a(0)}^j y_j + A_{a(1)}^{bc} p_b p_c + C_{a(0)}^{bj} p_b y_j = 0 \\ C_{j(0)} &= V_{j(0)} + M_{j(0)}^a p_a + D_{j(0)}^{ab} p_a p_b = 0 \end{aligned} \quad (4.8)$$

for all p, y . Taking zeroth, first and second derivatives at $p = y = 0$ yields

$$U_{a(1)} = K_{a(1)}^b = L_{a(0)}^j = A_{a(1)}^{bc} = C_{a(0)}^{bj} = 0, \quad V_{j(0)} = M_{j(0)}^a = D_{j(0)}^{ab} = 0 \quad (4.9)$$

To solve $C_a = C_j$ perturbatively for $p_a = -h_a, y_j = -h_j$ we expand

$$p_a = \sum_{n=0}^{\infty} p_a(n), \quad y_j = \sum_{n=1}^{\infty} y_j(n) \quad (4.10)$$

where $p_a(n) := -h_{a(n)}, y_j(n) := -h_{j(n)}$ are n -th order monomials wrt x, X, Y with coefficients depending on q, Q, P which are to be determined. Note that $p_a(0) \neq 0 = y_j(0)$ consistent with the perturbative scheme that requires p_a, y_j respectively to be a zeroth and first order quantity respectively.

Theorem.

Suppose that a solution $p_a(0)$ of $C_{a(0)} = 0$ can be found and that the x, X, Y independent matrices

$$R_a^b(q, Q, P) := K_{a(0)}^b + 2 A_{a(0)}^{cb} p_c(0), \quad S_j^k(q, Q, P) := N_{j(0)}^k + F_{j(0)}^{ck} p_c(0) \quad (4.11)$$

are non-degenerate. Then $C_a = 0 = C_j$ has a unique (up to the choice of root $p_a(0)$) perturbative solution. In particular $p_a(1) = 0$.

Remarks:

i.

Since $C_a(0) = 0$ is one of the *exact* field equations of the *purely symmetric* system, the assumption that a solution $p_a(0)$ exists is physically well justified because imposing the symmetry was *motivated* by the desire to find exact solutions.

ii.

The assumed regularity of R, S is a selection criterion for the split of the full canonical pair (k, i) into $(q, p), (x, y), (Q, P), (X, Y)$. Note that the regularity of R, S is a condition that one also imposes in usual first and second order perturbation theory and since R, S do not receive corrections at higher order, their inversion which enters into the iteration as displayed below does not get more involved at higher orders.

iii.

The solution constructed below is formal in the sense that nothing is known about the radius of convergence of the corresponding power series in x, X, Y (pointwise in q, x, Q, P, X, Y). Such a convergence analysis is beyond the scope of the present manuscript and is reserved for future analysis.

iv.

The proof displays the advantage of working with constraints polynomial in all variables when available as the range of the sums in (4.13) gets automatically truncated in terms of the polynomial degree of the coefficient functions.

Proof. :

The proof is by induction over $N = 0, 1, 2, \dots$ in solving $C_a^{(N)} = C_j^{(N)} = 0$. We do this by inserting the expansions (4.10) into the decomposition (4.5) and isolating homogenous perturbation orders. We start with the $N = 0, 1$ cases and use (4.9)

$$\begin{aligned}
C_{a(0)} &= U_{a(0)} + K_{a(0)}^b p_b(0) + A_{a(0)}^{bc} p_b(0) p_c(0) = 0 \\
C_{a(1)} &= U_{a(1)} + K_{a(1)}^b p_b(0) + K_{a(0)}^b p_b(1) + L_{a(0)}^j y_j(1) + A_{a(1)}^{bc} p_b(0) p_c(0) + 2A_{a(0)}^{bc} p_b(0) p_c(1) \\
&\quad + C_{a(0)}^{bj} p_b(0) y_j(1) \\
&= [K_{a(0)}^b + 2A_{a(0)}^{cb} p_c(0)] p_b(1) = R_a^b p_b(1) \equiv 0 \\
C_{j(0)} &= V_{j(0)} + M_{j(0)}^a p_a(0) + D_{j(0)}^{ab} p_a(0) p_b(0) \equiv 0 \\
C_{j(1)} &= V_{j(1)} + M_{j(1)}^a p_a(0) + M_{j(0)}^a p_a(1) + N_{j(0)}^k y_k(1) + D_{j(1)}^{ab} p_a(0) p_b(0) + 2D_{j(0)}^{ab} p_a(0) p_b(1) \\
&\quad + F_{j(0)}^{ak} p_a(0) y_k(1) \\
&= [V_{j(1)} + M_{j(1)}^a p_a(0) + D_{j(1)}^{ab} p_a(0) p_b(0)] + [N_{j(0)}^k + F_{j(0)}^{ak} p_a(0)] y_k(1) \\
&= [V_{j(1)} + M_{j(1)}^a p_a(0) + D_{j(1)}^{ab} p_a(0) p_b(0)] + S_j^k y_k(1) = 0
\end{aligned} \tag{4.12}$$

The first equation is supposed to be solved by $p_a(0)$ which thus is a known function depending only on q, Q, P . Thus also the matrices R, S in (4.11) only depend on q, Q, P . The second equation is equivalent to $p_a(1) = 0$ by virtue of the assumed regularity of R . The third equation is already identically satisfied due to (4.9) and the fourth equation uniquely determines $y_j(1)$ as a homogeneous linear function of x, X, Y by virtue of the assumed regularity of S .

Thus $p_a(0), p_a(1) = 0, y_j(0) = 0, y_j(1)$ are all determined by the the equations $C_{a(0)} = C_{a(1)} = C_{j(0)} = C_{j(1)} = 0$. The idea is that when including the next terms $C_{a(2)}, C_{j(2)}$ to obtain $C_a^{(2)}, C_j^{(2)}$, then solving $C_a^{(2)} = C_j^{(2)} = 0$ we can account for that by adding corrections $p_a(2), y_j(2)$ to $p_a(0), y_j(1)$. This can be repeated. We thus assume inductively that for some $N \geq 2$ all $p_a(n), y_j(n)$ for $n = 0, \dots, N-1$ have been found iteratively by solving $C_{a(n)} = C_{j(n)} = 0$ for $n = 0, \dots, N-1$. We now isolate $C_{a(N)}$ and $C_{j(N)}$ exploiting $p_a(0) = y_j(1) = 0$ and the relations (4.9). We display the excluded values of the integers $n, r, s \geq 0$ where we

sum over the occurring values n, r or n, r, s respectively subject to $n + r = N$ or $n + r + s = N$ respectively

$$\begin{aligned}
C_{a(N)} &= U_{a(N)} + \sum_{n \neq 1, r \neq 1, n+r=N} K_{a(n)}^b p_b(r) + \sum_{n \neq 0, r \neq 0, n+r=N} L_{a(n)}^j y_j(r) \\
&+ \sum_{n \neq 1, r, s \neq 1, n+r+s=N} A_{a(n)}^{bc} p_b(r) p_c(s) + \sum_{r, s \neq 0, n+r+s=N} B_{a(n)}^{jk} y_j(r) y_k(s) \\
&+ \sum_{n \neq 0, r \neq 1, s \neq 0, n+r+s=N} C_{a(n)}^{bj} p_b(r) y_j(s) \\
C_{j(N)} &= V_{j(N)} + \sum_{n \neq 0, r \neq 1, n+r=N} M_{j(n)}^a p_a(r) + \sum_{r \neq 0, n+r=N} N_{j(n)}^k y_k(r) \\
&+ \sum_{n \neq 0, r, s \neq 1, n+r+s=N} D_{j(n)}^{ab} p_a(r) p_b(s) + \sum_{r, s \neq 0, n+r+s=N} E_{j(n)}^{kl} y_k(r) y_l(s) \\
&+ \sum_{r \neq 1, s \neq 0, n+r+s=N} F_{j(n)}^{ak} p_a(r) y_k(s)
\end{aligned} \tag{4.13}$$

Due to $n + r = N$ or $n + r + s = N$ and $n \geq 0$ the top order of r or s in (4.13) can be at most N and only if $n = 0$ is an allowed value. If both r, s cannot take the value 0 then also neither of r, s can take the value N and if one of r, s cannot take the value 0 the other cannot take the value N . Thus, in $C_{a(N)}$ the only terms that allow for $r = N$ or $s = N$ are the second and fourth while in $C_{j(N)}$ the only terms that allow for $r = N$ or $s = N$ are the third and sixth. Isolating those and denoting the remainder as $C'_{a(N)}, C'_{j(N)}$ respectively which involves only the already known values of $p_a(n), y_j(n), n \leq N - 1$ we find

$$\begin{aligned}
0 &= C'_{a(N)} + [K_{a(0)}^b + 2A_{a(0)}^{cb} p_c(0)] p_b(N) = C'_{a(N)} + R_a^b p_b(N) \\
0 &= C'_{j(N)} + [N_{j(0)}^k + F_{j(0)}^{ck} p_c(0)] y_k(N) = C'_{j(N)} + S_j^k y_k(N)
\end{aligned} \tag{4.14}$$

which can be solved uniquely for $p_a(N), y_j(N)$ due to the regularity of both R, S . $\square$

Note:

i.

It seems that we have introduced more degrees of freedom $p_a(n), y_j(n); n = 0, 1, 2, \dots$ than we had originally (i.e. just p_a, y_j) and that we solved more equations $C_{a(n)} = 0, C_{b(n)} = 0$ than we had originally (i.e. only $C_a = 0, C_j = 0$). However this is not the case: The $p_a(n), y_j(n)$ are just auxiliary constructs, of interest is only their sum. When summed up in (4.10) up to order N yielding $-h_a^{(N)}, -h_j^{(N)}$ respectively, by virtue of the above construction, they give zero up to a term of order $N + 1$ when inserted into C_a, C_j . This works because for each N the equations $C_{a(N)} = 0 = C_{j(N)}$ involve only the variables $p_a(n), y_j(n); n \leq N$ and thus are not affected by adding higher order corrections to $h_a^{(n)}, h_j^{(n)}$. Thus we immediately get the $N - th$ order approximation of the reduced Hamiltonian

$$H^{(N)} := \dot{\tau}^a [h_a^{(N)}]_{q=\tau, x=\rho} + \dot{\rho}^j [h_j^{(N)}]_{q=\tau, x=\rho} \tag{4.15}$$

ii.

As detailed by the proof, the contributions $p_a(n), y_j(n)$ involve $n - th$ powers of the inverses of R, S which are functions of q, x, Q, P . Since in the final Hamiltonian we are only interested in the evaluation at the prescribed values $q = \tau(t), x = \rho(t)$ installing the gauge fixing conditions, we thus find that the physical Hamiltonian depends on inverse powers of R, S and thus inverse powers of functions of the observables Q, P while it depends only on positive powers of the observables X, Y . Negative powers in the physical Hamiltonian of just one of Q, P are not problematic in quantum theory as they just correspond to singular potentials and the corresponding operator can still be densely defined on a suitable domain. However, negative powers of both P, Q could be potentially problematic unless the functions of both P, Q of which inverse powers occur have suitable properties. For example these functions could be bounded from below by a positive constant. This is indeed the case in some examples of interest, including cosmology. Obviously, nothing can be said in general about this issue, it requires a case by case analysis. A possibility consists in performing an additional power expansion in at least one of Q, P around the integration constants p_0 of the previous section when they are present.

iii.

