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On the Relation between Operator Constraint –, Master Constraint –, Reduced Phase Space – and Path Integral Quantisation

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Abstract

Path integral formulations for gauge theories must start from the canonical formulation in order to obtain the correct measure. A possible avenue to derive it is to start from the reduced phase space formulation. In this article we review this rather involved procedure in full generality. Moreover, we demonstrate that the reduced phase space path integral formulation formally agrees with the Dirac's operator constraint quantisation and, more specifically, with the Master constraint quantisation for first class constraints. For first class constraints with non trivial structure functions the equivalence can only be established by passing to Abelian(ised) constraints which is always possible locally in phase space. Generically, the correct configuration space path integral measure deviates from the exponential of the Lagrangian action. The corrections are especially severe if the theory suffers from second class secondary constraints. In a companion paper we compute these corrections for the Holst and Plebanski formulations of GR on which current spin foam models are based.

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1 Introduction

Path integrals for scalar Quantum Field Theories (QFT) on Minkowski space are supposed to compute the S – Matrix for the Hamiltonian in question. A standard Folklore says that heuristically one should simply consider all “paths” between some initial and final scalar field configuration on a spatial hypersurfaces labelled by moments of time t_i, t_f respectively and integrate over the exponential of (i times) the action with “Lebesgue measure” in order to obtain the evolution kernel. More specifically, let Ω be a (normalised) ground state (provided it exists) for the Hamiltonian H on a Hilbert space \mathcal{H} , let Q be the configuration space of spatial scalar field configurations with “configuration Lebesgue measure” dq , let $Q_{t_i, t_f} = \times_{t \in [t_i, t_f]} Q$ be the set of paths, let $[Dq] = \prod_{t \in [t_i, t_f]} dq_t$ the “path Lebesgue measure”, then

$$\langle \psi_f, e^{i(t_f - t_i)H/\hbar} \psi_i \rangle_{\mathcal{H}} = \frac{\int_{Q_{t_i, t_f}} [Dq] \overline{\psi_f[q(t_f)]} \psi_i[q(t_i)] e^{iS_{t_i, t_f}[q, \dot{q}]/\hbar}}{\int_{Q_{t_i, t_f}} [Dq] \overline{\Omega[q(t_f)]} \Omega[q(t_i)] e^{iS_{t_i, t_f}[q, \dot{q}]/\hbar}} \quad (1.1)$$

and S_{t_i, t_f} is the classical (Lorentzian) action integrated over the time interval $[t_i, t_f]$. Here by Lorentzian action we mean the Legendre transform

$$S[q, \dot{q}] := \text{extr}_p \left\{ \int_{t_i}^{t_f} dt [p\dot{q} - H(p, q)] \right\} \quad (1.2)$$

where p denotes the momentum conjugate to q and H the Hamiltonian. This “theorem” is wrong for several reasons.

First of all, from the mathematical point of view, there is no Lebesgue measure on infinite dimensional spaces. Therefore one would like to consider $[DQ] \exp(iS/\hbar)$ as a (complex) measure on Q but this does not work because the modulus of a complex measure [2] is supposed to be normalisable which is obviously not the case here. If the Hamiltonian is bounded from below, it is therefore much more promising to consider, instead of the unitary group $\mathbb{R} \rightarrow \mathcal{B}(\mathcal{H}); t \mapsto \exp(itH/\hbar)$ the contraction semigroup $\mathbb{R}_+ \rightarrow \mathcal{B}(\mathcal{H}); t \mapsto \exp(-tH/\hbar)$. Here $\mathcal{B}(\mathcal{H})$ denotes the algebra of bounded operators on \mathcal{H} . Under these circumstances another Folklore theorem states that

$$\langle \psi_f, e^{-(t_f - t_i)H/\hbar} \psi_i \rangle_{\mathcal{H}} = \frac{\int_{Q_{t_i, t_f}} [Dq] \overline{\psi_f[q(t_f)]} \psi_i[q(t_i)] e^{-S_{t_i, t_f}^E[q, \dot{q}]/\hbar}}{\int_{Q_{t_i, t_f}} [Dq] \overline{\Omega[q(t_f)]} \Omega[q(t_i)] e^{-S_{t_i, t_f}^E[q, \dot{q}]/\hbar}} \quad (1.3)$$

where now S_{t_i, t_f}^E denotes the “Euclidean” action, that is, the Legendre transform¹

$$S^E[q, \dot{q}] := \text{extr}_p \left\{ \int_{t_i}^{t_f} dt [ip\dot{q} - H(p, q)] \right\} \quad (1.4)$$

While even under these circumstances the partition function

$$Z := \int_Q [Dq] e^{-S^E/\hbar} \overline{\Omega[q(t_f)]} \Omega[q(t_i)] \quad (1.5)$$

diverges, under fortunate circumstances it is possible to assign to $e^{-S^E} [Dq] / Z$ a well defined measure theoretic meaning on a proper σ –algebra \mathcal{Q} (with respect to which S^E is usually not even measurable). Whenever (1.3) can be made rigorous, it is called the Feynman – Kac formula [3, 4].

However, as it is well known [5], also from the physical point of view, (1.1) or (1.3) are wrong in general. This is because the strict derivation (see e.g. [6]) of, say (1.3) requires a skeletonisation of the time interval $[t_i, t_f]$ and

¹Usually one obtains the Euclidian action by Wick rotation $t \rightarrow it$. However, we insist on this definition because it does not rely on an analytic structure of the fields in the time coordinate which is not justified anyway. Our definition is formally correct also in circumstances where the Hamiltonian is not only quadratic in the momenta with constant coefficients, see below.

corresponding resolutions of the identity in terms of (generalised) position and momentum eigenvectors. That is to say, a priori one has to consider the complex hybrid action

$$S^C[q, p] := \int_{t_i}^{t_f} dt[ip\dot{q} - H(p, q)] \quad (1.6)$$

which is integrated over both momentum and configuration coordinates. If H depends on p only quadratically with constant coefficients, then one can perform the Gaussian integral and up to an (infinite) constant which drops out in the fraction (1.3) one arrives at the Folklore result. However, in more general situations the result is different. For instance, the Hamiltonian could still be quadratic in p but with q dependent coefficients which leads to a nontrivial modification of the “measure” $[Dq]$. More generally, however, the Hamiltonian may not be quadratic or even analytic in p in which case an exact configuration space path integral representation is not available, only a saddle point approximation is available (plus the corresponding perturbative treatment of the non Gaussian corrections). Notice that the saddle point approximation and subsequent integrating out of the momentum variables reproduces (1.4) up to a non trivial measure factor.

So far we have only considered scalar QFT on Minkowski space and even here we saw that the only correct derivation of the path integral proceeds via the Hamiltonian formulation, as stressed for instance in [5]. Additional technical and conceptual complications arise when we consider gauge theories and/or other background spacetime metrics. The simplest problem occurs for Yang – Mills type of gauge theories: Here the action is gauge invariant and if the measure is anomaly free (is gauge invariant as well) then one should divide by the (in general infinite) volume of the gauge group in order to give sense to both numerator and denominator in (1.3). If one considers QFT on non stationary background spacetimes then no natural Hamiltonian and vacuum exists [7] and the conceptual status of the path integral as a means to calculate scattering amplitudes becomes veiled. Even more veiled the situation becomes for totally constrained systems such as General Relativity on spatially compact four manifolds admitting globally hyperbolic metrics when there is no true Hamiltonian at all. In this case certainly also the notion of a Wick rotation breaks down which on Minkowski space allows to reconstruct the Lorentzian Wightman functions from the Euclidian Schwinger functions via the Osterwalder – Schrader reconstruction theorem [1]. Parts of the reconstruction theorem, namely the construction of a Hamiltonian and a Hilbert space from a measure satisfying a natural background independent generalisation of the OS axioms, can be generalised to background independent theories [8].

It transpires that especially in the context of realistic physical theories, that is, General Relativity coupled to (standard) matter, it is neither clear what the heuristic Ansatz (1.1) or (1.3) computes nor whether it is the correct formula for what it is supposed to do. One possibility to deal with these problems is to try to solve the constraints classically and then to quantize the reduced phase space equipped with the (pull back of the) Dirac bracket [6]. This can be done in two ways. The first option is to impose suitable gauge fixing conditions in order to render the system totally second class and then to quantize the corresponding pull back of the Dirac bracket together with the induced reduced Hamiltonian. The second option is to determine explicitly a sufficient number of Dirac observables and to quantise the symplectic structure induced by the Dirac bracket. While for rare examples independent means exist to determine those gauge invariants, for most systems the only practical way to determine a sufficient number of Dirac observables is via a choice of gauge fixing. Namely, as we will review in the next section (see also e.g. the appendix in the second reference of [10]), there is a one to one correspondence between a choice of gauge fixing and a preferred set of gauge invariant functions which generate the full algebra of gauge invariant functions. In that sense the two methods, gauge fixing and this so called relational approach, are completely equivalent. The method is physically very interesting because it not only provides a suitable algebra of gauge invariant objects but also a gauge invariant Hamiltonian which drives the time evolution of those invariants. Here the question of equivalence between different choices of gauge fixing arises. As we will review in the next section, the preferred algebras of invariants that one obtains via different choices of gauge fixing are isomorphic. Of course they differ in their physical interpretation but as Poisson algebras they are isomorphic, the physical quantum kinematics is not affected by the choice of gauge

fixing. The difference arises in the physical Hamiltonian, that is, in the quantum dynamics. The explicit form of the physical Hamiltonian as a function of the invariant generators of the algebra of gauge invariant functions depends absolutely sensitively on the choice of gauge fixing and therefore even classically the evolution of the invariants will differ drastically from each other for different choices. For some choices the Hamiltonian may be explicitly time independent and leads to a conservative reduced system, for others it may not be. Even more crucial the choice of gauge fixing becomes in the quantum theory. Already for finite dimensional systems, depending on the choice of gauge fixing the physical Hamiltonian and other composite invariants built from the generators of the gauge invariant algebra may have discrete or continuous spectrum [9]! Notice that we here talk about composite invariants that have the interpretation of a given non invariant f measured in terms of another non invariant T (the so called clock). If we change T to T' then its spectrum may switch from continuous to discrete or vice versa even though we talk about the same f and about the same Hilbert space representation!. In infinite dimensional situations the choice of gauge fixing has an even stronger influence for not only do we have to find a representation of the generators of the algebra of observables but in addition that algebra should support the physical Hamiltonian. One way to read Haag's theorem [11] is that Hamiltonians with different interaction terms cannot be implemented on the same Hilbert space. Thus generically different choices of gauge fixing will force us to choose different representations. For instance one may want to construct a cyclic representation built from application of the generators to a vacuum (ground state of the Hamiltonian). That vacuum of course depends on the Hamiltonian and even for free field theories those cyclic representations are typically unitarily inequivalent. In case that the physical Hamiltonian is explicitly time dependent, one is in addition confronted with the usual problem of QFT on curved spacetimes, namely that one has to decide at which point of time one wants to select a vacuum vector.

All of this certainly strongly affects the resulting reduced phase space path integral because it is based on the selected Hilbert space representation and the transition amplitudes between physical states do depend on the physical Hamiltonian. For any such choice, the path integral then does have the interpretation of (1.1) or (1.3) in terms of the reduced Hamiltonian.

An additional complication that we have not mentioned yet is the case of a system with second class constraints. Such a system is to be canonically quantised with respect to the Dirac bracket rather than the Poisson bracket. Typically the Dirac bracket destroys the canonically conjugacy of the global coordinates of the phase space that one started from. Since to find representations of such complicated Poisson algebras is usually prohibitively difficult one is forced to switch to local Darboux coordinates (by means of a canonical transformation with respect to the original Poisson bracket) which is always possible locally [6]. Such coordinates may be very difficult to find in practice. Assuming this to have done nevertheless, one can then construct the reduced phase space using a choice of gauge fixing as already described above and after having chosen a Hilbert space representation subordinate to that gauge fixing, the transition amplitudes in terms of the induced physical Hamiltonian.

From here on then mostly one proceeds rather formally. One assumes that one can choose a Schrödinger representation based on the reduced Darboux configuration space. By using well known skeletonisation techniques one then basically writes the transition amplitude between initial and final states Ψ_i, Ψ_f , as a path integral over the reduced Darboux phase space, replacing the reduced Hamiltonian operator by its classical function which results in the exponential of the reduced Hamiltonian Darboux action. In order to make contact with (1.1) one wants to rewrite this path integral as a path integral over the unreduced, original configuration space and in terms of the original Lagrangian. As is well known, this can be formally done and we will review this rather involved procedure in section 3. Basically one first extends the reduced Darboux phase space to the unreduced Darboux phase space thereby introducing δ distributions of the constraints and the gauge fixing condition as well as measure factors which cancel the Jacobian that arises when solving the δ distributions. One then observes that, in presence of the δ distributions the reduced Hamiltonian action can be written as the unreduced symplectic potential, in terms of the unreduced Darboux coordinates. Interestingly, the measure factors and the δ distributions combine in just the right way as to make the resulting expression

independent of the gauge fixing condition when considered as a measure on gauge invariant functions. This is similar to the Fadeev – Popov theorem [6] and we will review this result in section 3. This seems to be in contradiction to what we have said above about the dependence of the transition amplitudes on the gauge fixing condition. The resolution is that at this point the integral is *not* over gauge invariant functions, it is an integral over $\Psi_i \overline{\Psi}_f$ which are functions at initial and final points of time of the reduced Darboux coordinates which are not gauge invariant. More generally, in applications to scattering theory, we may be interested also in n-point functions so that the path integral is over functions of the reduced Darboux coordinates also at intermediate times (in fact we will use the method of a generating functional so that there is a dependence on the reduced Daroux coordinates *at all* times). One may, in the presence of the δ distributions, extend the non gauge invariant, reduced Darboux coordinates to gauge invariant functions which use the chosen gauge fixing condition. However, these extended functions now display a complicated dependence on all unreduced Darboux coordiantes which makes this extension practically useless. Even if one did perform the extension, while one can now change the dependence on the gauge fixing condition in the measure, one cannot get rid of it in the gauge invariantly extended functions². In any case, one next performs the canonical transformation that leads from the Darboux coordinates back to the original canonical coordinates which does not affect the symplectic potential and the Liouville measure but it affects the initial and final states. Then one exponentiates the δ functions and, by the technique introduced in [12], gets rid of the secondary second class constraints which leads to further changes in the measure. Finally, one integrates out the momenta. This is only possible if the reduced Darboux configuration coordinates, as functions of the original canonical coordinates, do not depend on the original momenta and if they do not leads in general to further changes in the measure while now the exponential of the covariant Lagrangian action appears.

The point of mentioning these in principle well known facts is twofold. The first is that we wish to stress that even if all the assumptions that we have listed can be verified, the correct Langragian configuration space measure may differ drastically from the naive one in (1.1). These deviations depend crucially on the dynamical content of the theory and cannot be discarded. The second point that we want to make is the dependence of the transition amplitudes on the chosen gauge fixing. This dependence is at first astonishing because one is used from Yang – Mills theory that the path integral does not depend on the gauge fixing and it even sounds dangerous because it seems as if this dependence implies that gauge invariance is broken. However, this is not the case: The dependence on the gauge fixing *is physically correct*. The reason is that in generally covariant systems the dynamics mixes with gauge invariance. In Yang – Mills theory this is not the case, there one has a gauge invariant Hamiltonian at one’s disposal which is not generated by a gauge fixing condition, it is simply there without further input. Gauge invariant functions in Yang – Mills theory can also be easily constructed without ever mentioning any gauge fixing, for instance Wilson loops or flux tubes between quarks. The gauge fixing condition comes in only when cancelling an otherwise infinite constant. This introduces a gauge fixing δ distribution and a Fadeev – Popov determinant into the measure whose combination is independent of the gauge fixing by construction, similar as in our discussion above. In contrast, in generally covariant systems a gauge fixing condition can be seen as *defining a preferred algebra of observables and a preferred dynamics thereof*. Gauge invariance is not at all broken, the dynamical system consisting of reduced Darboux phase space and reduced Hamiltonian as defined by a gauge fixing is in one to one correspondence with a dynamical system consting of a preferred algebra of Dirac observables and a gauge invariant physical Hamiltonian defined via the same gauge fixing (now interpreted as a choice of clocks). The two descriptions are equivalent. The gauge fixing dependence comes in because one needs a gauge fixing in order to arrive at the very notion of a dynamics, or in other words, at the very notion of an observer. This observer dependence of the classical and quantum theory has already been stressed in [13] and will be discussed in more detail in [14]. Let us stress again, as we have already said, that similar

²A special situation arises if one considers gauge transformations that tend to the identity in the infinite past and future and that the only non gauge invariant functions in the path integral are located at the infinite past and future. This is not the case for the n-point functions or the generating functional but for the rigging kernel between two kinemtical states. Now the dependence on the gauge fixing formally disappears from the path integral, of course modulo the representation theoretic caveats that we have mentioned.

as in Yang – Mills theories the gauge fixing dependence of the *measure* disappears when we restrict it (as a linear functional) to gauge invariant functions. However, the choice of those gauge invariant functions themselves and the corresponding physical Hamiltonian, in other words the physical interpretation of the theory, induced by a choice of gauge fixing (clock) is what makes the description gauge choice dependent. In contrast, in Yang – Mills theories such a choice of clocks is not necessary in order to arrive at useful gauge invariant functions. In principle, the generators of the algebra of gauge invariant functions for one choice of gauge fixing can be written as complicated functions of the generators for any other choice. However, this involves an infinite series of commutator functions about whose convergence nothing is known and which therefore is practically useless if not mathematically ill –defined.