The gauge condition $\rho^j = 0$ is particularly simple and adopted by many practitioners, it is also used in the partial reduction approach described in the next section. In this case, the lowest order for which the backreaction Hamiltonian (4.14) depends non-trivially on the gauge invariant perturbations X, Y is $N = 2$. To compute it, we need $p_a(0) = -h_{a(0)}, p_a(1) \equiv 0, p_a(2) = -h_{a(2)}, y_j(0) \equiv 0, y_j(1)$ while $y_j(2)$ is not needed to compute $H^{(2)} = \dot{\tau}^a [h_{a(0)} + h_{a(2)}]$. These can be computed iteratively using theorem 4. Using it, one finds the explicit formula for $y_j(1)$ is displayed in (6.11) assuming that $p_a(0)$ has been found. Thus, having $p_a(0), y_j(1)$ at our disposal we find from (4.13), (4.14)

$$h_{a(2)} = (R^{-1})_a^b [U_{a(2)} + K_{a(2)}^b p_b(0) + L_{a(1)}^j y_j(1) + A_{a(2)}^{bc} p_b(0) p_c(0) + B_{a(0)}^{jk} y_j(1) y_k(1) + C_{a(1)}^{bj} p_b(0) y_j(1)] \quad (4.16)$$

5 Reduction in stages

In the first subsection we outline the theory for partial classical and partial quantum reduction for general gauge systems combined with perturbation theory. Analogous to section 3 we develop both the gauge invariance and the reduction viewpoint. The gauge invariance viewpoint will be used in the next subsection in order to compare with [5] which uses the gauge invariance viewpoint applied to second order cosmological perturbation theory with backreaction. We will show that the results of [5] are precisely embedded into the approach developed here, opening the avenue for generalisation to higher order. Hence, the reduction viewpoint will be used in section 6 in order to display the details of *third order* perturbation theory in this partially reduced context for a general gauge system (not only cosmology).

We show that there is generically an obstacle whenever there are more than one unreduced remaining constraints when the latter are to be quantised which is one of the motivations to perform full reduction as compared to partial reduction. If on the other hand there is only one remaining constraint, then our perturbation theory applied in the partial reduction context, does not suffer from that quantisation obstacle, to arbitrary order. This is precisely the situation in cosmological perturbation theory.

It should be stressed that what is called a gauge invariant observable in the context of this section should better be called *partially* gauge invariant observable: They are just invariant with respect to the subset of constraints with respect to which the partial reduction is carried out. This is in contrast to the previous section where observable means a fully gauge invariant object. This abuse of notation common in cosmology arises for historical reasons: If one neglects backreaction then the unreduced constraint (there is only one in this case) becomes a physical Hamiltonian and no longer has the status of a constraint, in that sense the partially reduced variables are full observables.

5.1 Partial reduction and perturbation theory

It maybe desirable to carry out the reduction only partially with respect to a non-trivial subset of the constraints. For example for practical reasons one may wish to carry out a classical reduction with respect to the chosen subset of constraints and a quantum reduction with respect to the remaining subset of constraints. In order that this works, the chosen subset must form a closed subalgebra in the constraint algebra. In what follows we display the theory for the case that the classical reduction be performed with respect to the “non-symmetric constraints” C_j . This will enable us to compare a similar procedure developed in [5] for second order cosmological perturbation theory.

We first note that the subalgebra condition is not automatically satisfied if the structure functions κ_{jk}^a displayed in (2.11) are non-trivial. Thus, the first step must be to pass to an equivalent set of constraints $\tilde{C}_a, \tilde{C}_j$ for which the corresponding $\tilde{\kappa}_{jk}^a$ all vanish. Given the theory layed out in section 3, a good candidate for this are the constraints $\tilde{C}_a = \hat{C}_a = p_a + h_a, \tilde{C}_j = \hat{C}_j = y_j + h_j$ which are even Abelian with respect to all of $\hat{C}_a, \hat{C}_j$. Since we want to keep the C_a intact as much as possible for the purposes of quantisation, we may work instead with the equivalent constraint set $C_a, \tilde{C}_j := \hat{C}_j$ where $\hat{C}_j = y_j + h_j(q, x, Q, P, X, Y)$ is obtained by solving C_a for $p_a = -\tilde{h}_a(q, x, y, Q, P, X, Y)$ and then solving $C_j(q, p = -\tilde{h}(q, x, y, Q, P, X, Y), x, y, Q, P, X, Y) = 0$ for

$y_j = -h_j(q, x, Q, P, X, Y)$. However, as $\tilde{C}_j = \lambda_j^a C_a + \nu_j^k C_k$ and $C_j = (\nu^{-1})_j^k [\tilde{C}_k - \lambda_k^a C_a]$ for certain functions λ and invertible ν and given (2.11) we now find

$$\begin{aligned} \{C_a, C_b\} &= (\kappa')_{ab}{}^c C_c + (\kappa')_{ab}{}^j \tilde{C}_j \\ \{C_a, \tilde{C}_j\} &= (\kappa')_{aj}{}^b C_b + (\kappa')_{aj}{}^k \tilde{C}_k \\ \{\tilde{C}_j, \tilde{C}_k\} &= 0 \end{aligned} \quad (5.1)$$

for certain new structure functions κ' which can be explicitly computed from κ, λ, ν .

5.1.1 Gauge invariance viewpoint

As we wish to get rid of the constraints $\tilde{C}_j$ classically we want to still modify the constraint C_a into $\tilde{C}_a$ in order to achieve for the resulting yet further modified structure functions that $\tilde{\kappa}_{ab}{}^j = \tilde{\kappa}_{aj}{}^b = \tilde{\kappa}_{aj}{}^k = 0$. Given the theory layed out in section (3) this may be achieved as follows: Since the $\tilde{C}_j$ form a closed, Abelian subalgebra we may apply (3.3) with the partial set of Abelian Hamiltonian vector fields $X_j = \{\tilde{C}_j, \cdot\}$ instead of the full Abelianised set X_μ . That is, for any function F on phase space

$$O_F := F + \sum_{n=1}^{\infty} \frac{1}{n!} \tilde{G}^{j_1} \dots \tilde{G}^{j_n} [X_{j_1} \dots X_{j_n} \cdot F] \quad (5.2)$$

with the gauge fixing condition $\tilde{G}^j := -x^j$ (i.e. we set $\tau = 0$ in (3.3)).

Applied to $F = C_a$ we note that $X_j \cdot C_a$ is a linear combination of constraints via the second relation in (5.1), thus also $X_j \cdot X_k \cdot C_a$ is a linear combination of constraints etc. It follows that

$$\tilde{C}_a := O_{C_a} \quad (5.3)$$

together with $\tilde{C}_j$ forms an equivalent set of constraints as the zeroth order term with respect to the x^j in (5.3) starts with C_a . Moreover, (5.3) enjoys the following properties (see the list of properties displayed in section (3))

$$\begin{aligned} \{\tilde{C}_a, \tilde{C}_b\} &= O_{\{C_a, C_b\}}^* \\ \{\tilde{C}_j, \tilde{C}_a\} &= 0 \end{aligned} \quad (5.4)$$

The last relation says that $\tilde{C}_a$ is an observable with respect to the $\tilde{C}_j$ by construction of the “projector” $F \mapsto O_F$. The first relation can be further worked out using the Dirac bracket defined by the pair $(\tilde{C}_j, \tilde{G}^j)$

$$\{F, F'\}^* = \{F, F'\} - [\{F, \tilde{C}_j\} \{\tilde{G}^j, F'\} - \{F', \tilde{C}_j\} \{\tilde{G}^j, F\}] \quad (5.5)$$

For $F = C_a, F' = C_b$ both correction terms in (5.5) is a linear combination of constraints $C_a, \tilde{C}_j$. It follows that also $\{\tilde{C}_a, \tilde{C}_b\}$ is a linear combination of constraints $\tilde{C}_a, \tilde{C}_j$. The constraints $\tilde{C}_a$ can also be written (see section 3)

$$\tilde{C}_a = C_a(q \rightarrow O_q, p \rightarrow O_p, x \rightarrow 0, y \rightarrow \tilde{C} - O_h, Q \rightarrow O_Q, P \rightarrow O_P, X \rightarrow O_X, Y \rightarrow O_Y) \quad (5.6)$$

Since by construction $\{O_F, O_{F'}\} = \{O_F, O_{F'}\}^*$ and since with respect to the Dirac bracket we may set $\tilde{C}_j = 0$ before or after evaluating the bracket, we may pass to the partial constraint surface $\tilde{C}_j = 0$ and henceforth forget about the degrees of freedom $x^j, \tilde{C}_j$ which form a canonical pair and the partially reduced phase space is coordinatised by O_F with $F \in \{q, p, Q, P, X, Y\}$ while we set $\tilde{C}_j$ strongly to zero in (5.6), that is

$$\begin{aligned} \tilde{C}_a &= C_a(q \rightarrow O_q, p \rightarrow O_p, x \rightarrow 0, y \rightarrow -O_h, Q \rightarrow O_Q, P \rightarrow O_P, X \rightarrow O_X, Y \rightarrow O_Y), \\ h_j &= h_j(q \rightarrow O_q, x \rightarrow 0, Q \rightarrow O_Q, P \rightarrow O_P, X \rightarrow O_X, Y \rightarrow O_Y) \end{aligned} \quad (5.7)$$

Moreover, since x^j has vanishing Poisson brackets with $F \in \{q, p, Q, P, X, Y\}$ it follows that

$$\{O_F, O_{F'}\} = O_{\{F, F'\}^*} = O_{\{F, F'\}} = \{F, F'\} \quad (5.8)$$

for $F, F' \in \{q, p, Q, P, X, Y\}$ since then $\{F, F'\} = \text{const.}$ so that the $O_F, O_{F'}$ remain conjugate variables. Thus Poisson algebraically nothing is changed under the substitution $F \mapsto O_F$ for functions of q, p, Q, P, X, Y only, i.e. on this sector of the phase space the map O is an exact Poisson isomorphism or canonical transformation.

5.1.2 Reduction viewpoint

Alternatively to this gauge invariance (with respect to the $\tilde{C}_j$) viewpoint we may consider the partially reduced phase space where the reduction is with respect to the $\tilde{C}_j$. This is completely analogous to the previous section and the summary is that we can forget about the degrees of freedom x, y and the constraints C_j altogether and just keep the constraints C_a as long as we modify them into

$$\tilde{C}_a(q, p, Q, P, X, Y) = C_a(q, p, x = 0, y = -h(q, x = 0, Q, P, X, Y), Q, P, X, Y) \quad (5.9)$$

Here h_j was constructed perturbatively in the previous section. In particular these modified constraints close among themselves

$$\{\tilde{C}_a, \tilde{C}_b\} = \tilde{\kappa}_{ab}{}^c \tilde{C}_c \quad (5.10)$$

for certain $\tilde{\kappa}$ which are explicitly computed in the next section, see (6.2). To have a classical first class algebra (5.10) is a prerequisite for a consistent quantisation. The problem is that only the *exact* $\tilde{C}_a$ are granted to close among themselves, i.e. only when we invoke the entire series (4.10) that defines h_j and not only its N -th order truncation. The only exception is the case that the index a takes only one value. If that is not the case and if we construct $\tilde{C}_a$ perturbatively, then the closure of the approximated constraints will in general be violated thus prohibiting a consistent quantisation which, however, was the whole motivation for the only partial reduction with respect to C_j . Thus, the perturbation theory for h_j and thus $\tilde{C}_a$ developed in the previous section is granted to be viable for the partial reduction approach developed in this section only for systems for which there is only one symmetric constraint C_a as is the case for instance in cosmology but not for black holes. Thus, whenever the index range of a comprises at least two values we must resort to the full reduction process developed in section 4.

If on the other hand, if there is only one symmetric constraint C_a then the N -th order truncation $C_a^{(N)}(q, p, Q, P, X, Y)$ of the function

$$C_a(q, p, x = 0, y = -h^{(N)}(q, x = 0, Q, P, X, Y), Q, P, X, Y) \quad (5.11)$$

with respect to X, Y , where $h_j^{(N)}$ is the series (4.10) truncated at order N , will be a well motivated starting point for quantisation. The N -th order truncation of (5.11) is readily computed since $C_a(p, q, x, y, P, Q, X, Y)$ is polynomial in y as displayed in (4.5). Thus, e.g. for $N \geq 3$ using either the previous or the present section one would get a viable theory describing cosmological non-Gaussianities resulting from the self-interactions of the non-symmetric (that is in this case, inhomogeneous) degrees of freedom X, Y while there are only a finite number of degrees of freedom in the list q, p, Q, P (the homogeneous modes of all matter and geometry degrees of freedom). We display the details in section 6 for $N = 3$.

5.2 Comparison with the literature at second order

We first review the quite elaborate procedure developed in [5] and then show that it embeds very naturally into the context of the previous subsection, thus explaining the symplecto-geometric origin of the procedure followed in [5]. We only consider 2nd order perturbation theory in this section and keep the index a for easier comparison with the rest of this paper but keep in mind that eventually we are only interested in univalent index range of a .

We start again with the constraints C_a, C_j and, as motivated in section (2), truncate them at second and first order respectively

$$C_{a(1)} = 0, C_{j(0)} = 0, C_a^{(2)} = C_{a(0)} + C_{a(2)}, C_j^{(1)} = C_{j(1)} \quad (5.12)$$

We also recall the symmetric and non-symmetric brackets (2.12) as well as the following identities derived in section 2

$$\begin{aligned} \{C_{a(0)}, C_{b(0)}\}_S &= \{C_{a(0)}, C_{b(0)}\} = \kappa_{ab(0)}{}^c C_{c(0)}, \\ \{C_{j(1)}, C_{k(1)}\}_{\bar{S}} &= \kappa_{jk(0)}{}^a C_{a(0)} \\ \{C_{j(1)}, C_{a(0)}\}_S + \{C_{j(1)}, C_{a(2)}\}_{\bar{S}} &= \kappa_{ja(0)}{}^k C_{k(1)} + \kappa_{ja(1)}{}^b C_{b(0)} \end{aligned} \quad (5.13)$$

Since the $C_{j(1)}$ do not close among each other, the first step of [5] is to select some first order canonical variable L^j subject to the conditions

$$\{C_{j(1)}, L^k\}_{\bar{S}} = \delta_j^k, \{L^j, L^k\}_{\bar{S}} = 0 \quad (5.14)$$

In the present situation, a possible choice is

$$L^j := x^k (\sigma^{-1})_k^j, \sigma_j^k := \{C_{j(1)}, x^k\}_{\bar{S}} \quad (5.15)$$

Whenever such functions can be found we can consider the “improved” constraints

$$C'_{j(1)} = C_{j(1)} + \frac{1}{2} \kappa_{jk(0)} L^k C_{a(0)} \quad (5.16)$$

which enjoy the property (note that all zero order quantities have vanishing $\{.,.\}_{\bar{S}}$ bracket)

$$\{C'_{j(1)}, C'_{k(1)}\}_{\bar{S}} = \{C_{j(1)}, C_{k(1)}\}_{\bar{S}} + \frac{1}{2} [\kappa_{km(0)}^a \{C_{j(1)}, L^m\}_{\bar{S}} - \kappa_{jm(0)}^a \{C_{k(1)}, L^m\}_{\bar{S}}] C_{a(0)} = 0 \quad (5.17)$$

i.e. they are Abelian albeit only with respect to the non-symmetric bracket. We may replace $C_{j(1)}$ by $C'_{j(1)}$ free of charge in 2nd order perturbation theory because the totally constrained Hamiltonian reads

$$f^a C_a^{(2)} + g^j C_{j(1)} = [f^a - \frac{1}{2} g^j L^k \kappa_{jk(0)}^a] C_{a(0)} + f^a C_{a(2)} + g^j C'_{j(1)} = [f^a - \frac{1}{2} g^j L^k \kappa_{jk(0)}^a] C_a^{(2)} + g^j C'_{j(1)} + O(3) \quad (5.18)$$

where the third order correction can be dropped in 2nd order perturbation theory. In other words, the substitution of $C_{j(1)}$ by (5.16) can be induced by a redefinition of f^a up to a higher order correction of the Hamiltonian.

If we are interested in backreaction, it is not enough that (5.17) holds with respect to the non-symmetric bracket only, it should hold with respect to the full bracket. Therefore the second step of [5] consists in constructing a canonical transformation on the full phase space, at least to second order perturbation theory, from the canonical coordinates (q, p, x, y, Q, P, X, Y) to new canonical coordinates $(q', p', x', y', Q', P', X', Y')$ with $y'_j := C'_{j(1)}$, $(x')^j := L^j$. In other words the $\{.,.\}_{\bar{S}}$ canonical pair $(L^j, C'_{j(1)})$ as displayed in (5.14), (5.15), (5.16) and (5.17) is completed to a canonical pair on the full phase space which triggers corresponding changes in the other canonical coordinates. To derive this transformation one notices that [5]

$$(X')^J := X^J - L^j \{C_{j(1)}, X^J\}_{\bar{S}} = X^J - L^j \{C'_{j(1)}, X^J\}_{\bar{S}}, \quad Y'_J := Y_J - L^j \{C_{j(1)}, Y_J\}_{\bar{S}} = Y_J - L^j \{C'_{j(1)}, Y_J\}_{\bar{S}}, \quad (5.19)$$

are such that (x', y', X', Y') have canonical $\{.,.\}_{\bar{S}}$ brackets among each other since $\kappa_{jk(0)}^a C_{a(0)}$ and σ_j^k have vanishing $\{.,.\}_{\bar{S}}$ bracket. We will therefore use these x', y', X', Y' as candidates and try to compute q', p', Q', P' at least up to second order. To do this we compute the inversions of (5.15), (5.16) and (5.19) i.e.

$$x^j = \sigma_k^j (x')^k = (x')^k \{C'_{k(1)}, x^j\}_{\bar{S}}, \quad X^J = (X')^J + (x')^j \{C'_{j(1)}, X^J\}_{\bar{S}} \\ Y_J = Y'_J + (x')^j \{C'_{j(1)}, Y_J\}_{\bar{S}}, \quad y_j = (\sigma^{-1})_j^k [y'_k - (\sigma_{jk} x^k + \sigma_{jK} X^K + \sigma_j^K Y_K)] \quad (5.20)$$

where we have used that $C'_{j(1)}$ is linear in x, y, X, Y with coefficient functions σ depending on q, p, Q, P

$$C'_{j(1)} = \sigma_{jk} x^k + \sigma_j^k y_k + \sigma_{jK} X^K + \sigma_j^K Y_K \quad (5.21)$$

We will condense the notation by writing the variables in two groups corresponding to symmetric and non-symmetric degrees of freedom

$$r^\alpha = (q^a, Q^A), s_\alpha = (p_a, P_A), u^\rho = (x^j, X^J), v_\rho = (y_j, Y_J) \quad (5.22)$$

and may write the content of (5.20) compactly as

$$u^\rho = M_\lambda^\rho (u')^\lambda + M^{\rho\lambda} v'_\lambda, \quad v_\rho = \rho_\lambda (u')^\lambda + M_\rho^\lambda v'_\lambda \quad (5.23)$$

where the matrices M depend only on r, s and define by construction a linear canonical transformation $(u', v') \mapsto (u, v)$ at constant (r, s) . We plug (5.23) into the symplectic potential

$$2\Theta = s_\alpha dr^\alpha - ds_\alpha r^\alpha + v_\rho du^\rho - dv_\rho u^\rho \quad (5.24)$$

where the exterior derivative d acts on all phase space variables. If we collect the terms in which d acts on u', v' we know that this just replaces the (u, v) in (5.24) by (u', v') by virtue of M being canonical for each r, s . Thus

$$\begin{aligned} 2\Theta &= s_\alpha dr^\alpha - ds_\alpha r^\alpha + v'_\rho d(u')^\rho - dv'_\rho (u')^\rho + 2(\Delta s_\alpha) dr^\alpha - 2ds_\alpha (\Delta r^\alpha) \\ &= (s_\alpha + (\Delta s)_\alpha) d(r^\alpha + (\Delta r)^\alpha) - d(s_\alpha + (\Delta s)_\alpha) (r^\alpha + (\Delta r)^\alpha) + v'_\rho d(u')^\rho - dv'_\rho (u')^\rho + d(\cdot) + O(4) \\ 2(\Delta s)_\alpha &= v_\rho u^\rho_{,r^\alpha} - v_{\rho,r^\alpha} u^\rho, \quad -2(\Delta r)^\alpha = v_\rho u^\rho_{,s_\alpha} - v_{\rho,s_\alpha} u^\rho \end{aligned} \quad (5.25)$$

where in the last step we dropped a total differential and a term of fourth order in u, v because $\Delta r, \Delta s$ are of second order. The notation in the last line means that u, v are considered as functions of the independent coordinates u', v', r, s . Thus up to second order

$$(r')^\alpha = r^\alpha + (\Delta r)^\alpha, \quad s'_\alpha = s_\alpha + (\Delta s)_\alpha, \quad (5.26)$$

where in the expressions for $\Delta r, \Delta s$ we reexpress u', v' in terms of u, v . A closer look at $\Delta r, \Delta s$ shows that

$$2(\Delta r)^\alpha = \{v_\rho, r^\alpha\}_S u^\rho - v_\rho \{u^\rho, r^\alpha\}_S, \quad 2(\Delta s)_\alpha = \{v_\rho, s_\alpha\}_S u^\rho - v_\rho \{u^\rho, s_\alpha\}_S \quad (5.27)$$

where again u, v are functions of u', v', r, s as displayed in (5.23). We once more compactify the notation and write $t^A = (r^\alpha, s_\alpha)$, $w^{\mathcal{M}} = (u^\rho, v_\rho)$ and introduce the antisymmetric, constant symplectic structure matrices $\Omega^S, \Omega^{\bar{S}}$ defined by