In this paper we want to illustrate the complications sketched above for a general theory which will be the first result of this paper. While certainly bits and pieces of our description appear in various places in the literature, we hope that assembling them in the form presented here may add a certain amount of clarity to the question how reduced phase space and path integral quantisation fit together.

The second result of this paper will be to sketch how the path integral is related to Dirac’s operator constraint quantisation [15] and a particular incarnation of it, the so called Master Constraint Programme [16] for first class systems. As already mentioned, the reduced phase space rarely admits a global Darboux coordinate system and hence a quantisation of the unreduced phase space is much simpler. The price to pay is that one has to impose them as non –anomalous operators on that Hilbert space in order to compute the physical Hilbert space. There are certain heuristic group averaging methods [17] available in the literature which, as the name suggests, apply when the constraints form a Lie algebra. If they do not (structure functions), then not only are the constraints difficult to define without anomalies because of factor ordering difficulties but also group averaging is not applicable. It is for that reason that the Master Constraint Programme (MCP) was introduced. In the MCP, all constraints are encoded into one single Master constraint. The Master Constraint is a classically equivalent platform and is automatically free of anomalies so that group averaging (or direct integral decomposition) methods apply.

The central ingredient of the group averaging method is a (generalised) “projector” (or rigging map) from the kinematical Hilbert space into the physical one, equipped with an associated physical inner product. It can be expressed in terms of a path integral which in case of a true Lie algebra is readily recognised as (1.1) or (1.3) respectively. In case of the Master constraint that can also be established, however, the proof is somewhat more involved. Not surprisingly, the key to the understanding of how all of these methods fit together is how the reduced phase space description arises from the constraints and a suitable gauge fixing condition which in turn allows for a local Abelianisation of the constraints. It may seem astonishing that the gauge fixing condition enters the interpretation of the physical Hilbert space in such a prominent way. The reason for why that happens is that the physical Hilbert space can be considered as the closure of the set of vectors that one obtains by applying the algebra of gauge invariant observables to a cyclic physical state. However, the construction of that algebra and the interpretation of its elements is facilitated by considering the gauge invariant extension of the kinematical algebra as induced by a gauge fixing condition. In other words, while in the operator constraint method one only deals with manifestly gauge invariant objects, their interpretation again relies on a gauge fixing condition or equivalently on a choice of rods and clocks. Different such choices result in the same algebra but its generators (elementary observables) differ for each choice.

To summarise:

The correct path integral formula and its interpretation can only be obtained by following the Hamiltonian path, otherwise one misses important corrections to the measure. In the context of spin foam models [18] for Loop Quantum Gravity [19] this has been pointed already in [20] (see also [21, 22]). The corrections to the measure are not manifestly covariant as first indicated in [23] but seem to be required in order to maintain at least some form of spacetime

covariance as claimed in [24]. They should therefore be taken seriously in any realistic spin foam model for General Relativity. Work is now in progress which tries to implement these corrections. See also [22] where the covariance of the path integral with respect to the Bergmann – Komar group is discussed.

This article is organised as follows.

In section two we review Dirac’s analysis of gauge systems and the relation between gauge fixing and a gauge invariant description.

In section three we derive the path integral from the quantisation of the reduced phase space based on the natural generators of the algebra of invariants defined by a choice of gauge fixing conditions.

In section four we derive the same path integral starting from the unreduced (with respect to the first class constraints) phase space and implement the rigging map. In case that the first class algebra of constraints involves structure functions, using the rigging map technique requires to pass to new constraints that form an algebra. This is always (locally) possible because one can always (locally) Abelianise constraints.

In section five we use as an alternative route the MCP and show that again one arrives at the same path integral. This is to be expected because both constraint rigging and Master constraint rigging should provide the generalised projector on physical states, however, the technical mechanism by which this works is somewhat involved.

Finally in section six we summarise and conclude.

2 Classical Preliminaries: Gauge Fixing Versus Gauge Invariant Formulation

In an attempt to make this article self – contained we start with the classical theory. We will need the corresponding notation anyway for the path integral formulation. First we summarise the main ingredients of Dirac’s algorithm. Then we display the relation between the reduced phase space of gauge invariant observables and the pull back phase space as induced by a gauge fixing. As we will see, the two formulations are equivalent for suitable choices of gauge fixing.

2.1 Brief Review of Dirac’s Algorithm

We consider a theory with Lagrangian $L(q^a(t), v^a(t))$ and corresponding action

$$S = \int_{[t_1, t_2]} dt L(q^a(t), v^a(t)) \quad (2.1)$$

Here the index a takes values in a general set which may comprise discrete and/or continuous labels. We are interested in a theory with gauge symmetries so that the Lagrangian will be singular, that is, we cannot solve all the velocities $v^a = \dot{q}^a$ for the canonical momenta

$$p_a := \frac{\partial L}{\partial v^a} \quad (2.2)$$

By solving a maximal number of velocities v^α (whose number is equal to the rank of the matrix $\partial^2 L / \partial v^a \partial v^b$), i.e. a maximal number of the equations (2.2), in terms of the momenta p_α and the remaining velocities v^i , that is, $v^\alpha = v^\alpha(q^a, p_\alpha; v^i)$ such that $(v^\alpha) = (v^\alpha, v^i)$ (i.e. the indices α and i take values in index sets that partition the index set associated with a) we obtain the primary constraints

$$C_i = p_i - \left[\frac{\partial L}{\partial v^i} \right]_{v^\alpha = v^\alpha} \quad (2.3)$$

which does not depend on the v^i by assumption of the maximality of the v^α and contain the p_i only linearly. The canonical Hamiltonian (total Hamiltonian)

$$H_T = [v^\alpha p_\alpha - L(q, v)]_{v^\alpha = u^\alpha} \quad (2.4)$$

always has the structure [15, 19]

$$H_T = H'_0(q, p) + v^i C_i(q, p) \quad (2.5)$$

that is, it is an affine function of the v^i .

The further analysis of the system is now governed by Dirac's algorithm [15]:

One requires that the constraints are preserved by the Hamiltonian flow of H_T . Whenever $\{H_T, C_i\} = 0$ is not satisfied on the constraint surface, there are two possibilities: Either 1. $\{H_T, C_i\}$ does not involve the velocities v^i or 2. it does. In the first case we must add $\{H_T, C_i\}$ to the list of constraints in the second we solve all the equations of type 2 for some of the velocities v^i (assuming that the system of equations is not overdetermined). Iterating like this, one ends up, in general, with further constraints C_I , which are called secondary constraints, and the velocities are restricted to be of the form $v^i = v_0^i(q, p) + \lambda^m v_m^i(q, p)$. Here $v^i = v_0^i$ solves $\{H_T, C_j\} = \{H_c, C_j\} = 0$ for all j, J on the constraint surface $\{C_j = C_J = 0 \forall j, J\}$ and $(v_m^i)_m$ is a maximal linearly independent set of solutions of the system $v^i \{C_i, C_j\} = v^i \{C_i, C_J\} = 0$ for all j, J (on the constraint surface). The coefficients λ_m are free and phase space independent.

It follows that the

$$F_m := v_m^i C_i \quad (2.6)$$

are first class constraints, i.e. they weakly (i.e. on the constraint surface) Poisson commute with all constraints. By taking linear combinations of the constraints C_i, C_I (with phase space dependent coefficients) we isolate a maximal number of first class constraints. The constraints F_m are called primary first class constraints, the additional ones F_M are called secondary first class constraints. The remaining constraints among the set (C_i, C_I) which are linearly independent of the set $(F_\mu) := (F_m, F_M)$ are called second class constraints and are denoted by (S_Σ) .

The canonical Hamiltonian can now be written

$$H_T = H'_0 + \lambda^m F_m \quad (2.7)$$

where

$$H'_0 = H_0 + v_0^i C_i \quad (2.8)$$

is of first class by construction. It may therefore be an affine function of the F_μ (with phase space dependent coefficients)

$$H'_0 = H_0 + f^\mu F_\mu \quad (2.9)$$

The piece H_0 is referred to as the true Hamiltonian because it is not constrained to vanish. In totally constrained systems such as General Relativity it vanishes identically, that is, the canonical Hamiltonian is a linear combination of first class constraints. Notice that only the primary first class constraints appear in the canonical Hamiltonian with arbitrary coefficients λ^m and so one would associate gauge invariance only with respect to them. However, this is in general inconsistent because the Poisson algebra of primary first class constraints generically does not close, only the full set of first class constraints always does. In other words, since the Poisson bracket between two first class functions is first class and if O is weakly invariant under the F_m then also $2\{F_{[m}, \{F_n], O\}\} = \{\{F_m, F_n\}, O\}$ should be weakly zero. Furthermore, the time evolution of O with respect to H_c should be gauge invariant which gives

$$\{F_m, \{H_T, O\}\} = -\{H_T, \{O, F_m\}\} - \{O, \{F_m, H_T\}\} \approx \{\{F_m, H'_0\}, O\} \approx 0 \quad (2.10)$$

Hence gauge invariant quantities should be those that weakly Poisson commute with the minimal subset of first class constraints generated by the Poisson brackets between the $\{H_T, F_m\}$ (and higher order brackets with H_T) and between

the first class primary constraints among each other. For most systems of physical interest this exhausts all first class constraints and we will assume this to be the case here. In that situation the piece H''_0 of the Hamiltonian in (2.9) will therefore generically contain all secondary first class constraints as well, that is, the corresponding phase space functions f'' will be non – vanishing. See [6, 27, 28] for a discussion when this so called Dirac conjecture can be proved.

As far as the second class constraints are concerned, they are not associated with any gauge freedom. It is in fact inconsistent in general to require an observable to satisfy $\{S_\Sigma, O\} \approx 0$ as an application of the Jacobi identity reveals. This means that observables are not first class functions, they only have to weakly Poisson commute with the first class constraints, not with the second class constraints. Hence, to solve the second class constraints we simply have to restrict ourselves to the corresponding constraint surface. In other words, once we have computed the functions on phase space which have weakly vanishing Poisson brackets with all first class constraints, we should restrict them to the constraint surface defined by the second class constraints only. The induced symplectic structure between such observables f, f' on the total constraint surface is simply the pull back of the symplectic structure on the unconstrained phase space by the embedding of the constraint surface defined by the second class constraints into the full phase space. More precisely, let \mathcal{P} denote the unconstrained phase space and $\overline{\mathcal{P}} := \{m \in \mathcal{P}; S_\Sigma(m) = 0 \forall \Sigma\}$ the constraint surface defined by the second class constraints. Consider the corresponding embedding $J : \overline{\mathcal{P}} \rightarrow \mathcal{P}$. If Ω denotes the symplectic structure on \mathcal{P} then $\Omega^- := J^*\Omega$ denotes the pull – back symplectic structure on $\overline{\mathcal{P}}$. This is again a symplectic structure because it is closed and non degenerate which follows from the fact that the matrix

$$\Delta_{\Sigma\Sigma'} := \{S_\Sigma, S_{\Sigma'}\} \quad (2.11)$$

is non degenerate. The corresponding Poisson bracket is given by

$$\{J^*f, J^*f'\}^- = J^*\{f, f'\}^* \quad (2.12)$$

where

$$\{f, f'\}^* := \{f, f'\} - \{f, S_\Sigma\} (\Delta^{-1})^{\Sigma\Sigma'} \{S_{\Sigma'}, f'\} \quad (2.13)$$

denotes the Dirac bracket on the full phase space. We will prove this for the convenience of the reader in the next section.

The reduced phase space is defined by the Poisson algebra of gauge invariant observables, which are not weakly vanishing (i.e. which are not linear combinations of first class constraints) equipped with the pull-back of the Dirac bracket to the constraint surface defined by the second class constraints. Notice that the Dirac bracket generically changes the symplectic structure for the observables as compared to the Poisson bracket. However, it does not change the equations of motion defined by the canonical Hamiltonian as the Dirac bracket and the Poisson bracket between two functions coincide whenever at least one of them is a first class function.

2.2 Reduced Phase Space and Gauge Fixing

In principle the description of the previous subsection entails the complete information about the dynamics and the physical (gauge invariant) content of the theory. However, it does not provide an explicit description of the observables. Moreover, in totally constrained systems the equations of motion for the observables with respect to the canonical Hamiltonian are trivial which means that some important ingredient is missing in that case: A non vanishing physical Hamiltonian which drives the time evolution of the observables. In this section we give an explicit construction of the reduced phase space, provide a physical Hamiltonian and display the relation of our framework to gauge fixing.

We saw that we eventually obtain a constrained Hamiltonian system with first class constraints F_μ and second class

constraints S_Σ on a phase space with canonical pairs (q^a, p_a) , $a = 1, \dots, n$; $m \leq n$ with respect to the original Poisson bracket. As shown in [27], there always exists a local canonical transformation (with respect to the Poisson bracket) from the canonical pairs (q^a, p_a) to canonical pairs (Q^A, P_A) , (ϕ^μ, π_μ) , (x^σ, y_σ) such that

$$S_\Sigma = 0 \Leftrightarrow z_\Sigma = 0 \quad (2.14)$$

where the index σ takes half the range of that of Σ and where we denoted either x^σ or y_σ by z_Σ for some value of Σ . It is then clear that at least weakly the Dirac bracket and the Poisson bracket coincide on the (Q, P, π, ϕ) and that z has zero Dirac bracket with anything.

Next, if there is a true, gauge invariant Hamiltonian H_0 in (2.9) (not constrained to vanish) enlarge the phase space by an additional canonical pair (q^0, p_0) and additional first class constraint $F_0 = p_0 + H$. The reduced phase space and dynamics of the enlarged system is equivalent to the original one, hence we consider without loss of generality a system with no true Hamiltonian (totally constrained system). The canonical Hamiltonian of the system is then a linear combination of the first class constraints

$$H_T = \rho^\mu F_\mu \quad (2.15)$$

Here we have set $\rho^M = f^M$ for secondary first class constraints and $\rho^m = f^m + \lambda^m$ for primary first class constraints where f^μ is defined in (2.9).

A gauge fixing is defined by a set of gauge fixing functions G_μ with the property that the matrix with entries $M_{\mu\nu} := \{C_\mu, G_\nu\}$ has everywhere (on the unconstrained phase space) non vanishing determinant³. Notice that we allow for gauge fixing conditions that display an explicit time dependence. The conservation in time of the gauge fixing conditions

$$0 = \frac{d}{dt}G_\mu = \frac{\partial}{\partial t}G_\mu + \{H_c, G_\mu\} \approx \frac{\partial}{\partial t}G_\mu + \rho^\nu M_{\nu\mu} \quad (2.16)$$

uniquely fixes the ‘‘Lagrange multipliers’’ to be the following phase space dependent functions

$$\rho^\mu = -\frac{\partial G_\nu}{\partial t} (M^{-1})^{\nu\mu} =: \rho_0^\mu \quad (2.17)$$

At this point one may be puzzled by the following issue: The functions ρ^μ already depend on the phase space through f^μ . For the ρ^m we can always solve (2.17) for the free function λ^m . But for the ρ^M the solution (2.17) leads to a consistency condition on the already imposed gauge fixing conditions, in other words we should impose independent gauge fixing conditions only for the primary first class constraints⁴. This is indeed true as far as fixing the free coefficients in the canonical Hamiltonian is concerned. However, in view of the fact that all first class constraints generate gauge transformations, one has to eventually reduce with respect to all their gauge motions. Therefore it is mathematically and physically equivalent and mathematically much more convenient to regard all ρ^μ as free parameters, that is, to drop the phase space dependence of the f^M . Hence to fix the gauge we need gauge fixing

³Ideally, the gauge $G_\mu = 0$ should define a unique point in each gauge orbit.