$$2\Theta = \Omega^S_{AB} t^A dt^B + \Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} dw^{\mathcal{N}} \quad (5.28)$$

with inverse Ω^{AB}_S i.e. $\Omega^A_C (\Omega_S)_{CB} = \delta^A_B$ and similar for $\Omega^{\bar{S}}$. It is standard but also not difficult to check directly that with the non-vanishing Poisson bracket convention $\{y_j, x^k\}_{\bar{S}} = \delta^k_j$, $\{Y_J, X^K\}_{\bar{S}} = \delta^K_J$, $\{p_a, q^b\}_S = \delta^b_a$, $\{P_A, Q^B\}_S = \delta^B_A$ we have

$$\{F, G\}_S = -\Omega^{AB}_S F_{,A} G_{,B}, \quad \{F, G\}_{\bar{S}} = -\Omega^{\mathcal{MN}}_{\bar{S}} F_{,\mathcal{M}} G_{,\mathcal{N}} \quad (5.29)$$

with $F_{,A} := \partial F / \partial t^A$, $F_{,\mathcal{M}} := \partial F / \partial w^{\mathcal{M}}$. In this notation (5.23) becomes

$$w^{\mathcal{M}} = M^{\mathcal{M}}_{\mathcal{N}} (w')^{\mathcal{N}} \quad (5.30)$$

and (5.27) becomes (w is considered a function of w', t)

$$\begin{aligned} -2(\Delta t)^A &= \Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} \{w^{\mathcal{N}}, t^A\}_S \\ &= \Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} \{M^{\mathcal{N}}_{\mathcal{P}}, t^A\}_S (w')^{\mathcal{P}} \\ &= \Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} \{M^{\mathcal{N}}_{\mathcal{P}}, t^A\}_S (M^{-1})^{\mathcal{P}}_{\mathcal{Q}} w^{\mathcal{Q}} \end{aligned} \quad (5.31)$$

which expresses the corrections Δt in terms of w, t as M is also a function of t . Next

$$\begin{aligned} -2(\Delta t)^A &= -\Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} M^{\mathcal{N}}_{\mathcal{P}} \{(M^{-1})^{\mathcal{P}}_{\mathcal{Q}}, t^A\}_S w^{\mathcal{Q}} \\ &= -\Omega^{\bar{S}}_{\mathcal{MN}} w^{\mathcal{M}} M^{\mathcal{N}}_{\mathcal{P}} \{(w')^{\mathcal{P}}, t^A\}_S \end{aligned} \quad (5.32)$$

where in the second step we used that $\{.,.\}_S$ does not act on w and reintroduced $w' = M^{-1}w$ considered as a function of w, t . Since M is canonical wrt $\Omega^{\bar{S}}$ we have

$$\Omega^{\bar{S}}_{\mathcal{MN}} M^{\mathcal{M}}_{\mathcal{P}} M^{\mathcal{N}}_{\mathcal{Q}} = \Omega^{\bar{S}}_{\mathcal{PQ}} \Leftrightarrow \Omega^{\bar{S}}_{\mathcal{MN}} M^{\mathcal{N}}_{\mathcal{Q}} = \Omega^{\bar{S}}_{\mathcal{PQ}} (M^{-1})^{\mathcal{P}}_{\mathcal{M}} \quad (5.33)$$

and thus we can cast (5.32) into the simpler form

$$-2(\Delta t)^A = -\Omega^{\bar{S}}_{\mathcal{QP}} (M^{-1})^{\mathcal{Q}}_{\mathcal{M}} w^{\mathcal{M}} \{(w')^{\mathcal{P}}, t^A\}_S = -(w')^{\mathcal{M}} \Omega^{\bar{S}}_{\mathcal{MN}} \{(w')^{\mathcal{N}}, t^A\}_S \quad (5.34)$$

Reintroducing x', y', X', Y' we get

$$-2(\Delta t)^A = -y'_j \{(x')^j, t^A\}_S + (x')^j \{y'_j, t^A\}_S - Y'_J \{(X')^J, t^A\}_S + (X')^J \{Y'_J, t^A\}_S \quad (5.35)$$

To summarise we have shown that

$$\begin{aligned} y'_j &:= C'_{j(1)} = C_{j(1)} + \kappa_{jk(0)}^a C_a(0) L^k/2 \\ (x')^j &:= L^j = (\sigma^{-1})_k^j x^k, \quad \sigma_j^k = \{C_{j(1)}, x^k\}_{\bar{S}} \\ (X')^J &:= X^J - (x')^j \{C'_{j(1)}, X^J\}_{\bar{S}}, \quad Y'_J := Y_J - (x')^j \{C'_{j(1)}, Y_J\}_{\bar{S}}, \\ F' &= F + \frac{1}{2} [y'_j \{(x')^j, f\}_S - (x')^j \{y'_j, f\}_S + Y'_J \{(X')^J, f\}_S - (X')^J \{Y'_J, f\}_S], \quad F \in \{q^a, p_a, Q^A, P_A\} \end{aligned} \quad (5.36)$$

defines a canonical transformation with respect to the full Poisson bracket, up to 2nd order in x, y, X, Y , i.e. the failure from being an exact canonical transformation is an at least third order correction.

Therefore q', p', Q', P', X', Y' in (5.36) define observables with respect to $C'_{j(1)}$ up to second order corrections. It is however not clear that $C_a^{(2)} = C_{a(0)} + C_{a(2)}$ in (5.12) can be written in terms of these 2nd order observables up to higher order corrections. For this to be the case it would be necessary that $\{C'_{j(1)}, C_a^{(2)}\}$ is of second order modulo $C'_{k(1)}, C_a^{(2)}$ terms. Given (5.13) we compute the modifications of (5.13) that result from the substitution $C_{j(1)} \rightarrow C'_{j(1)}$. Using $\hat{\kappa}_{jk(0)}^a = \frac{1}{2} \hat{\kappa}_{jl(0)}^a (\sigma^{-1})_k^l$ we find for the full brackets (note that $C'_{j(1)}$ is still homogeneous linear in x, y, X, Y)

$$\begin{aligned} \{C'_{j(1)}, C'_{k(1)}\} &= \{C'_{j(1)}, C'_{j(1)}\}_{\bar{S}} + O(2) = O(2) \\ \{C'_{j(1)}, C_a^{(2)}\} &= \{C_{j(1)}, C_a^{(2)}\} + \{\hat{\kappa}_{jk(0)}^b x^k C_{b(0)}, C_a^{(2)}\} \\ &= \{C_{j(1)}, C_{a(0)}\}_S + \{C_{j(1)}, C_{a(2)}\}_{\bar{S}} + O(3) + \{\hat{\kappa}_{jk(0)}^b x^k C_{b(0)}, C_{a(0)}\}_S + \{\hat{\kappa}_{jk(0)}^b x^k C_{b(0)}, C_{a(2)}\}_{\bar{S}} + O(3) \\ &= \kappa_{ja(0)}^k C_{k(1)} + \kappa_{ja(1)}^b C_{b(0)} \\ &\quad + x^k [\{\hat{\kappa}_{jk(0)}^b, C_{a(0)}\}_S C_{b(0)} + \hat{\kappa}_{jk(0)}^b \kappa_{ab(0)}^c C_{c(0)}] + \hat{\kappa}_{jk(0)}^b \{x^k, C_{a(2)}\}_{\bar{S}} C_{b(0)} + O(3) \\ &=: \kappa_{ja(0)}^k C'_{k(1)} + \tilde{\kappa}_{ja(1)}^b C_{b(0)} + O(3) \end{aligned} \quad (5.37)$$

The $C'_{j(1)}$ close among themselves up to $O(2)$ corrections by construction but $C_a^{(2)}$ is not an observable with respect to $C'_{j(1)}$ up to $O(2)$ corrections, there is an $O(1)$ obstruction term proportional to $C_{a(0)}$. We thus modify $C_a^{(2)}$ by

$$C_a^{(2)} := C_a^{(2)} + \lambda_{a(2)}^b C_{b(0)} \quad (5.38)$$

where the $O(2)$ correction can be absorbed into a redefinition of the smearing function $(f')^a = f^a + \lambda_{b(2)}^a f^b$ up to higher order corrections since $(f')^a C_a^{(2)} - f^a C_a^{(2)} = O(4)$. Then

$$\begin{aligned} \{C'_{j(1)}, C_a^{(2)}\} &= \kappa_{ja(0)}^k C'_{k(1)} + \tilde{\kappa}_{ja(1)}^b C_{b(0)} + O(3) + \{C'_{j(1)}, \rho_{a(2)}^b C_{b(0)}\} \\ &= \kappa_{ja(0)}^k C'_{k(1)} + [\tilde{\kappa}_{ja(1)}^b + \{C'_{j(1)}, \rho_{a(2)}^b\}_{\bar{S}}] C_{b(0)} + O(3) \end{aligned} \quad (5.39)$$

The term proportional to $C_{b(0)}$ can be brought to vanish if the PDE system

$$\tilde{\kappa}_{ja(1)}^b + \{C'_{j(1)}, \rho_{a(2)}^b\}_{\bar{S}} = 0 \quad (5.40)$$

has a solution for which it is necessary that the corresponding integrability conditions

$$2\{C'_{[j(1)}, \tilde{\kappa}_{k]a(1)}^b + \{C'_{k(1)}, \rho_{a(2)}^b\}_{\bar{S}}\}_{\bar{S}} = 0 \quad (5.41)$$

hold which, using the Jacobi identity with respect to $\{.,.\}_{\bar{S}}$ translates into

$$2\{C'_{[j(1)}, \tilde{\kappa}_{k]a(1)}^b\}_{\bar{S}} = O(2) \quad (5.42)$$

which is not granted to hold, not even, if the index range of a, b is uni-valent. We also note for completeness that

$$\begin{aligned}
\{C_a^{(2)}, C_b^{(2)}\} &= \{C_{a(0)}, C_{b(0)}\}_S + \{C_{a(0)}, C_{b(2)}\}_S + \{C_{a(2)}, C_{b(0)}\}_S + \{C_{a(2)}, C_{b(2)}\}_{\bar{S}} + O(4) \\
&= \kappa_{ab(0)}^c C_{b(0)} + \kappa_{ab(0)}^c C_{b(2)} + \kappa_{ab(2)}^c C_{b(0)} + \kappa_{ab(1)}^j C_{j(1)} + \kappa_{ab(0)}^j C_{j(2)} + \\
&= \kappa_{ab(0)}^c C_c^{(2)} + O(2)
\end{aligned} \tag{5.43}$$

closes with itself but only up to $O(2)$ corrections which are of the same order as $C_a^{(2)}$ which is discomforting. However, if we wish $C_a^{(2)}$ to be gauge invariant with respect to $C'_{j(1)}$ up to $O(2)$ we must perform the substitution (if it exists) $C_a^{(2)} \rightarrow C_a'^{(2)} = \lambda_{a(2)}^b C_{b(0)} + C_a^{(2)}$ and then find

$$\{C_a'^{(2)}, C_b'^{(2)}\} = \kappa_{ab(0)}^c C_c'^{(2)} + O(2) \tag{5.44}$$

where the additional $O(2)$ corrections are all proportional to $C_{a(0)}$ with coefficients of the form $\{\lambda_{(2)}, \lambda_{(2)}\}_{\bar{S}}, \{\lambda_{(2)}, C_{(2)}\}_{\bar{S}}, \lambda_{\kappa(0)}$. Of course, (5.44) vanishes when a, b take only uni-valent range.