⁴As an example, in General Relativity the primary constraints demand that the momenta conjugate to lapse and shift vanish, the secondary constraints are the spatial diffeomorphism and Hamiltonian constraints respectively. All constraints are first class and the canonical Hamiltonian is a linear combination of all of them, in particular lapse and shift play the role of the f^M for the Hamiltonian and spatial diffeomorphism constraint respectively. A consistent gauge fixing would now be to first prescribe four functions purely built from the intrinsic metric and their conjugate momenta (independent of lapse and shift). Such conditions have vanishing Poisson brackets with respect to the primary constraints. Therefore equation (2.17) can be computed and prescribes lapse and shift as a function of intrinsic metric and conjugate momentum alone. The remaining four gauge fixing conditions for the velocities (Lagrange multipliers) of lapse and shift which are the coefficients of the primary constraints are now that they are the time derivatives (Poisson brackets with the canonical Hamiltonian) of the already prescribed functions for lapse and shift. These conditions are then consistent with the equations of motion, i.e. that the Lagrange multipliers are the time derivatives of lapse and shift. The corresponding matrix $\{F_\mu, G_\nu\}$ in this case is block diagonal. We could also have prescribed lapse and shift in the first place as functions of intrinsic metric and conjugate momentum and then would have to find four additional gauge fixing conditions on those variables whose equations of motion lead to the prescribed values of lapse and shift.

conditions for all first class constraints. We will see explicitly in the path integral formulation that one is forced to this point of view and that nevertheless one can restore the phase space dependence of the f^M when eventually reducing the path integral as one over configuration space (rather than the phase space). This will be detailed in section 3.3 where we will also see how it can be achieved that the original Lagrangian (which knows only about the primary constraints) is obtained in the exponent although one gauge fixes the secondary first class constraints as well.

By construction of the Dirac bracket, we can simply ignore the variables z for what follows and set them equal to zero where ever they occur. In terms of the remaining canonical pairs we can solve $F_\mu = G_\mu = 0$ for π_μ, ϕ^μ (and define the new constraint \tilde{F}, \tilde{G})

$$\tilde{F}_\mu := \pi_\mu + \tilde{h}_\mu(Q, P) = 0, \quad \tilde{G}_\mu := \phi^\mu - \tau^\mu(Q, P) = 0 \quad (2.18)$$

for certain functions \tilde{h}, τ which generically will be explicitly time dependent. The variables ϕ, π are called the gauge degrees of freedom and Q, P are called the true degrees of freedom (although typically neither of them is gauge invariant).

The reduced Hamiltonian $H_{\text{red}}(Q, P)$, if it exists, is supposed to generate the same equations of motion for Q, P as the canonical Hamiltonian does, when the constraints and the gauge fixing conditions are satisfied and the Lagrange multipliers assume their fixed values (2.17), that is,

$$\{H_{\text{red}}, f\} = \{H_{\text{can}}, f\}_{F=G=\rho-\rho_0=0} = [\rho_0^\mu \{F_\mu, f\}]_{F=G=\rho-\rho_0=0} \quad (2.19)$$

for any function $f = f(Q, P)$. For general gauge fixing functions the reduced Hamiltonian will not exist, the system of PDE's to which (2.19) is equivalent to, will not be integrable.

However, a so called coordinate gauge fixing condition $G_\mu = \phi^\mu - \tau^\mu$ with τ^μ independent of the phase space always leads to a reduced Hamiltonian as follows: We can always (locally) write the constraints in the form (at least weakly)

$$F_\mu = M_{\mu\nu}(\pi_\nu + h'_\nu(\phi, Q, P)) =: M_{\mu\nu} F'_\nu \quad (2.20)$$

where $\tilde{h}_\mu(Q, P) = h'_\mu(\phi = \tau, Q, P)$. Notice that the locally equivalent constraints F'_μ are actually Abelian by a general argument [6]. Then, noticing that $M_{\mu\nu} \approx \{F_\mu, G_\nu\}$, (2.19) becomes

$$\{H_{\text{red}}, f\} = [\rho_0^\mu M_{\mu\nu} \{h'_\nu, f\}]_{F=G=\rho-\rho_0=0} = [\dot{\rho}_\mu \{h'_\mu, f\}]_{G=0} = \{\dot{\rho}_I h'_I, f\} \quad (2.21)$$

with $\tilde{h}_\mu = h'_\mu(\phi = \tau, Q, P)$ and we used that f only depends on Q, P . This displays the reduced Hamiltonian as

$$H_{\text{red}}(Q, P; t) = \dot{\tau}^\mu(t) h_\mu(\phi = \tau(t), Q, P) \quad (2.22)$$

It will be explicitly time dependent unless $\dot{\tau}_I$ is time independent and h_μ is independent of ϕ , that is, unless those constraints can be deparametrised for which $\dot{\tau}_\mu \neq 0$. Hence, deparametrisation is crucial for having a conserved, reduced Hamiltonian system.

On the other hand, let us consider the gauge invariant point of view. Following the general framework [29, 30, 31, 32, 10, 33] it is possible to construct a gauge invariant extension of any gauge variant function $f(Q, P)$ off the gauge section $\phi = \tau$ by the following formula

$$O_f(\tau) = [\exp(\beta^\mu X_\mu) \cdot f]_{\beta=\tau-\phi} \quad (2.23)$$

where we have denoted the Abelian Hamiltonian vector fields X_μ by $X_\mu := \{\pi_\mu + h_\mu, \cdot\}$. It is easy to check that $\{O_f(\tau), F_\mu\} \approx 0$. Consider a one parameter family of flows $t \mapsto \tau^\mu(t)$ then with $O_f(t) := O_f(\tau(t))$ we find

$$\frac{d}{dt} O_f(t) = \dot{\tau}^\mu(t) \sum_{n=0}^{\infty} \frac{\beta^{\mu_1} \cdot \beta^{\mu_n}}{n!} X_\mu X_{\mu_1} \dots X_{\mu_n} \cdot f \quad (2.24)$$

On the other hand, consider $H_\mu(t) := O_{h_\mu}(\tau(t))$, then [32]

$$\begin{aligned} \{H_\mu(t), O_f(t)\} &= O_{\{h_\mu, f\}^*}(\tau(t)) = O_{\{h_\mu, f\}}(\tau(t)) = O_{X_\mu \cdot f}(\tau(t)) \\ &= \dot{\tau}^\mu(t) \sum_{n=0}^{\infty} \frac{\beta^{\mu_1} \cdot \beta^{\mu_n}}{n!} X_\mu X_{\mu_1} \dots X_{\mu_n} \cdot f \end{aligned} \quad (2.25)$$

Here the bracket $\{.,.\}^*$ denotes the Dirac bracket associated with the second class system (F_μ, G_μ) . In the second step we used that neither h_μ nor f depend on π_ν , in the third we used that f does not depend on ϕ^ν and in the last we used the commutativity of the X_ν . Thus the physical Hamiltonian that drives the time evolution of the observables is simply given by

$$H(t) := \dot{\tau}^\mu(t) h'_\mu(\tau(t), O_Q(t), O_P(t)) \quad (2.26)$$

where we used that (2.23) is a Poisson automorphism [32], that is,

$$\{O_f(\tau), O_g(\tau)\} = O_{\{f, g\}}(\tau) \quad (2.27)$$

Here $\{f, g\}^* = \{f, g\}$ for functions of Q, P only was exploited. This is exactly the same as (2.21) under the identification $f \leftrightarrow O_f(0)$. Hence we have shown that for suitable gauge fixings the reduced and the gauge invariant frameworks are equivalent. Notice that it was crucial in the derivation that (ϕ^μ, π_μ) and (Q^A, P_A) are two sets of canonical pairs. If that would not be the case, then it would be unclear whether the time evolution of the observables has a canonical generator.

The power of a manifestly gauge invariant framework lies therefore not in the gauge invariance itself. Rather, it relies on whether the gauge fixing can be achieved globally, whether it can be phrased in terms of separate canonical pairs, whether the observer clocks ϕ^μ are such that reduced Hamiltonian system is conserved and whether they do display the time evolution of observables as viewed by a realistic observer. See [10, 14] for a discussion of this point.

Our description sketched above shows that a useful, manifestly gauge invariant formulation implicitly also relies on a system of gauge fixing conditions. Namely, the gauge fixing conditions equip us first with a physical interpretation of the Dirac observables and second with a physical time evolution: $O_f(\tau)$ has the meaning of that relational observable, i.e. gauge invariant quantity, which in the gauge $\phi = \tau$ takes the value⁵ f . Its time evolution in terms of τ is driven by a gauge invariant Hamiltonian which arises by solving the constraints $F = 0$ in terms of the momenta π conjugate to ϕ . The gauge fixing condition thus prominently finds its way into the very interpretation of the physical (reduced) phase space. If we would choose different clocks ϕ' then different observables $O'_{f'}(\tau)$ would result. Due to (2.27), the algebra of the $O_f(\tau)$ among each other and of the $O'_{f'}(\tau)$ among each other respectively are isomorphic provided that f and f' only depend on the respective true degrees of freedom. In particular, both the $(O_{Q^A}(0), O_{P_A}(0))$ and $(O'_{Q'^A}(0), O'_{P'_A}(0))$ respectively provide a (local) system of coordinates on the reduced phase space and therefore one can translate between the two⁶. However, their physical interpretation and physical time evolution is entirely different. This crucial fact will also be reflected in the interpretation of the path integral.

Remark:

⁵One maybe tempted to run the following contradictory argument: $O_f(\tau)$ obviously coincides with f in the gauge $\phi = \tau$. Since it is also gauge invariant and since any other gauge can be reached from $\phi = \tau$ one may think that it takes the value f in any other gauge, say $\phi = \tau'$ which is obviously not the case by inspection. The catch is that in order to reach the gauge $\phi = \tau'$ from $\phi = \tau$ one must apply a gauge transformation to $O_f(\tau)$ which maps ϕ to $\phi + \tau' - \tau = \phi + \delta\tau$ and f to its corresponding image $f + \delta f$ under this gauge transformation. By gauge invariance we obtain $O_f(\tau) = O_{f+\delta f}(\tau + \delta\tau)$. Hence in the gauge $\phi = \tau'$ the observable takes the value $f + \delta f$ and not f . This is not in contradiction with gauge invariance because $f + \delta f$ and f are evaluated at different points on the same gauge orbit just in the right way as to give the same numerical value.

⁶Notice that when choosing different clock variables ϕ', π' we also have to choose different true degrees of freedom Q', P' . The algebra of the $O'_Q(0), O'_{P'}(0)$ is *not* isomorphic to the one of $O_Q(0), O_P(0)$, rather we have $\{O'_P(0), O'_Q(0)\} = O'_{\{P, Q\}^*}(0)$ where $\{.,.\}^*$ denotes the Dirac bracket associated with F, ϕ' . Thus, while $O_P(0), O_Q(0)$ and $O'_{P'}(0), O'_{Q'}(0)$ are conjugate pairs, $O'_P(0), O'_Q(0)$ are not.

Before closing this section we should mention that most of what we have sketched above is local in nature. Many issues in quantum theory are, however, of a more global nature and in order to capture those aspects one has to generalise the framework, using for instance techniques developed in [36]. Such an extension is, however, non trivial and unfortunately beyond the scope of the present paper whose main purpose is to remind of the difficulties that one generically faces when going from the canonical framework to the path integral formalism.

3 Reduced Phase Space Path Integral

This section is subdivided into three parts. In the first we make some general remarks about scattering theory in ordinary QFT which is closely related to the path integral and how this applies to our case. In the second we formally derive the reduced phase space integral as the generating functional of n -point functions. This path integral is an integral over the reduced phase space. In the third section we unfold this path integral and integrate over the unconstrained phase space whereby proper gauge fixing conditions and constraints have to be imposed.

Most of the material reviewed in this section is standard and the familiar reader can safely skip it. However, we tried to assemble this material in a way so that it is hopefully useful to researchers from different scientific communities and such that the paper is self contained.

3.1 Remarks about Scattering Theory

The central object of interest in QFT is the scattering matrix. Rigorous scattering theory is in fact a difficult subject even in ordinary QFT on Minkowski space. First of all, there is a notion of a free and interacting field φ and ϕ respectively which evolve according to the free and interacting Hamiltonian H_0 and H respectively. Here free means that H_0 does not contain any self – interaction. The physical assumption is that in the far future $t_f \rightarrow \infty$ and far past $t_i \rightarrow -\infty$ any outgoing and ingoing particles respectively do not interact. This is, of course, not really true. However, using the methods of local quantum physics, assuming that the theory has a mass gap⁷ one can prove that the vacuum correlators of the asymptotic fields reduce to those of the free field, where vacuum really means the interacting vacuum.

This means that the asymptotic fields generate from the interacting vacuum a Fock space \mathcal{H}_\pm which in general could be a proper subspace of \mathcal{H} . These states can be thought of as the rigorous substitutes for the states generated by the non existing asymptotic free field from the free vacuum. This is the famous framework of Haag and Ruelle, see [11] and references therein. The rigorous S – matrix is then defined by the scalar product between these asymptotic Fock states which one interprets as vector states in the Heisenberg picture under the free dynamics. The rigorous relation between the S – matrix elements and the time ordered n -point functions is then provided by the famous LSZ formula [11] which rests on the assumption of asymptotic completeness⁸, that is, $\mathcal{H} = \mathcal{H}_\pm$.

In most textbooks on QFT, the Haag – Ruelle theory is barely mentioned. Rather, one somehow postulates that the free and interacting fields can be implemented on the same Hilbert space. Then one can consider Fock states $\psi_\pm \equiv \psi_\pm^H$ created from the free vacuum by free field creation operators which one considers as vectors in the Heisenberg picture in the infinite past and future respectively because they are time independent. To obtain the corresponding Schrödinger picture states in that limit one just has to evolve via the free Hamiltonian to obtain $\psi_\pm^S(t) = e^{iH_0 t/\hbar} \psi_\pm^H$ as $t \rightarrow \pm\infty$. To map a Schrödinger state from the far past to the far future one should however use the interacting Hamiltonian H and get the evolved Schrödinger picture vector state $e^{iH(t_f-t_i)/\hbar} \psi_-^S(t_i)$. Thus the scattered Heisenberg picture state would

⁷The four momentum squared operator should have a pure point spectrum which is separated from the continuum.

⁸More in detail, in order to derive the LSZ formulae one needs the LSZ asymptotic conditions which state that the matrix elements of the interacting field between vector states in \mathcal{H}_+ and \mathcal{H}_- respectively converge to those of the free field. If asymptotic completeness holds, this is just weak convergence on \mathcal{H} which is implied by the strong convergence of the Haag – Ruelle theory.

be given by

$$\psi_{\text{scattered}}^H = \lim_{t_{\pm} \rightarrow \pm\infty} S(t_+, t_-) \psi_-^H \quad (3.1)$$

where

$$S(t_f, t_i) := V(t_f)^\dagger V(t_i) \quad V(t) = \exp(-itH/\hbar) \exp(itH_0/\hbar) \quad (3.2)$$

The formally unitary operators $V(t)$ in principle map the evolving free Heisenberg field operators to the evolving Heisenberg field operators. Using the differential equation for $U(t)$ and solving the resulting Dyson series one can formally derive the Gell – Mann and Low magic formula [11] for the scattering operator

$$S = T\{\exp(i \int_{\mathbb{R}} dt [H(t) - H_0])\}, \quad H(t) = e^{-iH_0 t/\hbar} H e^{iH_0 t/\hbar} \quad (3.3)$$

where the time ordering symbol T asks to order the latest operator to the left. Unfortunately, all of this is mathematically ill – defined: A tiny subset⁹ of the Haag – Kastler (or Wightman) axioms is sufficient to establish that the operator $V(t)$ is the identity operator (up to a phase). This is Haag’s famous theorem [11]. In other words, either there is no interaction or the magic formula is wrong. Indeed, (3.3) is ill – defined in perturbation theory and needs renormalisation. In order to avoid the implication of Haag’s theorem one can, as a regularisation, break translation invariance of the Hamiltonian in an intermediate step by multiplying its density by a function of compact support and then extend the support to infinity. This is also the technique underlying causal renormalisation theory [34].

It transpires that in ordinary QFT the scattering matrix is directly related to the time ordered n – point functions. As we are interested in applications to quantum gravity, we are in a somewhat different situation because we do not have the axiomatic framework of ordinary QFT at our disposal which relies on the metric considered as a background field. However, one can consider a Born – Oppenheimer type of approach with a representation of \mathfrak{A} in which the three – metric operator g acts by multiplication (see [35] for first steps towards a technical implementation). Then, at fixed metric argument of the vector state under consideration one can consider the resulting matter part of the Hamiltonian and apply the techniques of QFT on curved (in this case ultra – static) backgrounds [7] and the corresponding perturbation theory [37] in order to define scattering theory for matter. In particular, LSZ type of formulae then again apply. To define scattering theory for gravity in a background independent way one should consider background independent semiclassical states which are concentrated on a given three geometry and extrinsic curvature and identify their excitations with scattering states, see [35].

3.2 Path Integral for n – point functions

We are thus interested in the time ordered n – point functions. More in detail, suppose we have a representation of the $*$ algebra \mathfrak{A} generated by the elementary fields Q^A, P_A (or the corresponding C^* -algebra of Weyl elements) on a Hilbert space \mathcal{H} which supports the Hamiltonian H of the (conservative) system. We will assume that H is bounded from below and has at least one normalisable vacuum Ω , i.e. a unit vector state of minimal energy $E = \inf(\sigma(H))$ which is a cyclic vector for \mathfrak{A} . Without loss of generality we redefine H such that $E = 0$. Consider the Heisenberg picture operators $Q^A(t) = e^{-iHt/\hbar} Q^A e^{iHt/\hbar}$. As motivated in the previous subsection, we are interested in the time ordered n –point functions

$$\tau^{A_1 \dots A_n}(t_1, \dots, t_n) := \langle \Omega, T\{Q^{A_1}(t_1) \dots Q^{A_n}(t_n)\} \Omega \rangle \quad (3.4)$$

For $n > 1$ and pairwise distinct times we have

$$\tau^{A_1 \dots A_n}(t_1, \dots, t_n) = \sum_{\pi \in S_n} \prod_{k=1}^{n-1} [\theta(t_{\pi(k)} - t_{\pi(k+1)})] W^{A_{\pi(1)} \dots A_{\pi(n)}}(t_{\pi(1)}, \dots, t_{\pi(n)}) \quad (3.5)$$

⁹It is sufficient to retain the 1. uniqueness of the vacuum and 2. spatial translation invariance of the Hamiltonian (part of the Poincaré algebra) and 3. spatial translation invariance of the vacuum.

where we have defined the unordered Wightman functions

$$W^{A_1 \dots A_n}(t_1, \dots, t_n) := \langle \Omega, Q^{A_1}(t_1) \dots Q^{A_n}(t_n) \Omega \rangle \quad (3.6)$$

We should allow for more general operator insertions but $Q^A(t)$ contains information about $\dot{Q}^A(0) = [H, Q^A]/(i\hbar)$ which knows about P_A , hence any scalar product between vector states in the dense subspace $\mathfrak{A}\Omega$ can be approximated by linear combinations of the functions (3.6). Conversely, given suitable positivity requirements on the Wightman functions and their transformation properties under time translations we can reconstruct \mathcal{H} , Ω , H via the GNS construction. The latter arises via Stone's theorem from the fact that we can define a strongly continuous unitary group of time translations.

Using $H\Omega = 0$ we may write

$$W^{A_1 \dots A_n}(t_1, \dots, t_n) := \langle \Omega, e^{i(t_+ - t_1)H/\hbar} Q^{A_1} e^{iH(t_1 - t_2)/\hbar} Q^{A_2} \dots Q^{A_n} e^{iH(t_n - t_-)/\hbar} \Omega \rangle \quad (3.7)$$

for any t_{\pm} . By inserting resolutions of unity it follows that for suitable choices for ψ_i, ψ_f and times t_i, t_f we are interested in the matrix elements

$$\langle \psi_f, U(t_f - t_i) \psi_i \rangle_{\mathcal{H}}, \quad U(t) = \exp(itH/\hbar) \quad (3.8)$$

of the evolution operator between initial and final vectors prepared at initial and final times t_i, t_f respectively.

The path integral substitute for (3.8) is heuristically obtained by skeletonisation of the time interval $[t_i, t_f]$ followed by insertions of unity in terms of generalised position and momentum eigenvectors respectively¹⁰. Specifically, assuming that \mathcal{H} is a representation in which the operators Q^A act by multiplication, for time steps $\epsilon = (t_f - t_i)/N$ and integration variables $Q_n := Q(t_i + n\epsilon)$, $P_n := P(t_i + n\epsilon)$ we obtain formally

$$\langle \psi_f, U(t_f - t_i) \psi_i \rangle = \int \left\{ \prod_{n=0}^N [dQ_n] \right\} \left\{ \prod_{n=1}^N [dP_n] \right\} \overline{\psi_f(Q_N)} \psi_i(Q_0) \left[\prod_{n=1}^N \langle Q_n, e^{i\epsilon H/\hbar} P_n \rangle \langle P_n, Q_{n-1} \rangle \right] \quad (3.9)$$

where formally¹¹

$$[dQ] := \prod_A dQ^A, \quad [dP] := \prod_A dP_A \quad (3.10)$$

The assumption is now that as $N \rightarrow \infty$ we may approximate

$$\langle Q_n, e^{i\epsilon H/\hbar} P_n \rangle \approx \langle Q_n, P_n \rangle e^{i\epsilon H(Q_n, P_n)/\hbar} \quad (3.11)$$

which can be heuristically justified by expanding the exponential in powers of ϵ , ordering momentum and configuration operators to right and left respectively and neglecting all higher \hbar corrections. For certain Hamiltonian operators of Schrödinger type one can actually prove (3.11) (Trotter Product formula [4]) but in general this is a difficult subject. Making this assumption and using the position representation of the momentum eigenfunction

$$\langle Q, P \rangle = \prod_A \frac{\exp(-iQ^A P_A/\hbar)}{\sqrt{2\pi}} \quad (3.12)$$

¹⁰This assumes that the operators Q, P obey the canonical commutation relations. For more general algebras generalised eigenvectors may not exist because e.g. momenta do not commute with each other. In this case one must use different resolutions of the identity. We will here assume that \mathfrak{A} obeys the CCR, CAR and more general algebras can be treated analogously.

¹¹There is no Lebesgue measure in infinite dimensions. However, if the Hilbert space \mathcal{H} is rigorously defined as an L_2 space with a probability measure on a distributional extension of the classical configuration space, then (3.10) can be given a meaning. We will not consider these issues for our heuristic purposes and confine ourselves to drawing attention to the missing steps involved.

we obtain formally

$$\begin{aligned} \langle \psi_f, U(t_f - t_i), \psi_i \rangle &= \int \left\{ \prod_{n=0}^N [dQ_n] \right\} \left\{ \prod_{n=1}^N [d(P_n / \sqrt{2\pi})] \right\} \overline{\psi_f(Q_n)} \psi_i(Q_0) \times \\ &\exp\left(-i \frac{\epsilon}{\hbar} \sum_{n=1}^N \left\{ \left[\sum_A \frac{Q_n^A - Q_{n-1}^A}{\epsilon} P_{An} \right] - H(Q_n, P_n) \right\}\right) \end{aligned} \quad (3.13)$$

One now takes $N \rightarrow \infty$ and formally obtains

$$\langle \psi_f, U(t_f - t_i), \psi_i \rangle = \int [DQ] [DP / \sqrt{2\pi}] \overline{\psi_f(Q(t_f))} \psi_i(Q(t_i)) \exp\left(-\frac{i}{\hbar} \int_{t_i}^{t_f} dt \left\{ \left[\sum_A \dot{Q}^A P_A \right] - H(Q, P) \right\}\right) \quad (3.14)$$

where

$$[DQ] = \prod_{t \in [t_i, t_f]} \prod_A dQ^A(t) \quad (3.15)$$

and similar for $[DP]$. If the Hamiltonian is at most quadratic in P then one can formally perform the momentum integral. As an example, consider a Hamiltonian of the form

$$H(Q, P) = \frac{1}{2} G^{AB}(Q) P_A P_B + V(Q) \quad (3.16)$$

Examples of such Hamiltonians are for example the Hamiltonian constraint in General Relativity (neglecting the issue of gauge invariance for the moment) where the non trivial ‘‘supermetric’’ $G^{AB}(Q)$ is the Wheeler – DeWitt metric and the potential $V(Q)$ is related to the Ricci scalar of the three metric Q . (In)famously, neither G nor V are positive definite so that the Hamiltonian is not bounded from below in General Relativity.

In any case, for Hamiltonians of type (3.16) we can formally perform the Gaussian integral and obtain

$$\langle \psi_f, U(t_f - t_i), \psi_i \rangle = \mathcal{N} \int [DQ] [\sqrt{|\det(G)|}] \overline{\psi_f(Q(t_f))} \psi_i(Q(t_i)) \exp\left(-i \int_{t_i}^{t_f} dt \left\{ \frac{1}{2} (G^{-1})_{AB} \dot{Q}^A \dot{Q}^B - V(Q) \right\}\right) \quad (3.17)$$

where \mathcal{N} is an (infinite) numerical constant (a power of 2π and \hbar) and

$$[\sqrt{|\det(G)|}] = \prod_{t \in [t_i, t_f]} \sqrt{|\det(G)|} \quad (3.18)$$

is the functional determinant of the supermetric¹².

Notably, if G is a non trivial function of Q then it is *not true* that

$$\langle \psi_f, U(t_f - t_i), \psi_i \rangle = \mathcal{N} \int [DQ] \overline{\psi_f(Q(t_f))} \psi_i(Q(t_i)) \exp\left(-\frac{i}{\hbar} S[Q, \dot{Q}; [t_i, t_f]]\right) \quad (3.19)$$

with the classical action

$$S[Q, \dot{Q}; [t_i, t_f]] := \int_{t_i}^{t_f} dt L(Q, \dot{Q}), \quad L(Q, \dot{Q}) = \frac{1}{2} (G^{-1})_{AB} \dot{Q}^A \dot{Q}^B - V(Q) \quad (3.20)$$

Even worse is the case that the momentum dependence of the Hamiltonian is higher than quadratic so that the momentum integral can no longer be performed exactly. In that case one can at best perform a saddle point approximation or one has to rely on perturbation theory. We see that the correct path integral in general is over the phase space and

¹²In fact there is a sign factor involved which accounts for the signature of G . Equation (3.17) is only correct if the signature of G does not depend on Q .

involves the Hamiltonian action and not only over the configuration space involving only the Lagrangian action, so we will stick with (3.14) in what follows.

We still must provide a path integral formulation for the n -point functions. However, this is easy by noting that

$$W^{A_1 \dots A_n}(t_1, \dots, t_n) = \prod_{k=1}^n \int [dQ_k] \langle \Omega, U(t_+ - t_1) | Q_1 \rangle Q_1^{A_1} \times \\ \left[\prod_{k=1}^{n-1} \langle Q_k, U(t_k - t_{k+1}) | Q_{k+1} \rangle Q_{k+1}^{A_{k+1}} \right] \langle Q_n | U(t_n - t_-) | \Omega \rangle \quad (3.21)$$

where $\hat{Q}^A | Q \rangle = Q^A | Q \rangle$ was used. Combining (3.21) with (3.14) results in (for $t_+ > t_1 > \dots > t_n > t_-$)

$$W^{A_1 \dots A_n}(t_1, \dots, t_n) = \int [DQ] [DP / \sqrt{2\pi} \overline{\Omega(Q(t_+))}] \Omega(Q(t_-)) \times \\ \exp\left(-\frac{i}{\hbar} \int_{t_-}^{t_+} dt \left\{ \sum_A \dot{Q}^A P_A - H(Q, P) \right\}\right) \prod_{k=1}^n Q^{A_k}(t_k) \quad (3.22)$$

where

$$[DQ] = \prod_{t \in [t_-, t_+]} \prod_A dQ^A(t) \quad (3.23)$$

and similar for $[DP]$.

It is worth mentioning that in a rigorous setting [1, 8] one does not really consider matrix elements of the unitary operator $U(t) = \exp(itH/\hbar)$. Namely, consider the analytic continuation $t_k \mapsto it_k$ for $t_k > 0$, that is, the Schwinger functions

$$S^{A_1 \dots A_n}(t_1, \dots, t_n) := W^{A_1 \dots A_n}(it_1, \dots, it_n) \quad (3.24)$$

These are correlators of the $e^{tH/\hbar} Q^A e^{-tH/\hbar}$ and now the same formal manipulations as before lead us to consider the contraction semi-group $t \mapsto V(t) = \exp(-tH/\hbar)$, $t \geq 0$. One now obtains instead of (3.22) the formula

$$S^{A_1 \dots A_n}(t_1, \dots, t_n) = \int [DQ] [DP / \sqrt{2\pi} \overline{\Omega(Q(t_+))}] \Omega(Q(t_-)) \times \\ \exp\left(-\frac{1}{\hbar} \int_{t_-}^{t_+} dt \left\{ i \sum_A \dot{Q}^A P_A + H(Q, P) \right\}\right) \prod_{k=1}^n Q^{A_k}(t_k) \quad (3.25)$$

For Hamiltonians of the form (3.16) with positive definite G, V (subtract the energy gap if necessary) the formal Gaussian integration now gives

$$S^{A_1 \dots A_n}(t_1, \dots, t_n) = \mathcal{N} \int [DQ] [\sqrt{\det(G)}] \overline{\Omega(Q(t_+))} \Omega(Q(t_-)) \exp\left(-\frac{1}{\hbar} S_E[Q, \dot{Q}; [t_-, t_+]]\right) \prod_{k=1}^n Q^{A_k}(t_k) \quad (3.26)$$

with the ‘‘Euclidean’’ action

$$S[Q, \dot{Q}; [t_i, t_f]] := \int_{t_i}^{t_f} dt L_E(Q, \dot{Q}), \quad L_E(Q, \dot{Q}) = \frac{1}{2} (G^{-1})_{AB} \dot{Q}^A \dot{Q}^B + V(Q) \quad (3.27)$$

The path integral (3.26) has better chances to be rigorously defined because the ‘‘measure’’ has a damping factor rather than an oscillating one and so in the rigorous setting one *defines* (3.22) by backwards analytic continuation of (3.26) (when possible)¹³. Equation (3.26) (when it can be proved) is called the Feynman – Kac formula [1, 3, 4]. In what follows we therefore consider the Euclidian point of view.

¹³It is worth mentioning that in the axiomatic framework of local quantum physics [11] on Minkowski space the Schwinger functions are automatically symmetric although the Wightman functions are not which is a consequence of the locality axiom (bosonic operator valued distributions supported at spacelike separated points commute) and analyticity. In GR one does not expect to construct a Wightman QFT due to background independence which is why we insist on $t_k > t_{k+1}$.

In order to avoid any infinite constants we divide the contraction matrix by $1 = \langle \Omega, \Omega \rangle = \langle \Omega, V(t_+ - t_-)\Omega \rangle$ and obtain formally

$$S^{A_1 \dots A_n}(t_1, \dots, t_n) = \frac{\int [DQ] [DP] \overline{\Omega(Q(t_+))} \Omega(Q(t_-)) \exp(-\frac{1}{\hbar} \int_{t_-}^{t_+} dt \{[i \sum_A \dot{Q}^A P_A] + H(Q, P)\}) \prod_{k=1}^n Q^{A_k}(t_k)}{\int [DQ] [DP] \overline{\Omega(Q(t_+))} \Omega(Q(t_-)) \exp(-\frac{1}{\hbar} \int_{t_-}^{t_+} dt \{[i \sum_A \dot{Q}^A P_A] + H(Q, P)\})} \quad (3.28)$$

Even if one cannot integrate out the momenta in general, formula (3.28) reveals that what we are interested in is the measure formally given by

$$d\mu(Q) := \frac{1}{Z} [DQ] \exp(-S_E[Q]/\hbar) \overline{\Omega(Q(t_+))} \Omega(Q(t_-)) \quad (3.29)$$

where

$$\exp(-S_E[Q]/\hbar) := \int [DP] \exp(-\frac{1}{\hbar} \int_{t_-}^{t_+} dt \{[i \sum_A \dot{Q}^A P_A] + H(Q, P)\}) \quad (3.30)$$

is the exponential of the effective Euclidian action and

$$Z := \int [DQ] \exp(-S_E[Q]/\hbar) \overline{\Omega(Q(t_+))} \Omega(Q(t_-)) \quad (3.31)$$

is the partition function. None of the three quantities $[DQ]$, S_E , Z exists but in fortunate cases their combination can be rigorously defined as a measure on a suitable distributional extension of the space of configuration variables Q . The measure μ is known if we know all its moments or equivalently its generating functional

$$\chi[j] := \int d\mu(Q) e^{i \sum_A \int_{t_-}^{t_+} dt j_A(t) Q^A(t)} \quad (3.32)$$

from which the moments follow by (functional) derivation at zero current j .