Given these difficulties the procedure followed in the literature is to expand $C_a^{(2)}$ in terms of $q', p', x', y', Q', P', X', Y', P'$, to drop higher order terms and all terms proportional to y' (corresponding to a redefinition of g^j) and all powers of x' . Dropping the x' dependent terms is usually justified by arguing that x' is pure gauge and thus these terms cannot be observable. The so modified $C'_{a(2)}$ then satisfies $\{C'_{j(1)}, C_a'^{(2)}\} = O(2)$ by construction and trivially $\{C_a'^{(2)}, C_b'^{(2)}\} = 0$ for uni-valent range of a, b . However, the dropping of the x' dependent terms lacks a more profound justification other than providing a consistent model.

Given the theory developed in section 3 and specialised to the current situation in the previous subsection, one may wonder whether there is any connection between (5.36) and the observable “projector” O_F in 5.2. This is far from obvious:

1. In (5.36) an elaborate mixture and symmetric and non-symmetric brackets appears while in (5.2) just involves the full Poisson bracket.
2. In (5.36) the correction terms involve Poisson brackets of $F \in \{q, p, Q, P, X, Y\}$ with both $C'_{j(1)}$ and $(X')^j, Y'_j$ while in (5.2) only Poisson brackets between F and $\tilde{C}_j = y_j + h_j(q, x, Q, P, X, Y)$ are involved.
3. While both $C'_{j(1)} = C'_{j(1)}(q, p, x, y, Q, P, X, Y)$ and $\tilde{C}_j$ are related to the same original unperturbed C_j , they do not even depend on the same set of variables ($\tilde{C}_j$ does not depend on p).

Remarkably, still a precise relation between (5.36) and (5.2) can be established, thereby unveiling the symplecto-geometric origin of the quite elaborate set of formulae (5.36) and showing how to extend the framework of [5] to higher orders. It also justifies why the constrained Hamiltonian $f^a C_a^{(2)} + g^j C_{j(1)}$ can be replaced by an equivalent one which can be written just in terms of $q', p', y', Q', P', X', Y'$ while an explicit dependence on x' drops out: As we showed in the previous section, before engaging in perturbation theory, one can replace C_a, C_j by equivalent constraints (thereby redefining f^a, g^j in the Hamiltonian) $\tilde{C}_a, \tilde{C}_j$ such that with respect to the full bracket the $\tilde{C}_a$ close among themselves, the $\tilde{C}_a, \tilde{C}_j$ commute and the $\tilde{C}_j, \tilde{C}_k$ are Abelian. The exact reduction of the theory with respect to $\tilde{C}_j$ should therefore result in $\tilde{C}_a$ which is fully gauge invariant with respect to $\tilde{C}_j$ and thus cannot depend on x^j (which is such that $\{\tilde{C}_j, x^k\} = \delta_j^k$) explicitly. Indeed this is precisely achieved in (5.6) (partially gauge invariant viewpoint) or (5.9) (partial reduction viewpoint). As x, x' are linearly related in the perturbative treatment above, all explicit dependence on x' in $C_a^{(2)}$ should be eliminated.

A first hint that (5.36) and (5.2) cannot be unrelated is due to the appearance of the factor $1/2$ in $q' - q, p' - p, Q' - Q, P' - P$ which is missing in $X' - X, Y' - Y$: Such a factor would appear precisely in the second order term of the Taylor expansion in (5.2). Also the expansion parameter in (5.2) is x^j while in (5.36) for at least some of the terms it is $(x')^j$ and x, x' are linearly related. To understand the factor $1/2$ from the point of view of (5.2) let us temporarily assume (to be justified below) that we may substitute $(x')_j, y'_j = C'_{j(1)}$ by $x^j, \tilde{C}_{j(1)}$.

Let $X_j = \{\tilde{C}_{j(1)}, \cdot\}$ then

$$O_F = F - x^j \{\tilde{C}_{j(1)}, F\} + \frac{1}{2} x^j x^k \{\tilde{C}_{j(1)}, \tilde{C}_{k(1)}, F\} + O(3) \quad (5.45)$$

where we dropped higher order terms for second order perturbation theory: Since x is of first order, thus no matter what the result of the n -th order Poisson bracket calculation is, the terms proportional to x^n in (5.2) are at least of order n . We determine the terms at most of order two in (5.45) for a first order function $F_{(1)}$, i.e. a linear function of x, y, X, Y with coefficients depending on q, p, Q, P and a zeroth order function $F_{(0)}$ respectively. We have $\{\tilde{C}_{j(1)}, F_{(1)}\} = \{\tilde{C}_{j(1)}, F_{(1)}\}_{\bar{S}} + O(2)$ and thus the second term in (5.45) is contributing a quadratic correction. On the other hand

$$\{\tilde{C}_{j(1)}, \{\tilde{C}_{k(1)}, F_{(1)}\}\} = \{\tilde{C}_{j(1)}, O(0) + O(2)\} = \{\tilde{C}_{j(1)}, O(0)\}_S + \{\tilde{C}_{j(1)}, O(2)\}_{\bar{S}} + O(3) = O(1) \quad (5.46)$$

thus the third term in (5.45) is of third order and can be dropped. Next $\{\tilde{C}_{j(1)}, F_{(0)}\} = \{\tilde{C}_{j(1)}, F_{(0)}\}_S = O(1)$ and thus the second term in (5.45) is a quadratic correction and thus

$$\{\tilde{C}_{j(1)}, \{\tilde{C}_{k(1)}, F_{(0)}\}\} = \{\tilde{C}_{j(1)}, O(1)\} = \{\tilde{C}_{j(1)}, O(1)\}_{\bar{S}} + O(2) \quad (5.47)$$

Therefore the third term which contains the factor $1/2$ in (5.45) is also quadratic and does contribute when F is of zeroth order!

To see explicitly why the third term in (5.45) is mandatory in order that O_F be a second order observable when $F = F_{(0)}$ we compute assuming $\{\tilde{C}_{j(1)}, x^k\} = \delta_j^k$ (justified below)

$$\{\tilde{C}_{j(1)}, F - x^k \{\tilde{C}_{k(1)}, F\}\} = -x^k \{\tilde{C}_{j(1)}, \{\tilde{C}_{k(1)}, F\}\} \quad (5.48)$$

which is $O(2)$ for $F = F_{(1)}$ but only $O(1)$ for $F = F_{(0)}$. Thus for $F = F_{(0)}$ we include the third term in (5.45) and use $\{\tilde{C}_j, \tilde{C}_k\} = O(2)$ (justified below). Then

$$\begin{aligned} \{\tilde{C}_{j(1)}, O_F\} &= \{\tilde{C}_{j(1)}, F\} - \{\tilde{C}_{j(1)}, x^k \{\tilde{C}_{k(1)}, F\}\} + \frac{1}{2} \{\tilde{C}_{j(1)}, x^k x^l \{\tilde{C}_{k(1)}, \{\tilde{C}_{l(1)}, F\}\}\} \\ &= -x^k \{\tilde{C}_{j(1)}, \{\tilde{C}_{k(1)}, F\}\} + \frac{1}{2} [x^k \{\tilde{C}_{k(1)}, \{\tilde{C}_{j(1)}, F\}\} + x^l \{\tilde{C}_{j(1)}, \{\tilde{C}_{l(1)}, F\}\} \\ &\quad + x^k x^l \{\tilde{C}_{j(1)}, \{\tilde{C}_{k(1)}, \{\tilde{C}_{l(1)}, F\}\}\}] \\ &= \frac{1}{2} x^k [\{\tilde{C}_{k(1)}, \{\tilde{C}_{j(1)}, F\}\} - \{\tilde{C}_j, \{\tilde{C}_{k(1)}, F\}\}] + O(3) \\ &= \frac{1}{2} x^k \{\tilde{C}_{k(1)}, \{\tilde{C}_{j(1)}, F\}\} + O(3) = O(3) \end{aligned} \quad (5.49)$$

where we used the Jacobi identity.

Summarising, to second order

$$O_{X^J} = X^J - x^j \{\tilde{C}_{j(1)}, X^J\}, \quad O_{Y_J} = Y_J - x^j \{\tilde{C}_{j(1)}, Y_J\} \quad (5.50)$$

already look very close to $(X')^J, Y'_J$ in (5.36) while for $F \in \{q^a, p_a, Q^A, P_A\}$ the quantities O_F and F' in (5.36) are not obviously related except that they involve a factor $1/2$. To see how (5.2) and (5.36) are related nevertheless we must carry out the programme of the previous subsection to second order. The first step is to calculate $\tilde{C}_j = y_j + h_j(q, x, Q, P, X, Y)$ to first order where h_j is computed perturbatively in section 4. Thus we suppose to have found a solution $p_a(0)$ (a function of q, Q, P of $C_a(0) = 0$) and must solve $C_j = 0$ to first order in y which is explicitly given by (see (4.12) where what is denoted by S_j^k there is denoted by σ_j^k here)

$$\tilde{C}_{j(1)} = y_j + \{(\sigma^{-1})_j^k [\sigma_{jk} x^k + \sigma_{jJ} X^J + \sigma_j^J Y_J]\}_{p=p(0)} = \{(\sigma^{-1})_j^k [C'_{j(1)}]\}_{p=p(0)} \quad (5.51)$$

where the notation (5.21) was used. Note that $C'_{j(1)} = C_{j(1)}$ when $p = p(0)$ since these two functions differ by a term proportional to $C_{a(0)}$ which vanishes at $p = p(0)$ by definition.

This provides the first connection between the formalisms. The second is that $(x')^j = \sigma_k^j x^k$ so that

$$[(x')^j C'_{j(1)}]_{p=p(0)} = x^j \tilde{C}_{j(1)} \quad (5.52)$$

It follows that to second order

$$\begin{aligned} O_{X^J} &= X^J - x^j \{ \tilde{C}_{j(1)}, X^J \} = X^J - x^j \{ \tilde{C}_{j(1)}, X^J \}_{\bar{S}} = X^J - (x')^j \{ [C'_{j(1)}]_{p=p(0)}, X^J \}_{\bar{S}} \\ &= X^J - (x')^j \{ [C'_{j(1)}]_{p=p(0)}, X^J \}_{\bar{S}} = (X')^J_{p=p(0)} \end{aligned} \quad (5.53)$$

and similarly $O_{Y_J} = [Y'_J]_{p=p(0)}$.