The apparent drawback of these formulae is that they involve the exact ground state Ω of the interacting Hamiltonian H which is difficult if not impossible to compute analytically. However, and here is where the Euclidian formulation again is helpful, notice that so far the choices for t_{\pm} were arbitrary except that $t_k \in [t_-, t_+]$, in particular, in the original correlator the dependence on t_{\pm} is through $e^{-t_+ H} \Omega = \Omega$ and $e^{t_- H} \Omega = \Omega$. Now suppose in addition that $\exp(-tH)$ for $t > 0$ has a positive integral kernel, i.e. maps a.e. positive functions to strictly positive functions which is usually the case. Then it follows from [38] that $E = 0$ is a simple eigenvalue and the unique (up to a phase) ground state Ω is a strictly positive function. It can be obtained from any a.e. positive $\Omega_0 \in \mathcal{H}$ via the strong limit

$$\Omega := \lim_{t \rightarrow \infty} \frac{e^{-tH} \Omega_0}{\|e^{-tH} \Omega_0\|} \quad (3.33)$$

It follows that by taking the limit $t_{\pm} \rightarrow \pm\infty$ we can replace Ω by Ω_0 in (3.29) – (3.32) because the factors of $\|e^{-tH} \Omega_0\|$ cancel in numerator and denominator. We will assume this to have done for what follows. Remarkably, the choice of the reference vector Ω_0 is rather arbitrary.

Having justified the replacement of Ω by Ω_0 in the Euclidean regime, we analytically continue the time parameter backwards to define the time ordered n-point functions and thus the exponential becomes a pure phase.

3.3 Unfolding the Reduced Phase Space Path Integral

We would like to rewrite the path integral over the reduced phase space coordinatised by the chosen true degrees of freedom in terms of the unconstrained phase space. This is of course standard, see e.g. [6], but we review this procedure here for the sake of completeness. It is, however, a rather involved procedure.

3.3.1 Preliminary Results

The virtue of the gauge fixing conditions G is that the system $C := \{S, F, G\}$ is now a total second class system so that one can treat all constraints on equal footing. We will do this first in the adapted system of Darboux coordinates $(Q^A, P_A), (\phi^\mu, \pi_\mu), (x^\sigma, y_\sigma)$ which is related to the original system (q^a, p_a) by a (local) canonical transformation and then show that the resulting expression is actually invariant under canonical transformations.

Theorem 3.1.

Let $C = \{C_{\mathcal{A}}\}$ be a second class system of constraints on a phase space with canonical coordinates \underline{z} and symplectic structure ω on the unconstrained phase space Γ . Denote the constraint surface by $\bar{\Gamma} := \{m \in \Gamma; C_{\mathcal{A}}(m) = 0 \forall \mathcal{A}\}$ which is a submanifold of Γ . Consider an embedding $J: \hat{\Gamma} \rightarrow \Gamma$ with $J(\hat{\Gamma}) = \bar{\Gamma}$ where $\hat{\Gamma}$ is a model manifold of with coordinates x^i for $\bar{\Gamma}$.

i.

$\hat{\omega} := J^* \omega$ is a symplectic structure on $\hat{\Gamma}$.

ii.

Let Ω^* be the degenerate symplectic structure on Γ defined by the Dirac bracket corresponding to C . Let $f, g \in C^1(\Gamma)$. Then $J^* (\{f, g\}^*) = \{J^* f, J^* g\}^\wedge$ where $\{.,.\}^\wedge$ is the Poisson bracket associated with $\hat{\omega}$.

iii.

The relation between the Liouville measures μ_L and $\hat{\mu}_L$ on Γ and $\hat{\Gamma}$ respectively is

$$\hat{\mu}_L[J^* f] = \mu_L[\sqrt{\det(\{C, C\})} \delta(C) f] \quad (3.34)$$

for any measurable function f .

We note that the right hand side of (3.34) does not make any reference to the chosen embedding J .

Proof.

i.

Obviously $d\hat{\omega} = J^* d\Omega = 0$ establishes closure. Non – degeneracy follows from the fact that J has maximal rank.

ii.

Let

$$M_{\mathcal{A}\mathcal{B}} := \{C_{\mathcal{A}}, C_{\mathcal{B}}\} \quad (3.35)$$

then¹⁴

$$[\omega^*]^{IJ} = \omega^{IJ} + (M^{-1})^{\mathcal{A}\mathcal{B}} \omega^{IK} \omega^{JL} C_{\mathcal{A},K} dC_{\mathcal{B},L} \quad (3.36)$$

where $\omega^{IJ} \omega_{JK} = \delta_K^I$. Using that $\{f, g\} = \omega^{IJ} f_{,J} g_{,I}$ and

$$\{J^* f, J^* g\}^\wedge = \hat{\omega}^{ij} (J^* f)_{,i} (J^* g)_{,j} = \hat{\omega}^{ij} J_{,i}^I f_{,I} J_{,j}^J g_{,J} \quad (3.37)$$

with $\hat{\omega}^{ij} \hat{\omega}_{jk} = \delta_k^i$, we see that the claim is equivalent to

$$\hat{\omega}^{ij} J_{,i}^I J_{,j}^J = [\omega^*]^{IJ} \quad (3.38)$$

on \bar{M} . To verify (3.38) we notice that $\sigma_{\mathcal{A}} := (C_{\mathcal{A},I}), \sigma_i := (\omega_{IJ} J_{,i}^J)$ is a linearly independent set of one forms on M and it suffices to check (3.38) in this basis. From $J^* C_{\mathcal{A}} \equiv 0$ for all \mathcal{A} we immediately have

$$J_{,i}^I C_{\mathcal{A},I} = 0 \quad (3.39)$$

¹⁴Our conventions are as follows: $i_{\chi_f} \omega + df := 0$ defines the Hamiltonian vector field χ_f associated to f while $\{f, g\} := -\chi_f[g] = -i_{\chi_f} dg = i_{\chi_g} i_{\chi_f} \omega$ defines the Poisson bracket. The corresponding matrix is denoted by $\omega^{IJ} := \{z^I, z^J\}$.

on \overline{M} and by construction of the Dirac bracket it is not difficult to see that contraction of (3.38) with $\sigma_{\mathcal{A}}$ results in zero on both sides. Contraction with $\sigma_i \sigma_j$ results in the identity

$$\begin{aligned} & \hat{\omega}^{kl} J_{,k}^I J_{,l}^J \sigma_{iI} \sigma_{jJ} = \hat{\omega}^{kl} \hat{\omega}_{ki} \hat{\omega}_{lj} = \hat{\omega}_{ji} \\ & = [\omega^*]^{IJ} \sigma_{iI} \sigma_{jJ} = \omega^{IJ} \sigma_{iI} \sigma_{jJ} = \omega^{IJ} \omega_{IK} \omega_{JL} J_{,i}^K J_{,j}^L \omega_{LK} J_{,i}^K J_{,j}^L \end{aligned} \quad (3.40)$$

where we used (3.39) and

$$\hat{\omega}_{ij} = (J^* \omega)_{ij} = \omega_{IJ} J_{,i}^I J_{,j}^J \quad (3.41)$$

iii.

Recall that for finite ($2n$ -) dimensional systems the Liouville measure is simply $\mu_L := \wedge^n \omega = \text{Pf}(\omega)[dz]$ where $\text{Pf}(\omega) = \sqrt{\det(\omega)}$ denotes the Pfaffian of the matrix ω_{IJ} . We adopt here the same formula for infinite dimensions, ignoring as usual that the Lebesgue measure $[dz]$ does not exist. Using (3.35) we solve the δ distribution in (3.34) in terms of the embedding J which we write in the form $z = (x, y) = J(x) = (x, Y(x))$. Here x, y are separate sets of canonical pairs so that ω_{IJ} becomes block diagonal and the block matrices $\omega_{\mathcal{A}\mathcal{B}}, \omega_{ij}$ are constant. We obtain

$$\mu_L[\sqrt{\det(\{C, C\})} \delta(C) f] = \int [dz] \sqrt{\det(\omega) \det(M)}(z) \delta(C(z)) f(z) = \int [dx] \left(\sqrt{\frac{\det(\omega) \det(M)}{[\det(c)]^2}} f \right)(J(x)) \quad (3.42)$$

where $c_{\mathcal{A}\mathcal{B}} := C_{\mathcal{A},\mathcal{B}}$. Here we used $C_{\mathcal{A}}(x, y) = C_{\mathcal{A}}(x, Y(x)) + c_{\mathcal{A}\mathcal{B}}[y - Y(x)]^{\mathcal{B}} + \dots = c_{\mathcal{A}\mathcal{B}}[y - Y(x)]^{\mathcal{B}} + \dots$. We have

$$M_{\mathcal{A}\mathcal{B}} = \omega^{IJ} C_{\mathcal{A},I} C_{\mathcal{B},J} = \omega^{CD} C_{\mathcal{A},C} C_{\mathcal{B},D} + \omega^{ij} C_{\mathcal{A},i} C_{\mathcal{B},j} \quad (3.43)$$

Equation (3.39) takes the form

$$C_{\mathcal{A},i} + C_{\mathcal{A},\mathcal{B}} Y_{,i}^{\mathcal{B}} = 0 \quad (3.44)$$

so that (3.43) can be written

$$M_{\mathcal{A}\mathcal{B}} = c_{\mathcal{A}\mathcal{C}} c_{\mathcal{B}\mathcal{D}} [\omega^{CD} + \omega^{ij} Y_{,i}^{\mathcal{C}} Y_{,j}^{\mathcal{D}}] \quad (3.45)$$

Let us introduce the abbreviations

$$Y_{,i}^{\mathcal{A}} := Y_{,i}^{\mathcal{A}}, \quad Y_{,\mathcal{A}}^i := \omega_{\mathcal{A}\mathcal{B}} \omega^{ij} Y_{,j}^{\mathcal{B}} \quad (3.46)$$

then

$$M_{\mathcal{A}\mathcal{B}} = c_{\mathcal{A}\mathcal{C}} c_{\mathcal{B}\mathcal{D}} \omega^{\mathcal{E}\mathcal{D}} [\delta_{\mathcal{E}}^{\mathcal{C}} - Y_{,\mathcal{E}}^{\mathcal{C}} Y_{,\mathcal{E}}^i] \quad (3.47)$$

Consider now the matrices

$$K_{\mathcal{B}}^{\mathcal{A}} := Y_{,\mathcal{B}}^{\mathcal{A}} Y_{,\mathcal{B}}^i, \quad k_{,\mathcal{B}}^j := Y_{,\mathcal{B}}^{\mathcal{A}} Y_{,\mathcal{A}}^j \quad (3.48)$$

The key identity is now

$$\det(1 - K) = \det(1 - k) \quad (3.49)$$

To prove this we use the identity (supposing that k has rank m)

$$\det(1 - k) = 1 + \sum_{l=1}^m (-1)^l \delta_{j_1}^{[i_1} \dots \delta_{j_l}^{i_l]} k_{i_1}^{j_1} \dots k_{i_l}^{j_l} \quad (3.50)$$

The same formula holds for $\det(1 - K)$ just that K may have a different rank n and that summation indices are \mathcal{A} rather than i . Now each term in the sum of (3.50) is a polynomial in the traces $\text{tr}(k^r)$, $r > 0$ with a coefficient that does not depend on m . However, $\text{tr}(k^r) = \text{tr}(K^r)$ for any r . So the only possible difference in the two quantities is the range of l . However, notice that

$$\delta_{j_1}^{[i_1} \dots \delta_{j_l}^{i_l]} k_{i_1}^{j_1} \dots k_{i_l}^{j_l} = Y_{\mathcal{A}_1}^{[i_1} \dots Y_{\mathcal{A}_l}^{i_l]} Y_{i_1}^{\mathcal{A}_1} \dots Y_{i_l}^{\mathcal{A}_l} = Y_{[\mathcal{A}_1}^{i_1} \dots Y_{\mathcal{A}_l}^{i_l]} Y_{i_1}^{\mathcal{A}_1} \dots Y_{i_l}^{\mathcal{A}_l} \quad (3.51)$$

is completely skew in either set of indices, hence the sum anyway extends to $\min(m, n)$ only.

We conclude with $\det(\omega) = \det((\omega_{ij})) \det((\omega_{\mathcal{A}\mathcal{B}}))$ that

$$\frac{\det(\omega) \det(M)}{\det(c^2)} = \det((\omega_{ik})) \det((\delta_j^k - k_j^k)) = \det((\omega_{ij} - \omega_{\mathcal{A}\mathcal{B}} Y_{,i}^{\mathcal{A}} Y_{,j}^{\mathcal{B}})) = \det(\hat{\omega}_{ij}) \quad (3.52)$$

□

Corollary 3.1.

The measure μ_G on Γ defined by (3.34) in terms of a gauge fixing condition G , as a linear functional is in fact independent of the gauge fixing condition when restricted to gauge invariant functions f .

Proof. By definition of a gauge fixing condition G for a first class constraint set $\{F\}$, it defines a section of the first class constraint surface (i.e. it defines a hypersurface that intersects each gauge orbit in precisely one point) and it can be reached from any point on the same gauge orbit. Hence any two gauge fixings G, G' are related by a gauge transformation φ which can be written as a composition of canonical transformations of the form $\exp(\beta^\mu \{F_\mu, \cdot\})$ for real valued (phase space independent) parameters. By the first class property, there exist matrices L, M, N such that $\varphi \cdot F_\mu = L_\mu^\nu F_\nu$ and $\varphi \cdot S_\Sigma = M_\Sigma^{\Sigma'} S_{\Sigma'} + N_\Sigma^\mu F_\mu$ where L, M are non-singular¹⁵. In matrix notation $\varphi \cdot F = L \cdot F$, $\varphi \cdot S = M \cdot S + N \cdot F$. This can be inverted

$$F = (L^{-1}) \cdot (\varphi \cdot F), \quad S = (M^{-1}) \cdot [(\varphi \cdot S) - N \cdot (L^{-1}) \cdot (\varphi \cdot F)] \quad (3.53)$$

By assumption, f is (weakly) gauge invariant, $f(m) \approx f(\varphi \cdot m)$ and the Liouville measure is invariant under canonical transformations (since the symplectic structure is), $d\mu_L(\varphi \cdot m) = d\mu_L(m)$.

We exhibit the dependence of the measure (3.34) on G by μ_G . Notice that in terms of $\{C\} = \{F, G, S\}$ we have

$$\begin{aligned} \det(\{C, C\})_{C=0} &= \det \begin{pmatrix} \{F_\mu, F_\nu\} & \{F_\mu, G_\nu\} & \{F_\mu, S_{\Sigma'}\} \\ \{G_\mu, F_\nu\} & \{G_\mu, G_\nu\} & \{G_\mu, S_{\Sigma'}\} \\ \{S_\Sigma, F_\nu\} & \{S_\Sigma, G_\nu\} & \{S_\Sigma, S_{\Sigma'}\} \end{pmatrix}_{C=0} = \det \begin{pmatrix} 0 & \{F_\mu, G_\nu\} & 0 \\ \{G_\mu, F_\nu\} & \{G_\mu, G_\nu\} & \{G_\mu, S_{\Sigma'}\} \\ 0 & \{S_\Sigma, G_\nu\} & \{S_\Sigma, S_{\Sigma'}\} \end{pmatrix}_{C=0} \\ &= \{[\det(\{F, G\})]^2 \det(\{S, S\})\}_{C=0} \end{aligned} \quad (3.54)$$

¹⁵At least for β^μ close to zero.

Using the automorphism property of canonical transformations $[\varphi \cdot f](m) = f(\varphi \cdot m)$ etc. and (3.53) we have

$$\begin{aligned}
\mu_{\varphi \cdot G}(f) &= \int_M d\mu_L(m) \delta(S(m)) \delta([\varphi \cdot G](m)) \delta(F(m)) |\det(\{F, \varphi \cdot G\}(m))| \sqrt{\det(\{S, S\}(m))} f(m) \\
&= \int_M d\mu_L(m) \delta((M^{-1}[\varphi \cdot S - NL^{-1}\varphi \cdot F])(m)) \delta(G(\varphi \cdot m)) \delta((L^{-1}[\varphi \cdot F])(m)) |\det(\{L^{-1}\varphi \cdot F, \varphi \cdot G\}(m))| \times \\
&\quad \sqrt{\det(\{M^{-1}[\varphi \cdot S - NL^{-1}\varphi \cdot F], M^{-1}[\varphi \cdot S - NL^{-1}\varphi \cdot F]\}(m))} f(\varphi \cdot m) \\
&= \int_M d\mu_L(m) |\det(M)(m)| |(\det(L)(m))| \delta([\varphi \cdot S](m)) \delta(G(\varphi \cdot m)) \delta([\varphi \cdot F](m)) |\det(\{L^{-1}\{\varphi \cdot F, \varphi \cdot G\}\}(m))| \times \\
&\quad \sqrt{\det(M^{-1}\{\varphi \cdot S, \varphi \cdot S\}(M^{-1})^T - NL^{-1}\{\varphi \cdot F, \varphi \cdot S\}(M^{-1})^T \\
&\quad - M^{-1}\{\varphi \cdot S, \varphi \cdot F\})(NL^{-1})^T + NL^{-1}\{\varphi \cdot F, \varphi \cdot F\})(NL^{-1})^T)(m))} f(\varphi \cdot m) \\
&= \int_M d\mu_L(m) |\det(M)(m)| |(\det(L)(m))| \delta([\varphi \cdot S](m)) \delta(G(\varphi \cdot m)) \delta([\varphi \cdot F](m)) |\det(\{L^{-1}\{\varphi \cdot F, \varphi \cdot G\}\}(m))| \times \\
&\quad \sqrt{\det(M^{-1}\{\varphi \cdot S, \varphi \cdot S\}(M^{-1})^T)(m)} f(\varphi \cdot m) \\
&= \int_M d\mu_L(m) \delta([\varphi \cdot S](m)) \delta(G(\varphi \cdot m)) \delta([\varphi \cdot F](m)) |\det(\{\varphi \cdot F, \varphi \cdot G\}(m))| \times \\
&\quad \sqrt{\det(\{\varphi \cdot S, \varphi \cdot S\}(m))} f(\varphi \cdot m) \\
&= \int_M d\mu_L(\varphi \cdot m) \delta(S(\varphi \cdot m)) \delta(G(\varphi \cdot m)) \delta(F(\varphi \cdot m)) |\det(\{F, G\}(\varphi \cdot m))| \times \\
&\quad \sqrt{\det(\{S, S\}(\varphi \cdot m))} f(\varphi \cdot m) \\
&= \mu_G(f)
\end{aligned} \tag{3.55}$$

where in the third step we used that Poisson brackets with L, M, N do not contribute since the δ -distributions have support at $\varphi \cdot F = \varphi \cdot S = 0$, in the fourth we used the first class property and again the support of the δ distributions, in the fifth we cancelled the determinants of the matrices L, M , in the sixth we exploited the Poisson automorphism property of φ as well as the invariance of the Liouville measure and in the last we performed a trivial relabeling. \square

The statements of theorem 3.1 and corollary 3.1 show that the measure μ_G (3.34) is the correct extension to the full phase space of the pull – back measure defined by a gauge fixing condition and that correlators among gauge invariant functions are actually independent of the gauge fixing condition. For instance, in terms of the gauge invariant observables $O_f^{(G)}$, where we have exhibited the dependence on G , we have $\mu_{G'}[O_f^{(G)}] = \mu_G[O_f^{(G)}]$ for any $G' = \varphi \cdot G$.

This can also be understood geometrically: Given two gauge fixing conditions G, G' we obtain $\hat{\omega}_G = J_G^* \omega$, $\hat{\omega}_{G'} = J_{G'}^* \omega$ from the corresponding embeddings $J_G : \hat{M} \rightarrow \overline{M}_G$, $J_{G'} : \hat{M} \rightarrow \overline{M}_{G'}$. Now clearly¹⁶

$$\begin{aligned}
\overline{M}_{\varphi \cdot G} &= \{m \in M; S(m) = F(m) = \varphi^* G(m) = 0\} \\
&= \{m \in M; M^{-1}(m)[S(\varphi(m)) - N(m)L^{-1}(m)F(\varphi(m))]L^{-1}F(\varphi(m)) = G(\varphi(m)) = 0\} \\
&= \{m \in M; S(\varphi(m)) = F(\varphi(m)) = G(\varphi(m)) = 0\} \\
&= \{\varphi^{-1}(\varphi(m)) \in M; S(\varphi(m)) = F(\varphi(m)) = G(\varphi(m)) = 0\} \\
&= \varphi^{-1}(\overline{M}_G)
\end{aligned} \tag{3.56}$$

so that

$$J_{\varphi \cdot G} = \varphi^{-1} \circ J_G \tag{3.57}$$

and therefore from the fact that φ is canonical $\varphi^* \omega = \omega$

$$\hat{\omega}_{\varphi \cdot G} = J_{\varphi \cdot G}^* \omega = J_G^* \omega = \hat{\omega}_G \tag{3.58}$$

¹⁶In abuse of notation we write $\varphi \cdot m = \varphi(m)$ i.e. we identify the action of the exponential map with the corresponding diffeomorphism.

Remark:

The fact that φ is canonically generated by first class constraints featured crucially into this argument. This has the following relevance:

Suppose we are given a system which as gauge symmetry has spatial diffeomorphism invariance in D spatial directions. Suppose that the field content consists, possibly among other things, of GR minimally coupled to D scalar fields ϕ_1, \dots, ϕ_n . From the curvature of the metric and higher derivatives we can also form D algebraically independent scalars R_1, \dots, R_n . Suppose that at least locally they define a coordinate system so that $x \mapsto \phi(x) := (\phi_1(x), \dots, \phi_n(x))$ and $x \mapsto R(x)$ defines a (local) diffeomorphism. Pick any fixed diffeomorphism φ_0 . Then both $G = \phi - \varphi_0$ and $G' = R - \varphi_0$ are bona fide gauge fixing conditions. However, there does not exist any canonically generated diffeomorphism $\varphi_\xi = \exp(\{\int d^D x \xi^a(x) C_a(x), \cdot\})$ with phase space independent ξ such that $\varphi_\xi \cdot G = G'$. The reason is that the spatial diffeomorphism constraint does not mix field species. It is true that we can find a phase space dependent function $\hat{\xi}[\phi, R]$ defined by $\varphi_{\hat{\xi}} \circ \phi = R$ such that $[\varphi_{\hat{\xi}} \cdot G]_{\xi=\hat{\xi}} = G'$, however, due to the phase space dependence of $\hat{\xi}$ it is not true that $[\varphi_{\hat{\xi}} \circ]_{\xi=\hat{\xi}} = \varphi_{\hat{\xi}} \circ$. The latter is also a canonical transformation with generator $\int d^D x \hat{\xi}^a C_a$ but it does not generate the searched for field dependent diffeomorphism, provided it exists at all. Notice that corollary 3.1 remains true for field dependent $\hat{\xi}$, just the matrices L, M, N look different, this is not the point, the point is that it is not clear that a canonical transformation exists which maps ϕ to R . It may therefore be true that gauge fixings separate into equivalence classes depending on whether such phase space dependent gauge transformations exist or not. If that was the case, then it would not be true that the measure (3.34) as a linear functional on gauge invariant functions would be independent of the gauge fixing condition, it would depend at least on the equivalence class.

3.3.2 From reduced Darboux coordinates to unreduced Darboux coordinates

In order to combine the results of sections 3.2 and 3.3.1 we notice that the parameter manifold \hat{M} (which is the same for any gauge fixing) can be identified with the manifold equipped with Darboux coordinates $\{Q^A, P_A\}$. These are adapted to our choice of G such that $F = G = 0$ or equivalently $F' = G = 0$ can be solved for $\{\phi^\mu, \pi_\mu\}$ in terms of $\{Q^A, P_A\}$ which also defines the embedding J_G . In particular, if \hat{f} only depends on $\{Q^A, P_A\}$ then we can form our preferred observables $O_{\hat{f}}^{(G)}$ and due to the identity $\hat{f} = J_G^* O_{\hat{f}}^{(G)}$ we find from (3.34)

$$\hat{\mu}_L[\hat{f}] = \mu_G[O_{\hat{f}}^{(G)}] = \mu_{\varphi \cdot G}[O_{\hat{f}}^{(G)}] \quad (3.59)$$

where corollary 3.1 was used. Of course, for practical calculations the precise expression for $O_{\hat{f}}^{(G)}$ in terms of $Q^A, P_A, \phi^\mu, \pi_\mu$ is rather cumbersome to use. However, due to the δ distribution $\delta(G)$ involved in μ_G obviously

$$\hat{\mu}_L[\hat{f}] = \hat{\mu}_G[O_{\hat{f}}^{(G)}] = \mu_G[\hat{f}] \quad (3.60)$$

so that we can drop the gauge invariant extension under the path integral at the price of having to keep the G dependence in $\mu_G G$ because \hat{f} is not gauge invariant so that corollary 3.1 does not apply. Even if we keep $O_{\hat{f}}^{(G)}$ rather than \hat{f} , still the G dependence does not disappear because while we can drop it from μ_G , it remains in $O_{\hat{f}}^{(G)}$ which is a specific type of Dirac observable which uses the structure G . This is in accordance with what we said in the introduction.

We are now ready to extend the reduced Darboux coordinate phase space path integral of section 3.2 to all Darboux coordinates: The Liouville measure used there is precisely given by $\hat{\mu}_L$ because in Darboux coordinates $\det(\hat{\omega}) = 1$. Furthermore, for our choice of gauge fixing $G^\mu = -\phi^\mu + \tau^\mu(t)$ and $F'_\mu = \pi_\mu + h'_\mu(\phi, Q, P)$ we have $|\det(\{F', G\})| = 1$ and since $S'_\sigma = z_\Sigma = (x^\sigma, y_\sigma)$ in Darboux coordinates are canonical pairs we have $\det(\{S', S'\}) = 1$. It is therefore trivial to write the generating functional of n -point functions as a path integral over the entire phase space by simply

using formula (3.34) at each point of time

$$\begin{aligned}\chi[j] &:= \frac{Z[j]}{Z[0]} \\ Z[j] &:= \int [DQ DP D\phi D\pi Dx Dy] \delta[G] \delta[S'] \delta[F'] |\det\{F', G\}| \sqrt{\det\{S', S'\}} \overline{\Omega_0(Q(+\infty))} \Omega_0(Q(-\infty)) \times \\ &\quad \exp(-i\frac{1}{\hbar} \int_{\mathbb{R}} dt \{[\sum_A \dot{Q}^A P_A] - H_{\text{red}}(Q, P; t)\}) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A(t)}\end{aligned}\quad (3.61)$$

where for instance

$$\delta[F'] = \prod_t \delta(F'(t)), \quad \det\{S', S'\} := \prod_t \det\{S'(t), S'(t)\} \quad (3.62)$$

and

$$S^{A_1 \dots A_n}(t_1, \dots, t_n) = i^{-n} \left[\frac{\delta^n \chi[j]}{\delta j_{A_1}(t_1) \dots j_{A_n}(t_n)} \right]_{j=0} \quad (3.63)$$

Here we have explicitly kept $\det\{S', S'\} = 1$ because we will see that (3.61) is covariant under changing to equivalent constraints. To remind the reader, we recall that the possibly explicitly time dependent reduced Hamiltonian is given by

$$H_{\text{red}}(Q, P; t) = \dot{\tau}^\mu(t) h'_\mu(\phi = \tau(t), Q, P) \quad (3.64)$$

where F_μ at $S = 0$ or equivalently $S' = 0$ was brought into the equivalent form $F'_\mu = \pi_\mu + h'_\mu(\phi, Q, P)$ which motivated the use of a gauge fixing of the form $G^\mu = \tau^\mu(t) - \phi^\mu$.

Formula (3.61) achieves the goal to extend the reduced phase space path integral to the full phase space, albeit in the specific, local Darboux coordinates that were picked by motivations from quantum theory¹⁷ and the constraint structure of the theory and in terms of the convenient equivalent constraints S', F' .

3.3.3 Restoring the Original Canonical Coordinates and Constraints

The next step will be to restore the original Darboux coordinates (q^a, p_a) as well as the original constraints S, F rather than S', D' . To that end we notice the identity

$$\begin{aligned}& \int dt [P_A \dot{Q}^A - H_{\text{red}}(\tau; Q, P)] \\ &= \int dt [P_A \dot{Q}^A - \dot{\tau}^\mu h_\mu(\tau; Q, P)] \\ &= \int dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu + \pi_\mu [\dot{\tau}^\mu - \dot{\phi}^\mu] - \dot{\tau}^\mu [\pi_\mu + h_\mu(\tau; Q, P)]] \\ &= \int dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu + \pi_\mu G^\mu - \dot{\tau}^\mu \tilde{F}_\mu]\end{aligned}\quad (3.65)$$

Since the path integral is supported at $G^\mu = \tau^\mu - \phi^\mu = 0$, $F'_\mu = \pi_\mu + h'_\mu = 0$, $S'_\Sigma := z_\Sigma = (x^\sigma, y_\sigma) = 0$ we can rewrite (3.65) *under the integral* in the form

$$\int dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu + y_\sigma \dot{y}^\sigma] \quad (3.66)$$

Now for certain, phase dependent, non singular matrices M, N we have $F' = M \cdot F$, $S' = N \cdot S$. But then

$$\delta(F') |\det\{F', G\}| = \delta(F) |\det\{F, G\}|, \quad \delta(S') \sqrt{\det\{S', S'\}} = \delta(S) \sqrt{\det\{S, S\}} \quad (3.67)$$

¹⁷Due to the second class constraints, the use of such coordinates is mandatory because otherwise the representation theory of the reduced symplectic structure becomes too difficult.

is covariant under change to equivalent constraints. This allows us to immediately restore the original constraints in (3.61) although everything is still written in terms of the unreduced and adapted darbox coordinates $(Q, P), (\phi, \pi), (x, y)$. However, that system of coordinates originates from the original system of canonical pairs (q^a, p_a) by a canonical transformation [6]. Accordingly, by applying the inverse canonical transformation α , we can restore the system of coordinates (q, p) which leaves the Liouville measure in (3.61) invariant, which leaves (3.66) invariant up to a total differential which we assume to vanish at t_{\pm} , which reexpresses F, G, S in terms Darbox coordinates in terms of the original coordinates and finally is covariant with respect to the Poisson brackets involved because e.g. $\alpha(\{F, G\}) = \{\alpha(F), \alpha(G)\}$. Therefore, (3.61) can be rewritten as

$$\begin{aligned}\chi[j] &:= \frac{Z[j]}{Z[0]} \\ Z[j] &:= \int [Dq Dp] \delta[G] \delta[S] \delta[F] |\det\{F, G\}| \sqrt{\det\{S, S\}} \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \\ &\quad \exp\left(-\frac{i}{\hbar} \int_{\mathbb{R}} dt \left[\sum_a \dot{q}^a p_a \right] e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)}\right)\end{aligned}\quad (3.68)$$

Notice that the effect of the reduced Darbox coordinates did not completely disappear: The initial and final state depend on Q as well as the exponential involving the current j . But $Q = Q[q, p]$ may be a complicated function of the original canonical coordinates q, p .