Recall $y'_j = C'_{j(1)}$ and let $\tilde{y}_j = (\sigma^{-1})^k_j y'_k$ so that $\tilde{C}_{j(1)} = [\tilde{y}_j]_{p=p(0)}$. For $F \in \{q, p, Q, P\}$ note that all brackets with F are automatically $\{.,.\}_{\bar{S}}$ brackets which do not act on x, y, X, Y . Then

$$\begin{aligned} -2(F' - F) &= y'_j \{ (x')^j, F \} - (x')^j \{ y'_j, F \} + Y'_J \{ (X')^J, F \} - (X')^J \{ Y'_J, F \} \\ &= y'_j \{ (x')^j, F \} - (x')^j \{ y'_j, F \} - Y'_J \{ (x')^j \{ y'_j, X^J \}_{\bar{S}}, F \} + (X')^J \{ (x')^j \{ y'_j, Y_J \}_{\bar{S}}, F \} \\ &= y'_j \{ (x')^j, F \} - x^k [(\sigma^{-1})^j_k \{ y'_j, F \} + Y'_J \{ (\sigma^{-1})^j_k \{ y'_j, X^J \}_{\bar{S}}, F \} - (X')^J \{ (\sigma^{-1})^j_k \{ y'_j, Y_J \}_{\bar{S}}, F \}] \\ &= y'_j \{ (x')^j, F \} - x^k [\tilde{y}_k, F] + (\sigma^{-1})^j_k \tilde{y}_l \{ \sigma^l_j, F \} + Y'_J \{ \tilde{y}_k, X^J \}_{\bar{S}}, F \} - (X')^J \{ \tilde{y}_k, Y_J \}_{\bar{S}}, F \} \\ &= y'_j \{ (x')^j, F \} - x^k [\tilde{y}_k, F] - y'_j \{ \sigma^{-1} \}^j_k, F \} + Y'_J \{ \tilde{y}_k, X^J \}_{\bar{S}}, F \} - (X')^J \{ \tilde{y}_k, Y_J \}_{\bar{S}}, F \} \\ &= 2y'_j \{ (x')^j, F \} - x^k [\tilde{y}_k, F] + Y'_J \{ \tilde{y}_k, X^J \}_{\bar{S}}, F \} - (X')^J \{ \tilde{y}_k, Y_J \}_{\bar{S}}, F \} \\ &= 2y'_j \{ (x')^j, F \} \\ &\quad - x^k [\{ A_{kj}, F \} x^j + \{ B_{jJ}, F \} X^J + \{ C^J_j, F \} Y_J + (Y_J + x^j B_j) \{ C^J_k, F \} + (X^J - x^j C^J_j) \{ B_{kJ}, F \}] \\ &= 2y'_j \{ (x')^j, F \} - x^k [\{ A_{kj}, F \} x^j + 2\{ B_{jJ}, F \} X^J + 2\{ C^J_j, F \} Y_J + x^j \{ B_j \} \{ C^J_k, F \} - C^J_j \{ B_{kJ}, F \}] \end{aligned} \quad (5.54)$$

where in the last step we used the abbreviations

$$\tilde{y}_j = y_j + (\sigma^{-1})^k_j [\sigma_{kl} x^l + \sigma_{kJ} X^J + \sigma^J_k Y_J] =: y_j + A_{jk} x^k + B_{jJ} X^J + C^J_j Y_J \quad (5.55)$$

On the other hand with $\bar{A}_{jk} := [A_{jk}]_{p=p(0)}$ and similar for $\bar{B}_{jJ}, \bar{C}^J_j$ as well as $\bar{y}_j := [\tilde{y}_j]_{p=p(0)} = \tilde{C}_{j(1)}$ we have

$$\begin{aligned} -2(O_F - F) &= 2x^k \{ \bar{y}_k, F \} - x^k x^j \{ \bar{y}_k, \{ \bar{y}_j, F \} \} \\ &= 2x^k \{ \bar{y}_k, F \} - x^k x^j \{ \bar{y}_k, \{ \bar{y}_j, F \} \}_{\bar{S}} + O(4) \\ &= 2x^k \{ \bar{y}_k, F \} - x^k x^j \{ \bar{y}_k, [\{ \bar{A}_{jl}, F \} x^l + \{ \bar{B}_{jJ}, F \} X^J + \{ \bar{C}^J_j, F \} Y_J] \}_{\bar{S}} \\ &= 2x^k \{ \bar{y}_k, F \} - x^k x^j [\{ \bar{A}_{jk}, F \} + \{ \bar{B}_{jJ}, F \} C^J_k - \{ \bar{C}^J_j, F \} B_{kJ}] \\ &= 2x^k [\{ \bar{A}_{kj}, F \} x^j + \{ \bar{B}_{kJ}, F \} X^J + \{ \bar{C}^J_k, F \} Y_J] - x^k x^j [\{ \bar{A}_{jk}, F \} + \{ \bar{B}_{jJ}, F \} C^J_k - \{ \bar{C}^J_j, F \} B_{kJ}] \\ &= x^k [\{ \bar{A}_{kj}, F \} x^j + 2\{ \bar{B}_{kJ}, F \} X^J + 2\{ \bar{C}^J_k, F \} Y_J] + x^k x^j [\{ \bar{C}^J_j, F \} B_{kJ} - \{ \bar{B}_{jJ}, F \} C^J_k] \end{aligned} \quad (5.56)$$

where we have used that A_{jk} is symmetrically projected.

Comparing (5.36) and (5.56) we find that to second order, modulo a term proportional to the constraints y'_j , we have $O_F = F'$ except that for O_F we set $p = p(0)$ before evaluating the brackets $\{.,.\}_{\bar{S}}$ involving F while for F' we do not do that. Nevertheless both expressions fulfill the same purpose, namely they define observables with respect to $\tilde{C}_{j(1)}$ and $C'_{j(1)}$ respectively. The reason for this is clear: From the relation

$$\{C_{j(1)}, C_{k(1)}\}_{\bar{S}} = \kappa_{jk(0)}^a C_{a(0)} \quad (5.57)$$

we find from using $\bar{y}_j = [(\sigma^{-1})^k_j y'_k]_{p=p(0)} = [(\sigma^{-1})^j_k C_{k(0)}]_{p=p(0)}$ and the fact that restricting $p = p(0)$ does not affect the $\{.,.\}_{\bar{S}}$ bracket that $\{ \bar{y}_j, \bar{y}_k \}_{\bar{S}} = 0$ just like $\{ y'_j, y'_k \}_{\bar{S}} = 0$. Thus the two descriptions agree at second order, we are using equivalent sets of constraints. Note that while the constraints $\tilde{C}_j$ use $p = p(0)$ in their construction, the constraints $\tilde{C}_a = O_{C_a}$ do not, the variable p is not yet eliminated in this partial reduction approach.

The advantage of working with the approach developed in this paper is that it directly generalises to higher orders. In the next section we develop higher order perturbation theory for partially reduced gauge systems with backreaction which is directly relevant for cosmology.

6 Partially reduced perturbation theory

We display here the explicit formulae for third order partially reduced perturbation theory, i.e. the explicit formulae for the remaining constraints C_a in the presence of the reduction of C_j . Again we will keep the index range a arbitrary but note that unless the range is uni-valent the subsequent perturbative constraints do not close at finite order (although the unperturbed constraints do). The results of this section are directly relevant for cosmological perturbation theory.

The non-perturbative expression is given by

$$\tilde{C}_a(q, p, Q, P, X, Y) := C_a(q, p, x = 0, y = -h(q, x = 0, Q, P, X, Y), Q, P, X, Y) \quad (6.1)$$

where $h = \sum_{n=1}^{\infty} h_{j(n)}$ is found using theorem 4 which is a perturbative method for determining $h_j(q, x, Q, P, X, Y)$.

Conceptually, h_j results from solving $C_a = 0$ for $p_a = -\hat{h}_a(q, x, y, Q, P, X, Y)$ and solving

$C_j(q, p = -\hat{h}(q, x, y, Q, P, X, Y), x, y, Q, P, X, Y) = 0$ for $y_j = -h_j(q, x, Q, P, X, Y)$. Although by the general theory reviewed in sections 3, 5.1 it is clear that the (6.1) close, it is instructive to verify this by direct computation. To that end we introduce the collective configuration coordinates $k^\alpha = (q^a, Q^A, X^J)$ and momentum coordinates $i_\alpha = (p_a, P_A, Y_J)$ on which $\tilde{C}_a$ still depends. We use the notation $F_{y=-h, x=0}$ to mean that we *first* replace $y = -h(q, x, Q, P, X, Y)$ to obtain $F'(q, p, x, Q, P, X, Y) = F(q, p, x, y = -h(q, x, Q, P, X, Y), Q, P, X, Y)$ and then set $x = 0$ to obtain $\tilde{F}(q, p, Q, P, X, Y) = F'(q, p, x = 0, Q, P, X, Y)$. Direct computation yields

$$\begin{aligned} \{\tilde{C}_a, \tilde{C}_b\} &= \frac{\partial \tilde{C}_a}{\partial i_\alpha} \frac{\partial \tilde{C}_b}{\partial k^\alpha} - a \leftrightarrow b \\ &= ([\frac{\partial C_a}{\partial i_\alpha}]_{y=-h, x=0} - [\frac{\partial C_a}{\partial y^j}]_{y=-h, x=0} [\frac{\partial h_j}{\partial i_\alpha}]_{x=0}) ([\frac{\partial C_b}{\partial k^\alpha}]_{y=-h, x=0} - [\frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} [\frac{\partial h_k}{\partial k^\alpha}]_{x=0}) - a \leftrightarrow b \\ &= \{\frac{\partial C_a}{\partial i_\alpha} \frac{\partial C_b}{\partial k^\alpha} - a \leftrightarrow b\}_{y=-h, x=0} \\ &\quad - \{[\frac{\partial C_a}{\partial y^j}]_{y=-h, x=0} [\frac{\partial h_j}{\partial i_\alpha}]_{x=0} [\frac{\partial C_b}{\partial k^\alpha}]_{y=-h, x=0} + [\frac{\partial C_a}{\partial i_\alpha}]_{y=-h, x=0} [\frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} [\frac{\partial h_k}{\partial k^\alpha}]_{x=0} - a \leftrightarrow b\}_{y=-h, x=0} \\ &\quad + \{[\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} [\frac{\partial h_j}{\partial i_\alpha} \frac{\partial h_k}{\partial k^\alpha} - j \leftrightarrow k]_{x=0}\} \\ &= \{C_a, C_b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial x^j} - a \leftrightarrow b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} \{[h_j]_{x=0}, C_b\} - a \leftrightarrow b\}_{y=-h, x=0} \\ &\quad + [\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} \{[h_j]_{x=0}, [h_k]_{x=0}\} \\ &= \{C_a, C_b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} \{y_j + [h_j]_{x=0}, C_b\} - a \leftrightarrow b\}_{y=-h, x=0} \\ &\quad + [\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} \{[h_j]_{x=0}, [h_k]_{x=0}\} \\ &= \{C_a, C_b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} (\{\tilde{C}_j, C_b\} + \{y_k, h_j\} \frac{\partial C_b}{\partial y^k}) - a \leftrightarrow b\}_{y=-h, x=0} + [\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} \{h_j, h_k\}_{x=0} \\ &= \{C_a, C_b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} \{\tilde{C}_j, C_b\} - a \leftrightarrow b\}_{y=-h, x=0} \\ &\quad + [\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} \{-\{y_k, h_j\} + \{y_j, h_k\} + \{h_j, h_k\}_{x=0}\} \\ &= \{C_a, C_b\}_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} \{\tilde{C}_j, C_b\} - a \leftrightarrow b\}_{y=-h, x=0} + [\frac{\partial C_a}{\partial y^j} \frac{\partial C_b}{\partial y^k}]_{y=-h, x=0} \{\tilde{C}_j, \tilde{C}_k\}_{x=0} \\ &= [(\kappa')_{ab}{}^c C_c + (\kappa')_{ab}{}^j \tilde{C}_j]_{y=-h, x=0} - \{\frac{\partial C_a}{\partial y^j} [(\kappa')_{jb}{}^c C_c + (\kappa')_{jb}{}^k \tilde{C}_k] - a \leftrightarrow b\}_{y=-h, x=0} \\ &= [(\kappa')_{ab}{}^c + 2 \frac{\partial C_{[a}}{\partial y_j} (\kappa')_{b]j}{}^c]_{y=-h, x=0} \tilde{C}_c =: \tilde{\kappa}_{ab}^c \tilde{C}_c \end{aligned} \quad (6.2)$$