Remark:

Notice that at this stage we can formally get rid of the gauge fixing condition in (3.68) by the ‘‘Fadeev – Popov trick’’ if we pay a price: As we have already remarked before, due to the presence of $\delta[G]$ we may replace everywhere the non gauge invariant Q by $O_Q^{(G)}$. Then the exponent, as a symplectic potential and the measure $[Dq] [Dp]$, which is formally the Liouville measure associated with ω , is gauge invariant since gauge transformations are canonical transformations. Also $\{S, S\}, F$ are weakly gauge invariant due to the first class property and since canonical transformations preserve Poisson brackets. Hence, after the gauge invariant extension of Q , the only non – gauge invariant ingredient of the integrand of $Z[j]$ in (3.61) is $\delta[G]$. In fact, $\alpha_{\beta}(G) = G - \beta$ where we have introduced the gauge transformations $\alpha_{\beta} := \exp(\beta^{\mu} \{F'_{\mu}, \cdot\})$ which, since the constraints F' are Abelian, have the Abelian group \mathfrak{G} structure $\alpha_{\beta} \circ \alpha_{\beta'} = \alpha_{\beta+\beta'}$. Since the remaining ingredients are all gauge invariant, we may replace G by $\alpha_{\beta}(G)$ for any β . Now extend both numerator $Z[j]$ and denominator $Z[0]$ by the infinite ‘‘gauge volume’’ constant $\int [D\beta]$ with ‘‘Haar measure’’ $[D\beta]$. We can then trivially integrate out the $\delta[\alpha_{\beta}(G)] = \delta[G - \beta]$ and find

$$\begin{aligned}\chi[j] &:= \frac{\tilde{Z}[j]}{\tilde{Z}[0]} \\ Z[j] &:= \int [Dq] [Dp] \delta[S] \delta[F] \sqrt{\det\{S, S\}} \overline{\Omega_0(O_Q^{(G)}[q, p](+\infty))} \Omega_0(O_Q^{(G)}[q, p](-\infty)) \times \\ &\quad \exp\left(-\frac{i}{\hbar} \int_{\mathbb{R}} dt \sum_a \dot{q}^a p_a\right) e^{i \int_{\mathbb{R}} dt j_A(t) O_Q^{(G)}[q, p](t)}\end{aligned}\quad (3.69)$$

The price that we have to pay is that we have to replace Q^A by $O_{Q^A}^{(G)} =: O_{Q^A}$ etc. which is an even more complicated function of q, p . This makes this method of getting rid of the gauge fixing condition useless in practice. The only exception is when we consider zero current $j = 0$ and restrict to gauge transformations that are the identity in the infinite past and future. Then the gauge invariant extension in the argument of Ω_0 and more general boundary states is not necessary and the argument just displayed goes through. The restriction to such asymptotically trivial gauge transformations however means that we set the constraints to zero by hand on the kinematical Hilbert space.

3.3.4 Restoring the Lagrangian

The idea is now to exponentiate the constraints and to rewrite the total resulting exponent in terms of the classical action. Thus we introduce Lagrange multipliers λ^μ for all first class constraints and μ^Σ for all second class constraints and write

$$\begin{aligned}\chi[j] &:= \frac{Z[j]}{Z[0]} \\ Z[j] &:= \int [Dq] [Dp] [D\lambda] [D\mu] \delta[G] |\det\{F, G\}| \sqrt{\det\{S, S\}} \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \\ &\quad \exp\left(-\frac{i}{\hbar} \int_{\mathbb{R}} dt \left[\sum_a \dot{q}^a p_a - \sum_\mu \lambda^\mu F_\mu - \sum_\Sigma \mu^\Sigma S_\Sigma \right]\right) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)}\end{aligned}\quad (3.70)$$

The final task is to remove the secondary constraints so that the action appears in covariant form after Legendre transformation, i.e. with primary constraints only. The technique for doing this is well known [12]. We will not treat the general case with secondary constraints of arbitrary high but finite order N (i.e. one has secondary, tertiary, .. N -ary constraints). For a systematic classification of such systems and a convenient choice of basis of those constraints see e.g. [39] and references therein. Here we pick a typical situation of particular interest for General Relativity. The general case will be even more complicated with even more modifications to the measure than we encounter below:

We assume that the canonical Hamiltonian has the following structure

$$H = H'_0 + v_f \cdot F^{(1)} + v_s \cdot S^{(1)}, \quad H^{(0)'} = -q_f \cdot \tilde{F}^{(2)} \quad (3.71)$$

As the notation suggests, $F^{(1)}$ is a vector with entries consisting of primary first class constraints while $S^{(1)}$ is a vector with entries consisting of primary second class constraints. The vector $\tilde{F}^{(2)}$ is related to a set of secondary second class constraints that we will derive shortly. Usually $F^{(1)}, S^{(1)}$ simply express the fact that the momenta p_f, p_s conjugate to q_f, q_s respectively vanish because the Lagrangian does not depend on the velocities v_f, v_s . It is also usually the case that $\tilde{F}^{(2)}$ does not depend on q_f, p_f, p_s but on q_s . Thus we assume that (we do not denote indices)

$$\{F^{(1)}, F^{(1)}\} = \{F^{(1)}, S^{(1)}\} = \{S^{(1)}, S^{(1)}\} = \{F^{(1)}, \tilde{F}^{(2)}\} = 0 \quad (3.72)$$

while the terms not proportional to $F^{(1)}, S^{(1)}$ of

$$S^{(2)} := \{\tilde{F}^{(2)}, S^{(1)}\} \quad (3.73)$$

defines a vector of secondary second class constraints. We abuse notation by identifying that vector with (3.73) in order not to have to introduce indices. Notice that

$$\{H, F^{(1)}\} = \{H'_0, F^{(1)}\} = \tilde{F}^{(2)} \quad (3.74)$$

thus justifying the name secondary first class constraint.

It is also often the case that the $\tilde{F}^{(2)}$ close on themselves, that is

$$\{\tilde{F}^{(2)}, \tilde{F}^{(2)}\} \propto \tilde{F}^{(2)} \quad (3.75)$$

which we also will assume. Correspondingly,

$$\{H, \tilde{F}^{(2)}\} = \{H'_0, \tilde{F}^{(2)}\} + \{v_s \cdot S^{(1)}, \tilde{F}^{(2)}\} \propto \tilde{F}^{(2)}, S^{(2)} \quad (3.76)$$

does not produce tertiary constraints. These assumptions imply by the Jacobi identity that

$$\{F^{(1)}, S^{(2)}\} = -\{\tilde{F}^{(2)}, \{S^{(1)}, F^{(1)}\}\} - \{S^{(1)}, \{F^{(1)}, \tilde{F}^{(2)}\}\} = 0 \quad (3.77)$$

Finally

$$\{H, S^{(2)}\} = q_f \cdot \{\tilde{F}^{(2)}, S^{(2)}\} + v_s \cdot \{S^{(1)}, S^{(2)}\} \quad (3.78)$$

and we assume that the matrix $\{S^{(1)}, S^{(2)}\}$ is invertible. Hence the Dirac algorithm does not produce any tertiary constraints and the velocity v_s must be fixed in order to equate (3.78) to zero. Accordingly the Hamiltonian becomes

$$H = q_f \cdot [\tilde{F}^{(2)} - \{\tilde{F}^{(2)}, S^{(2)}\} \{S^{(1)}, S^{(2)}\}^{-1} \cdot S^{(1)}] + v_f \cdot F^{(1)} =: q_f \cdot F^{(2)} + v_f \cdot F^{(1)} \quad (3.79)$$

a linear combination of first class constraints. Thus in terms of the previous notation, the first class constraints F_μ comprise $F^{(1)}, F^{(2)}$, the second class constraints S_Σ comprise $S^{(1)}, S^{(2)}$ and finally the primary constraints C_i comprise $F^{(1)}, S^{(1)}$.

This is a simple but non trivial situation often encountered in concrete models and this concrete form now enables us to explicitly carry out the steps outlined in [12]: In (3.65) by an obvious change of notation we write

$$\begin{aligned} \chi[j] &:= \frac{Z[j]}{Z[0]} \\ Z[j] &:= \int [Dq] [Dp] [D\lambda_1] [D\lambda_2] [D\mu_1] [D\mu_2] \delta[G] |\det\{F, G\}| \sqrt{\det\{S, S\}} \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \\ &\quad \exp\left(-\frac{1}{\hbar} \int_{\mathbb{R}} dt \left\{ i \left(\sum_a \dot{q}^a p_a - \lambda_1 \cdot F^{(1)} - \lambda_2 \cdot F^{(2)} - \mu_1 \cdot S^{(1)} - \mu_2 \cdot S^{(2)} \right) \right\} \right) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)} \\ &:= \int [Dq] [Dp] [D\lambda_1] [D\lambda_2] [D\mu_1] [D\mu_2] \delta[G] |\det\{F, G\}| \sqrt{\det\{S, S\}} \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \\ &\quad \exp\left(-\frac{1}{\hbar} \int_{\mathbb{R}} dt \left\{ i \left(\sum_a \dot{q}^a p_a - \lambda_1 \cdot F^{(1)} - \lambda_2 \cdot \tilde{F}^{(2)} - \mu_1 \cdot S^{(1)} - \mu_2 \cdot S^{(2)} \right) \right\} \right) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)} \end{aligned} \quad (3.80)$$

where in the second step we have shifted the integration variable μ_1 in order to absorb the contribution $\mu_0 \cdot S^{(1)} = \tilde{F}^{(2)} - \tilde{f}^{(2)}$.

We now perform a canonical transformation with generator $\mu_2 \cdot S^{(1)} / \lambda'_2$ at each time $t \in [t_-, t_+]$ which we assume to become the identity at t_\pm . Here λ'_2 is the unique component of λ_2 such that $\lambda_2 \cdot \{\tilde{F}^{(2)}, S^{(1)}\} = \lambda'_2 S^{(2)}$ modulo terms proportional to $F^{(1)}, S^{(1)}$. This transformation preserves the Liouville measure, the symplectic potential $\int dt p_a \dot{q}^a$ and $\overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A(t)}$ since in this example under consideration Q^A is among the coordinates independent of q_s . If we assume that $G = G^{(1)}, G^{(2)}$ do not involve q_s then also G is invariant. Indeed, one can choose $G^{(1)}, G^{(2)}$ to be gauge fixing conditions on $q_f^{(1)} := q_f$ and $q_f^{(2)}$ respectively which are both independent of $q_s = q_s^{(1)}$ so that $q_s^{(1)}, q_s^{(2)}, q_f^{(1)}, q_f^{(2)}, Q^A$ comprises a complete system of configuration coordinates. Furthermore, clearly $F^{(1)}, S^{(1)}$ are invariant. But, denoting the canonical transformation by α , we have

$$\begin{aligned} \alpha(\lambda_2 \cdot \tilde{F}^{(2)}) &= \lambda_2 \cdot \tilde{F}^{(2)} - \mu_2 \cdot S^{(2)} - \frac{1}{2\lambda'_2} \mu_2 \cdot \{S^1, S^{(2)}\} \cdot \mu_2 + O(\mu_2^3, F^{(1)}, S^{(1)}) \\ \alpha(\mu_2 \cdot S^{(2)}) &= \mu_2 \cdot S^{(2)} + \frac{1}{\lambda'_2} \mu_2 \cdot \{S^1, S^{(2)}\} \cdot \mu_2 + O(\mu_2^3) \end{aligned} \quad (3.81)$$

Since integrating again over λ_1, μ_1 enforces $F^{(1)} = S^{(1)} = 0$ we can drop terms proportional to $F^{(1)}, S^{(1)}$.

Next, $\alpha(\{F, G\}) = \{\alpha(F), \alpha(G)\} = \{\alpha(F), G\}$ under the assumptions made. This will in general depend non trivially on μ_2 through $\alpha(\tilde{F}^{(2)})$. Likewise $\alpha(\{S, S\}) = \{\alpha(S), \alpha(S)\}$ will in general depend non trivially on μ_2 through $\alpha(S^{(2)})$. Consider $|\det\{F, G\}|, \sqrt{\det\{S, S\}}$ as expanded in powers of μ_2 . Also, since

$$\alpha(\lambda_2 \cdot \tilde{F}^{(2)} + \mu_2 \cdot S^{(2)}) = \lambda_2 \cdot \tilde{F}^{(2)} + \frac{1}{2\lambda'_2} \mu_2 \cdot \{S^{(1)}, S^{(2)}\} \cdot \mu_2 + O(\mu_2^3) \quad (3.82)$$

let us power expand $\alpha(\delta(F))\delta(S)$ around that quadratic term and perform the Gaussian integral. Since $\det(\{S, S\}) = \det(\{S^{(1)}, S^{(2)}\})^2$ this yields

$$Z[j] = \int [Dq] [Dp] [D\lambda_1] [D\lambda_2|\lambda_2'|^{1/2}] [D\mu_1] \delta[G] |\det\{F, G\}| \sqrt[4]{\det\{S, S\}} V \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \exp\left(-\frac{1}{\hbar} \int_{\mathbb{R}} dt \left\{ i \left(\sum_a \dot{q}^a p_a - \lambda_1 \cdot F^{(1)} - \lambda_2 \cdot \tilde{F}^{(2)} - \mu_1 \cdot S^{(1)} \right) \right\} e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)} \right) \quad (3.83)$$

where the local factor V accounts for the additional contributions just mentioned. The integral over $p_f = F^{(1)}, p_s = S^{(1)}$ produces $\delta(\lambda_1 - v_f)\delta(\mu_1 - v_s)$ and cancels the integral over λ_1, μ_1 . Denoting $\{q'^\alpha\} = \{q_f^{(2)}, q_s^{(2)}, Q^A\}$, $\{p'_\alpha\} = \{q_f^{(2)}, q_s^{(2)}, Q^A\}$ we are left with

$$Z[j] = \int [Dq] [Dp'] [D\lambda_2|\lambda_2'|^{1/2}] \delta[G] |\det\{F, G\}| \sqrt[4]{\det\{S, S\}} V \overline{\Omega_0(Q[q, p](+\infty))} \Omega_0(Q[q, p](-\infty)) \times \exp\left(-\frac{1}{\hbar} \int_{\mathbb{R}} dt \left\{ i \left(\sum_a \dot{q}'^a p'_a - \lambda_2 \cdot \tilde{F}^{(2)} \right) \right\} e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q, p](t)} \right) \quad (3.84)$$

Now, by definition (see also section 2.1), solving $p'_\alpha = \partial L(q'^\beta, q_f, q_s; v'^\beta) / \partial v'^\alpha$ for v'^α yields $v' = u'^\alpha(q'^\beta, q_f, q_s; p'_\beta)$ and

$$H'_0 = q_f \tilde{F}^{(2)}(q^s, q'^\beta; p'_\beta) = [v'^\alpha p'_\alpha - L(q'^\beta, q_f, q_s; v'^\beta)]_{v'=u'} \quad (3.85)$$

As is well known, the inverse of this Legendre transformation is

$$L = [v'^\alpha p'_\alpha - H'_0(q'^\beta, q_f, q_s; p'_\beta)]_{p'=\partial L/\partial v'} \quad (3.86)$$

Therefore a saddle point expansion about the extremum $p' = \partial L / \partial v'$ of the exponent in (3.84) yields

$$Z[j] = \int [Dq] [D\lambda_2|\lambda_2'|^{1/2}] \delta[G] |\det\{F, G\}| \sqrt[4]{\det\{S, S\}} V' \overline{\Omega_0(Q[q](+\infty))} \Omega_0(Q[q](-\infty)) \times \exp\left(\frac{i}{\hbar} \int_{\mathbb{R}} dt L(q_f = \lambda_2, q_s, q'^b; v'^b)\right) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q](t)} \quad (3.87)$$

where V'/V accounts for the additional modifications that come from the saddle point approximation and the corresponding corrections. *Notice that a possible dependence on p in Q^A prohibits the saddle point approximation beyond its zeroth order term!* Assuming that Q^A is independent of p as it is the case in this example under consideration and assuming that $G^{(1)}$ really is a coordinate condition on q_f and noticing that $F, S, G^{(2)}, V'$ do not depend on q_f we have after relabeling $\lambda_2 \rightarrow q_f$

$$Z[j] = \int [Dq] [|q_f'|^{1/2}] \delta[G^{(2)}] |\det\{F, G\}| \sqrt[4]{\det\{S, S\}} V' \overline{\Omega_0(Q[q](+\infty))} \Omega_0(Q[q](-\infty)) \times \exp\left(\frac{i}{\hbar} \int_{\mathbb{R}} dt L(q_f, q_s, q'^b; v'^b)\right) e^{i \int_{\mathbb{R}} dt j_A(t) Q^A[q](t)} \quad (3.88)$$

which is our final result.

To summarise:

The path integral can be brought into a form only involving a configuration integral and the exponent of the covariant action, but there is a non trivial measure factor depending on S, F, G, V' which accounts for the correct implementation of the dynamics. Missing that factor means quantising an entirely different system. The measure is not covariant with respect to the Lagrangian symmetries, however, by construction it is covariant with respect to the Hamiltonian symmetries generated by the first class constraints [22]. As is well known from classical Noether theory, these two

symmetries coincide only on shell, that is, when the equations of motion hold, i.e. in the semiclassical sector of the path integral (critical points of the action). But that is hardly surprising. The quantum effects, that is, the fluctuations and higher correlations will receive corrections coming from the measure factor and one completely misses them if one postulates the naive covariant measure $[dq] \exp(iS)$. Notice also that the path integral remembers the gauge fixing condition explicitly through the dependence of the wave functions, as well as the exponential of the current, on Q^A only, rather than all of q^a , which are adapted to G .