where in the third step we used that $[h_j]_{x=0}$ does not depend on x, y , in the fourth we combined the second and third term using $\partial/\partial x^j(\cdot) = \{y_j, \cdot\}$, in the fifth we noted that the $y_j + [h_j]_{x=0} = [\tilde{C}_j]_{x=0}$ and that $\{[h_j]_{x=0}, [h_k]_{x=0}\} = \{h_j, h_k\}_{x=0}$ as h_j does not depend on y , in the seventh and eighth we combined terms, in the ninth we used that the set of constraints $C_a, \tilde{C}_j$ closes and whose structure constants were defined in (5.1), in the tenth we used that $\tilde{C}_j = 0$ when $y = -h$ and that $\tilde{C}_a = [C_a]_{y=-h, x=0}$. Note that at the reduced level $\tilde{C}_j \equiv 0$.

Our task is now to expand $\tilde{C}_a$ to N -th order in X, Y . We collect the relevant formulae from (4.5), (4.6)

$$\begin{aligned} C_a &= U_a + K_a^b p_b + L_a^j y_j + A_a^{bc} p_b p_c + B_a^{jk} y_j y_k + C_a^{bj} p_b y_j \\ U_a &= u_a + u_a^A P_A + u_a^J Y_J + u_a^{AB} P_A P_B + u_a^{JK} Y_J Y_K + u_a^{AJ} P_A Y_J \\ K_a^b &= k_a^b + k_a^{bA} P_A + k_a^{bJ} Y_J \\ L_a^j &= l_a^j + l_a^{jA} P_A + l_a^{jJ} Y_J \end{aligned} \quad (6.3)$$

where the functions A, B, C, u, k, l only depend on q, x, Q, X . We denote by $\bar{A}, \bar{B}, \bar{C}, \bar{u}, \bar{k}, \bar{l}$ their evaluation at $x = 0$ and by $\bar{A}_{(n)}$ etc. the homogeneous n -th order contribution to its expansion with respect to X . Also $\bar{U}, \bar{K}, \bar{L}$ just mean replacement of u, k, l in U, K, L by $\bar{u}, \bar{k}, \bar{l}$.

We are supposed to evaluate (6.3) at $y = -h$ and require the knowledge of the coefficients $h_{j(n)}$ for $n \leq N$ that were constructed by the iterative scheme of theorem 4. We denote by $\bar{h}_j$ the evaluation of $h_j(q, x, Q, P, X, Y)$ at $x = 0$ and by $\bar{h}_{j(n)}$ the n -th order contribution of its expansion with respect to X, Y . Then the exact expression is

$$\tilde{C}_a = \bar{U}_a + \bar{K}_a^b p_b - \bar{L}_a^j \bar{h}_j + \bar{A}_a^{bc} p_b p_c + \bar{B}_a^{jk} \bar{h}_j \bar{h}_k - \bar{C}_a^{bj} p_b \bar{h}_j \quad (6.4)$$

and the n -th order homogeneous contribution to its expansion with respect to X, Y is

$$\tilde{C}_{a(n)} = \bar{U}_{a(n)} + \bar{K}_{a(n)}^b p_b - \sum_{r+s=n} [\bar{L}_{a(r)}^j + \bar{C}_{a(r)}^{bj} p_b] \bar{h}_{j(s)} + \bar{A}_{a(n)}^{bc} p_b p_c + \sum_{r+s+t=n} \bar{B}_{a(r)}^{jk} \bar{h}_{j(s)} \bar{h}_{k(t)} \quad (6.5)$$

where

$$\begin{aligned} \bar{U}_{a(n)} &= \bar{u}_{a(n)} + \bar{u}_{a(n)}^A P_A + \bar{u}_{a(n-1)}^J Y_J + \bar{u}_{a(n)}^{AB} P_A P_B + \bar{u}_{a(n-2)}^{JK} Y_J Y_K + \bar{u}_{a(n-1)}^{AJ} P_A Y_J \\ \bar{K}_{a(n)}^b &= \bar{k}_{a(n)}^b + \bar{k}_{a(n)}^{bA} P_A + \bar{k}_{a(n-1)}^{bJ} Y_J \\ \bar{L}_{a(n)}^j &= \bar{l}_{a(n)}^j + \bar{l}_{a(n)}^{jA} P_A + \bar{l}_{a(n-1)}^{jJ} Y_J \end{aligned} \quad (6.6)$$

while

$$\tilde{C}_a^{(N)} = \sum_{n=0}^N \tilde{C}_{a(n)} \quad (6.7)$$

To determine the top order of $\bar{h}_{j(r)}$ needed to evaluate $\tilde{C}_{a(n)}$ we recall (4.9), (4.13) and (4.14): We note that due to $h_{j(0)} \equiv 0$ also $\bar{h}_{j(0)} = 0$ therefore the third term in (6.5) involves only $s, t \leq n-1$. Next from (4.9) we see that $\bar{L}_{a(0)}^j \equiv 0 \equiv \bar{C}_{a(0)}^{bj}$ so that $\bar{L}_{a(0)}^j = 0 = \bar{C}_{a(0)}^{bj}$. Therefore also in the second term of (6.5) only involves $s \leq n-1$. Thus we only need $\bar{h}_{j(r)}$, $r = 1, \dots, n-1$ to determine $\tilde{C}_{a(n)}$ which in turn requires to know $h_{j(r)}$, $r = 1, \dots, n-1$. By (4.13) and (4.14) the computation of both $h_{a(n)}, h_{j(n)}$ requires knowledge of $h_{b(r)}, h_{k(r)}$; $r \leq n-1$. The latter are obtained by solving $C_{a(r)} = C_{j(r)} = 0$ for $r \leq n-1$. Thus to find $h_{j(r)}$, $r \leq n-1$ we need to perturbatively solve $C_{a(s)} = 0$, $0 \leq n-2$ and $C_{j(s)} = 0$, $s \leq n-1$ or in other words we must perturbatively solve $C_a^{(r)}$, $r \leq n-2$ and $C_j^{(r)}$, $r \leq n-1$. For instance to find $\tilde{C}_{a(3)}$ we must solve $C_{a(0)}, C_{a(1)} = 0$ and $C_{j(0)} = C_{j(1)} = C_{j(2)} = 0$ and since $C_{a(1)} \equiv 0 \equiv C_{j(0)}$ corresponding to $h_{a(1)} = h_{j(0)} = 0$ we just need to solve $C_{a(0)} = C_{j(1)} = C_{j(2)}$. It should be stressed that while the solutions $p_a(r) = -h_{a(r)}$ of (4.13), (4.14) enter the construction of $\tilde{C}_a$ via h_j , in $\tilde{C}_a$ the variable p is otherwise still unconstrained.

The object (6.7) is to be contrasted with the strategy outlined in section 2 where one expands the unperturbed C_a, C_j to order $N, N-1$ respectively with respect to x, y, X, Y relying on the assumption that the smearing functions f^a, g^j respectively are to be considered as zeroth and second order quantities respectively. We compare this with $\tilde{C}_a^{(N)}$, which, as just derived, is obtained by 1. perturbatively solving the system $C_a^{(N-2)} = C_j^{(N-1)} = 0$

for $-y_j = h_j^{(N-1)} = h_{j(1)} + \dots + h_{j(N-1)}$, 2. restricting to $x = 0$ to find $\bar{h}_j^{(N-1)} = [h_j^{(N-1)}]_x = 0$ and 3. expanding C_a evaluated at $x^j = 0, y_j = -\bar{h}_j^{(N-1)}$ up to N -th order in X, Y . Common to both procedures is that both involve $C_a^{(N)}, C_j^{(N-1)}$ but the crucial difference is that in the second procedure $C_a^{(N)}$ acquires the non-trivial modification $C_a^{(N)} \rightarrow \tilde{C}_a^{(N)}$ and forgets about $C_j^{(N-1)}$ while in the first procedure one keeps both $C_a^{(N)}, C_j^{(N-1)}$ and hopes that these form a closed system of constraints which, as we have seen in section 2, is not the case. The modification $C_a^{(N)} \rightarrow \tilde{C}_a^{(N)}$ is just the perturbative counter part of switching from C_a, C_j to equivalent constraints (i.e. they have the same kernel) $\tilde{C}_a, \tilde{C}_j$ for which the crucial property holds that the $\tilde{C}_j$ close among themselves (even Abelian) and that the $\tilde{C}_a$ are invariant with respect to them so that a partial reduction with respect to the $\tilde{C}_j$ can be carried out.

Accordingly, $\tilde{C}_a^{(N)}$ has a profound justification while $C_a^{(N)'}$ does not. A sign of that can be seen from the fact that (6.7) can be shown to close, *with respect to the full bracket* up to higher order corrections of order at least $N + 1$. To see this, we split the exact $\tilde{C}_a = \tilde{C}_a^{(N)} + Z_{a(N+1)}$ where $Z_{a(N+1)} = O(N + 1)$ contains the higher order terms of $\tilde{C}_a$ with respect to X, Y . Then using (6.2)

$$\begin{aligned}
\{\tilde{C}_a^{(N)}, \tilde{C}_b^{(N)}\} &= \{\tilde{C}_a - Z_{a(N+1)}, \tilde{C}_b - Z_{b(N+1)}\} \\
&= \{\tilde{C}_a, \tilde{C}_b\} - \{\tilde{C}_a, Z_{b(N+1)}\} + \{\tilde{C}_b, Z_{a(N+1)}\} + \{Z_{a(N+1)}, Z_{b(N+1)}\} \\
&= \tilde{\kappa}_{ab}^c \tilde{C}_c - \{\tilde{C}_a, Z_{b(N+1)}\}_{\bar{S}} + O(N + 1) + \{\tilde{C}_b, Z_{a(N+1)}\}_{\bar{S}} + O(N + 1) + O(2N) \\
&= \tilde{\kappa}_{ab}^c \tilde{C}_c^{(N)} - \{\tilde{C}_{a(0)} + \tilde{C}_{a(2)} + O(3), Z_{b(N+1)}\}_{\bar{S}} + \{\tilde{C}_{b(0)} + \tilde{C}_{b(2)} + O(3), Z_{a(N+1)}\}_{\bar{S}} + O(N + 1) \\
&= \tilde{\kappa}_{ab}^c \tilde{C}_c^{(N)} - \{\tilde{C}_{a(2)}, Z_{b(N+1)}\}_{\bar{S}} + \{\tilde{C}_{b(2)}, Z_{a(N+1)}\}_{\bar{S}} + O(N + 1) \\
&= \tilde{\kappa}_{ab}^c \tilde{C}_c^{(N)} + O(N + 1)
\end{aligned} \tag{6.8}$$

where we used that $\{\cdot, \cdot\}_{\bar{S}}$ does not decrease orders, that $\tilde{C}_{a(0)}$ has vanishing $\{\cdot, \cdot\}_{\bar{S}}$ brackets and that $\tilde{C}_{a(1)} \equiv 0$. To see the latter we note from (6.5) and that $h_{j(0)} = 0$

$$\tilde{C}_{a(1)} = \bar{U}_{a(1)} + \bar{K}_{a(1)}^b p_b - [\bar{L}_{a(0)}^j + \bar{C}_{a(0)}^{bj} p_b] \bar{h}_{j(1)} + \bar{A}_{a(0)}^{bc} p_b p_c = 0 \tag{6.9}$$

since by (4.9)

$$U_{a(1)} = K_{a(1)}^b = L_{a(0)}^j = A_{a(1)}^{bc} = C_{a(0)}^{bj} = 0 \tag{6.10}$$

for all q, x, P, Q, X, Y hence also at $x = 0$.

Note that the proof of (6.8) uses the non-perturbative result (6.2). The result (6.8) shows that the failure of the $\tilde{C}_a^{(N)}$ to close exactly is of higher order $O(N+1)$ and thus formally decays to zero as $N \rightarrow \infty$. It is exactly zero for any N if the range of a, b is only univalent. Since only approximately closing constraints are not suitable for operator constraint quantisation, the partial reduction procedure is presumably not helpful for multivalent range of a, b . See, however, [12] where only approximately closing constraints are considered as second class constraints which opens a quantisation strategy based on second class constraints (Dirac bracket formalism). Yet, the result (6.8) can be used as a motivation to follow the approach to perturbation theory for partially reduced gauge systems with backreaction proposed in the present article at least in the classical theory. It is conceptually clear and simple and does not need the split of Poisson brackets into background and perturbation brackets, no canonical transformations are involved. Yet, it can be seen as a natural extension of the established method [5] as shown in the previous section. That (6.8) closes up to corrections of order higher than $C_a^{(N)}$ itself is also to be contrasted with (5.43) for second order which only closes up to the same order.

We finish this section by exemplifying the procedure and write $\tilde{C}_a^{(3)}$ with all details supplied, following the notation of theorem 4. This requires to know $y_j(1) = -h_{j(1)}, y_j(2) = -h_{j(2)}$ and, as an intermediate step, $p_a(0)$ in the notation of theorem 4. Here $p_a(0)$ solves $C_{a(0)} = 0$ and is supposed to be a known function of q, Q, P . Following the steps of theorem (4) we find successively in terms of the zeroth order matrix $S_j^k(q, Q, P) := N_{j(0)}^k + 2 F_{j(0)}^{ck} p_c(0)$, which is assumed to be regular

$$\begin{aligned}
h_{k(1)} &= (S^{-1})_k^j [V_{j(1)} + M_{j(1)}^a p_a(0) + D_{j(1)}^{ab} p_a(0) p_b(0)] \\
h_{k(2)} &= (S^{-1})_k^j [V_{j(2)} + M_{j(2)}^a p_a(0) - N_{j(1)}^k h_{k(1)} + D_{j(2)}^{ab} p_a(0) p_b(0) + E_{j(0)}^{kl} h_{k(1)} h_{l(1)} - F_{j(1)}^{ak} p_a(0) h_{k(1)}]
\end{aligned} \tag{6.11}$$

which are to be restricted to $x = 0$ thus yielding $\bar{h}_{j(1)}, \bar{h}_{j(2)}$ and inserted into (6.5) for $n = 2, 3$ to find $\tilde{C}_{a(2)}, \tilde{C}_{a(3)}$ while $\tilde{C}_{a(0)} = C_{a(0)}$, $\tilde{C}_{a(1)} = C_{a(1)} = 0$ remain unmodified. Then $\tilde{C}_a^{(3)} = \sum_{n=0}^3 \tilde{C}_{a(n)}$. Note again that $p_a(0)$ which solves $C_{a(0)} = 0$ just enters $h_{j(1)}, h_{j(2)}$ but the unconstrained p still remains intact in all other parts of $\tilde{C}_{a(n)}$ in particular in $C_{a(0)}$ and all coefficients in U, K, L, A, B, C (6.5).

We note that in full reduction to order N we require both h_a, h_j to order N and not only to order $N-2, N-1$ respectively which then gives directly the reduced Hamiltonian

$$H^{(N)}(t) = \dot{\tau}^a(t) \left[\sum_{n=0}^N h_{a(n)} \right]_{q=\tau, x=\rho} + \dot{\rho}^j(t) \left[\sum_{n=0}^N h_{j(n)} \right]_{q=\tau, x=\rho} \quad (6.12)$$

subject to the gauge fixing conditions $q^a = \tau^a, x^j = \rho^j$, as functions of Q, P, X, Y . Thus, to obtain for instance $H^{(3)}$ we require in addition $h_{a(2)}, h_{a(3)}$ if $\dot{\rho} = 0$ and in addition $h_{j(3)}$ if $\dot{\rho} \neq 0$ all of which can be obtained analogously.

Therefore at low orders of N the amount of work in partial reduction, when applicable, is significantly lower than for full reduction which comes at the price of having still to perform a quantum reduction of the $\tilde{C}_a^{(N)}$. At higher orders the difference in the amount of work involved becomes insignificant so that a full reduction seems preferable.

7 Conclusion and outlook

The present project was partly motivated by the desire to understand the seminal work [5] from a broader perspective. In [5] an elegant approach to classical and quantum (partially, i.e. with respect to the non-homogeneous gauge transformations) gauge invariant second order cosmological theory including backreaction is developed. The intention of the present study was to extract the symplecto-geometric origin of the methods developed in [5] with the aim to generalise them to higher orders, different symmetries and more general gauge systems. In fact, the generalisation of (cosmological) perturbation theory to higher orders is a much debated subject and to the best of our knowledge there is no conclusion in the literature how to proceed, the challenge being to define a perturbative notion of gauge invariance [6, 7].

We were intrigued by the fact that in [5] sophisticated canonical transformations are employed in order to generate gauge invariant variables which at least in part of its variables strongly reminded us of the first few terms in the Taylor expansion of relational Dirac observables [3]. In fact, we used the relational approach before [11] but using additional matter that is designed to drastically simplify the occurring tasks listed below and to arrive at an exact solution.

We believe that the present work at least partly succeeded in unveiling the broader structure underlying the work of [5]. The central ingredients are as follows:

1.
Starting from a physically motivated Killing symmetry, one can naturally split the symplectic structure into a symmetric and a non-symmetric sector.
2.
The first class constraints of the underlying constraints also naturally split into “symmetric” and “non-symmetric” subsets corresponding to a split of the tensors smearing those constraints.
3.
One then further splits the degrees of freedom into pure gauge and true degrees of freedom respectively. That additional split is less canonical, the only requirement being that the gauge degrees of freedom allow to gauge fix the constraints. This yields altogether four sets: symmetric or non-symmetric gauge degrees of freedom and symmetric or non-symmetric true degrees of freedom.
4.
As is well known, in that situation one may pass *in principle* to the reduced phase space. This step requires solving the constraints, the gauge fixing conditions and the stability conditions on the gauge fixings for the Lagrange multipliers (smearing function). For sufficiently complicated gauge systems, this step cannot be carried out exactly. The observation is (see theorem 4) that precisely in the presence of the symmetry one may solve

these three sets of equations perturbatively where we identify the perturbations with the non-symmetric degrees of freedom. Responsible for this is that the symmetry imposes that the first order of the symmetric constraint and the zeroth order of the non-symmetric constraint vanish identically on the full phase space. This allows to establish a well defined hierarchy of equations which can be solved iteratively and explicitly.

5.

One may use the reduction process of 4. in two versions, the fully gauge invariant version and the partially gauge invariant version. They turn out to be of similar complexity. In the full version, all constraints, symmetric and non symmetric, are reduced in a single step. The non-trivial task is then to develop the perturbation theory of the reduced (or physical) Hamiltonian. In the partial version, only a subset of the constraints are reduced. These are in general not just the non-symmetric constraints because these generically lack the important feature of forming a Poisson subalgebra even before perturbing them. The first non-trivial step is therefore to pass to an equivalent set of symmetric and non-symmetric constraints. After the corresponding partial reduction, the remaining task is to develop the perturbation theory for the accordingly reduced remaining symmetric constraints which in their exact version are exactly partially gauge invariant with respect to the non-symmetric constraints. It is the partial version that is the direct analog of [5] and when considering the second order of our approach we find exact match with results of [5].

We may apply the general theory developed in this work, among others, to the following tasks:

i. Higher order cosmological perturbation theory

We have written out all perturbative and iterative formulae for a general gauge system in sections 4, 5 and 6 and in principle one just has to specialise them to the system and the order that one is interested in. What one needs are the usual perturbative expansions of the constraints but its ingredients have to be combined in a non standard way in order that gauge invariance be maintained. Of particular importance is for instance third order cosmological perturbation theory with an eye towards non-Gaussianities [25] and the needed expressions in Hamiltonian language are already available [26].

ii. Spherically symmetric black holes

There is a rich literature on spherically symmetric spacetimes and their perturbations [9]. To the best of our knowledge, this has not been done yet including backreaction and also only to second order which is technically already quite challenging. If these backreaction formulae are worked out one would in principle be able to study quantum backreaction in Hawking radiation, perhaps even black hole evaporation [27]. As in this case the partial reduction would leave still an infinite number of constraints, given the complications that we have pointed throughout the paper regarding quantisation, one would prefer here the fully reduced approach. We have recently started this programme in [14].

iii. Axi-symmetric black holes

What we have said about Schwarzschild type black holes literally also applies to axi-symmetric (Kerr type) black holes [10].

iv. Quantum Backreaction

This paper and most of the literature is concerned with classical backreaction. In [28] we have developed an approach to quantum backreaction based on quantum mechanical space adiabatic perturbation theory (SAPT) [29] which is a perturbative expansion in addition to that with respect to the non-symmetric degrees of freedom, it is based on a mass hierarchy which typically makes the symmetric degrees of freedom “slower” than the “faster” non-symmetric ones. It seems natural to extend the ideas of [28] to the black hole context. A challenge will be to extend the Moyal product techniques of [29] to the case (black holes) that the slow sector is still a field theory rather than a quantum mechanical system as in the case of cosmology. Also, as pointed out in [5] as well as in [28], additional canonical transformations on the full phase space are generically required in order to allow for Fock type quantisations of the non-symmetric fields because masses and couplings of the fast fields are generically non-constant functions of the slow fields which calls for Hilbert-Schmidt type of conditions.

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