Finally we should mention that performing the momentum space integral will be technically impossible to do exactly and the saddle point approximation may only be a poor substitute for it yielding large errors the possibility for which we indicated by V' which, however, will also be hard to do exactly or even perturbatively. Even if it can be done perturbatively, the corresponding series may not converge. Especially in such situations, a naive quantisation based on the configuration space path integral with the exponent of the classical action as weight may have little to do with the correct quantisation of the system.

4 Operator Constraint Quantisation Path Integral

In this section we are going to derive the path integral formulation using Dirac's operator constraint formalism in the language of rigging maps using the always locally available linearised constraints. For more global, rigorous results, see e.g. [40].

As already mentioned, in the presence of second class constraints, operator constraint quantisation is in general impossible if one does not pass to local Darboux coordinates with respect to the Dirac bracket because otherwise one does not find representations of the canonical commutation relations. Hence we assume that we have passed from the global conjugate pairs (q^a, p_a) to local conjugate pairs $(z_\Sigma) = (x^\sigma, y_\sigma), (\phi^\mu, \pi_\mu), (Q^A, P_A)$ in terms of which the second and first class constraints respectively can be reformulated as $S_\Sigma = 0 \Leftrightarrow z_\Sigma = 0$ and $F_\mu = 0 \Leftrightarrow F'_\mu = \pi_\mu + h'_\mu(\phi; Q, P) = 0$. The F'_μ are Abelian $\{F'_\mu, F'_\nu\} = 0$ and first class $\{F'_\mu, z_\Sigma\} = 0$ while $\{y_\sigma, x^{\sigma'}\} = \delta_{\sigma}^{\sigma'}$ and thus the Dirac bracket on functions of ϕ, π, Q, P reduces to the Poisson bracket.

On the assumption that the constraints F'_μ can be quantised without anomalies on the kinematical Hilbert space $\mathcal{H}_{\text{kin}} = L_2(dQd\Phi)$, that is, $[F'_\mu, F'_\nu] = 0$ we define a rigging map heuristically as (one has to be careful with domains and ranges and η should be defined as anti-linear map, however we do not need to enter the discussion of these niceties here, see [17] for further information)

$$\eta : \mathcal{H}_{\text{kin}} \rightarrow \mathcal{H}_{\text{phys}}; \psi \mapsto [\eta(\psi)](\phi, Q) = \int [d\beta/(2\pi)] [e^{i\beta^\mu F'_\mu} \psi](\phi, Q) \quad (4.1)$$

In the case at hand we can easily bring (4.1) into a form from which it is obvious that it solves the constraints $F'_\mu = 0$. First of all we notice that (4.1) can be formally written as

$$\eta(\psi) = \prod_{\mu} \delta(F'_\mu) \psi \quad (4.2)$$

where the order of the δ distributions is irrelevant due to the Abelianess of the constraints. This is not the case for the F_μ which is why the heuristic projector defined in [41] does not solve the constraints. This is already a hint that (4.1) indeed solves the constraints. To actually prove it we notice that $e^{i\beta^\mu \pi_\mu} \psi(\phi) = \psi(\phi - \beta)$ and so (we suppress the Q argument in what follows)

$$[\eta(\psi)](\phi) = \int [d\beta/(2\pi)] V(\beta) \psi(\phi - \beta) = \int [d\beta/(2\pi)] V(\phi - \beta) \psi(\beta) \quad (4.3)$$

where

$$V(\beta) = e^{\beta^\mu [\pi_\mu + h'_\mu(\phi)]} e^{-i\beta^\mu \pi_\mu} \quad (4.4)$$

Using

$$e^{i\beta^\mu \pi_\mu} h'_\nu(\phi) e^{-i\beta^\mu \pi_\mu} = h'_\nu(\phi - \beta) \quad (4.5)$$

we derive

$$\frac{1}{i} \frac{\partial V(\beta)}{\partial \beta^\mu} = V(\beta) h'_\mu(\phi - \beta) \quad (4.6)$$

Denoting $\beta(t) := \beta_1 + t(\beta_2 - \beta_1)$ it follows

$$V(\beta_2) - V(\beta_1) = \int_0^1 dt_1 \frac{d}{dt_1} V(\beta(t_1)) = i \int_0^1 dt_1 V(\beta(t_1)) \dot{\beta}^\mu(0) h'_\mu(\phi - \beta(t_1)) \quad (4.7)$$

where we noticed that $\dot{\beta}(t) = \dot{\beta}(0) = \beta_2 - \beta_1 = \text{const.}$ Equation (4.7) can be iterated into a Dyson series: We need

$$\beta_{t_1}(t_2) = \beta_1 + t_2(\beta(t_1) - \beta_1) = \beta_1 + t_1 t_2 (\beta_2 - \beta_1) = \beta(t_1 t_2) \quad (4.8)$$

so that

$$\begin{aligned} V(\beta(t_1)) - V(\beta_1) &= \int_0^1 dt_2 \frac{d}{dt_2} V(\beta_{t_1}(t_2)) = i \int_0^1 dt_2 V(\beta_{t_1}(t_2)) t_1 \dot{\beta}^\mu(0) h'_\mu(\phi - \beta_{t_1}(t_2)) \\ &= i \int_0^{t_1} dt_2 V(\beta(t_2)) \dot{\beta}^\mu(0) h'_\mu(\phi - \beta(t_2)) \end{aligned} \quad (4.9)$$

Accordingly we obtain for any β_2, β_1

$$V(\beta_1)^{-1} V(\beta_2) = T_l \exp(i \int_0^1 dt [\beta_2 - \beta_1]^\mu h'_\mu(\phi - \beta_1 - t(\beta_2 - \beta_1))) \quad (4.10)$$

where the path ordering symbol T_l orders the earliest time to the left. Choosing $\beta_1 = \phi, \beta_2 = \phi - \beta$ we find

$$V(\phi - \beta) = V(\phi) T_l \exp(-i \int_0^1 dt \beta^\mu h'_\mu(t\beta)) =: V(\phi) U(\beta) \quad (4.11)$$

where, using again (4.10) with $\beta_2 = \phi, \beta_1 = 0$ and noticing from the definition (4.4) that $V(0) = 1$

$$V(\phi) = T_l \exp(i \int_0^1 dt \phi^\mu h'_\mu(\phi(1-t))) = T_r \exp(i \int_0^1 dt \phi^\mu h'_\mu(\phi t)) \quad (4.12)$$

where we have performed the change of variables $t \mapsto 1-t$ which switches T_l to T_r which orders the earliest time to the right. For later use we notice the identity

$$U(\beta) = V(\beta)^{-1} = V(\beta)^\dagger \quad (4.13)$$

which establishes unitarity of $V(\beta)$ (as an operator on $L_2(dQ)$) and can easist be demonstrated by writing $V(\beta)$ in the form

$$V(\beta) = \lim_{N \rightarrow \infty} e^{\frac{i}{N} \beta^\mu h'_\mu(\beta)} e^{\frac{i}{N} \beta^\mu h'_\mu(\frac{N-1}{N} \beta)} e^{\frac{i}{N} \beta^\mu h'_\mu(\frac{N-2}{N} \beta)} \dots e^{\frac{i}{N} \beta^\mu h'_\mu(\frac{1}{N} \beta)} \quad (4.14)$$

The point of these manipulations is that we can now write

$$[\eta(\psi)](\phi, Q) = V(\phi) [\eta'(\psi)](Q), \quad [\eta'(\psi)](Q) = \int [d\beta / (2\pi)] V(\beta)^{-1} \psi(\beta, Q) \quad (4.15)$$

Obviously $\eta'(\psi)$ no longer depends on ϕ so that the rigging map essentially produces functions whose ϕ dependence is restricted to be of the form $V(\phi) \Psi(Q)$ for suitable $\Psi \in L_2(dQ)$. In order to show that such functions really solve

$F'_\mu = 0$ it is very crucial that $[F'_\mu, F'_\nu] = 0$, otherwise this does not hold. Essentially, the proof boils down to showing (we again suppress the Q dependence)

$$\left[\frac{\partial}{\partial\phi^\mu} - ih'_\mu(\phi)\right]V(\phi) = 0 \quad (4.16)$$

This almost looks like a parallel transport equation on ϕ space with respect to a one form $-ih'_\mu(\phi)$ with values in a Lie algebra of (anti – self adjoint) operators on $L_2(dQ)$ defined on a common dense and invariant domain and $V(\phi)$ looks like its holonomy along the path $t \mapsto t\phi$. The difference with the parallel equation is of course that the latter is an ODE while (4.16) is a system of PDE's so that the issue of integrability arises and so the following theorem is not trivial (notice that we *do not* need to assume $\partial_{[\mu}h'_{\nu]} = 0$). Its validity rests on the fact that

$$[F'_\mu, F'_\nu] = -\{2\partial_{[\mu}(-ih'_{\nu]} + [(-ih'_\mu), (-ih'_\nu)]\} = 0 \quad (4.17)$$

i.e. that the curvature of the connection $-ih'_\mu$ vanishes.

Theorem 4.1.

Equation (4.16) holds pointwise in ϕ space on a dense set of analytic vectors¹⁸ for the operator $h'(\phi) = \phi^\mu h'_\mu(\phi)$.

Proof. Let $V_0(\phi) := 1$ for $N \in \mathbb{N}_0$ and for $N > 0$

$$V_N(\phi) = 1 + \sum_{n=1}^N i^n \int_0^1 dt_1 \phi^{y_1} h'_{\nu_1}(t_1\phi) \dots \int_0^{t_{n-1}} dt_n \phi^{y_n} h'_{\nu_n}(t_n\phi) \quad (4.18)$$

Clearly $\lim_{N \rightarrow \infty} V_N(\phi) = V(\phi)$ converges on analytic vectors for $h'(\phi) := \phi^\mu h'_\mu(\phi)$. We define for $N > 0$ the remainder

$$R_N(\phi) = -i^{N-1} \sum_{n=1}^N \int_0^1 dt_1 \phi^{y_1} h'_{\nu_1}(t_1\phi) \dots \int_0^{t_{n-1}} dt_n t_n \phi^{y_n} \{[h'_\mu, h'_{\nu_1}]\}(t_n\phi) \dots \int_0^{t_{N-1}} dt_N \phi^{y_N} h'_{\nu_N}(t_N\phi) \quad (4.19)$$

and prove by induction for $N > 0$ that

$$\partial_\mu V_N(\phi) = ih'_\mu(\phi) V_{N-1}(\phi) + R_N(\phi) \quad (4.20)$$

By definition, on analytic vectors of $h'(\phi)$ the norm of the remainder converges (pointwise in ϕ space) to zero (it is of order $1/[(N-1)!]$) so that once that (4.20) is established, the proof is complete.

For $N = 1$ we obtain

$$\begin{aligned} \partial_\mu V_1(\phi) &= i \int_0^1 dt [h'_\mu(t\phi) + t\phi^y (\partial_\mu h'_\nu)(t\phi)] \\ &= i \int_0^1 dt \left[\frac{d}{dt} [t h'_\mu(t\phi)] + 2t\phi^y (\partial_{[\mu} h'_{\nu]})(t\phi) \right] \\ &= ih'_\mu(\phi) - \int_0^1 dt \{t\phi^y ([h'_\mu, h'_\nu])(t\phi)\} \\ &= ih'_\mu(\phi)V_0(\pi) + R_1(\phi) \end{aligned} \quad (4.21)$$

where in the third step we used

$$[F'_\mu, F'_\nu] = 0 \Leftrightarrow 2i\partial_{[\mu}h'_{\nu]} + [h'_\mu, h'_\nu] = 0 \quad (4.22)$$

¹⁸A vector ψ is called analytic for an operator A if $\|A^n \psi\| < \infty$ for all n and $\sum_{n=0}^\infty t^n \|A^n \psi\|/(n!) < \infty$ for some $t > 0$.

Assuming that (4.20) holds up to N we compute

$$\begin{aligned}
& \partial_\mu(V_{N+1} - V_N) = i^{N+1} \partial_\mu \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&= i^{N+1} \sum_{n=1}^{N+1} \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-1}} dt_n [h'_\mu(t_n \phi) + t_n \phi^{v_n} (\partial_\mu h'_{v_n})(t_n \phi)] \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&= i^{N+1} \sum_{n=1}^{N+1} \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-1}} dt_n \left[\frac{d}{dt_n} (t_n h'_\mu(t_n \phi)) + 2t_n \phi^{v_n} (\partial_\mu h'_{v_n})(t_n \phi) \right] \dots \dots \\
&\quad \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&= i^{N+1} \sum_{n=1}^{N+1} \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-2}} dt_{n-1} \phi^{v_{n-1}} h'_{v_{n-1}}(t_{n-1} \phi) \int_0^{t_{n-1}} dt_n \left[\frac{d}{dt_n} (t_n h'_\mu(t_n \phi)) \right] \times \\
&\quad \times \int_0^{t_n} dt_{n+1} \phi^{v_{n+1}} h'_{v_{n+1}}(t_{n+1} \phi) \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&\quad - i^N \sum_{n=1}^{N+1} \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-1}} dt_n t_n \phi^{v_n} ([h'_\mu, h'_{v_n}](t_n \phi)) \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&= R_{N+1} + i h'_\mu(\phi) [V_N(\phi) - V_{N-1}(\phi)] \\
&\quad + i^{N+1} \sum_{n=2}^{N+1} \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-2}} dt_{n-1} \phi^{v_{n-1}} h'_{v_{n-1}}(t_{n-1} \phi) t_{n-1} h'_\mu(t_{n-1} \phi) \times \\
&\quad \times \int_0^{t_{n-1}} dt_{n+1} \phi^{v_{n+1}} h'_{v_{n+1}}(t_{n+1} \phi) \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&\quad - i^{N+1} \sum_{n=1}^N \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-2}} dt_{n-1} \phi^{v_{n-1}} h'_{v_{n-1}}(t_{n-1} \phi) \int_0^{t_{n-1}} dt_n t_n h'_\mu(t_n \phi) \phi^{v_n} h'_{v_n}(t_n \phi) \times \\
&\quad \times \int_0^{t_n} dt_{n+2} \phi^{v_{n+2}} h'_{v_{n+2}}(t_{n+2} \phi) \dots \int_0^{t_N} dt_{N+1} \phi^{v_{N+1}} h'_{v_{N+1}}(t_{N+1} \phi) \\
&= R_{N+1} + i h'_\mu(\phi) [V_N(\phi) - V_{N-1}(\phi)] \\
&\quad - i^{N-1} \sum_{n=1}^N \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-1}} dt_n \phi^{v_n} h'_{v_n}(t_n \phi) t_n h'_\mu(t_n \phi) \dots \int_0^{t_{N-1}} dt_N \phi^{v_N} h'_{v_N}(t_N \phi) \\
&\quad + i^{N-1} \sum_{n=1}^N \int_0^1 dt_1 \phi^{v_1} h'_{v_1}(t_1 \phi) \dots \int_0^{t_{n-1}} dt_n t_n h'_\mu(t_n \phi) \phi^{v_n} h'_{v_n}(t_n \phi) \dots \int_0^{t_{N-1}} dt_N \phi^{v_N} h'_{v_N}(t_N \phi) \\
&= R_{N+1} + i h'_\mu(\phi) [V_N(\phi) - V_{N-1}(\phi)] - R_N \tag{4.23}
\end{aligned}$$

In the fourth step we have separated two contributions and the second is easily recognized as the definition of R_{N+1} . The non trivial step was the fifth one where we performed an integration by parts in the first contribution which produces two sums. We have set $t_0 = 1$ in the first sum and in the second in the last term the integral over t_{N+2} etc. is just unity. In the sixth step we have relabeled in the first sum in the n -th term $t_{n+1} \rightarrow t_n, \dots, t_{N+1} \rightarrow t_N$ and then reset the summation range to $n = 1, \dots, N$. In the second sum in the n -th term we have relabeled $t_{n+2} \rightarrow t_{n+1}, \dots, t_{N+1} \rightarrow t_N$ which combines the two sums to $-R_N$.

Thus, by assumption (4.20)

$$\partial_\mu V_{N+1} = [\partial_\mu V_N - i h'_\mu V_{N-1} - R_N] + i h'_\mu V_N + R_{N+1} = i h'_\mu V_N + R_{N+1} \tag{4.24}$$

□

Having shown that the rigging map is well defined and produces solutions to the constraints F'_μ we can compute the physical inner product between states $\eta(\psi)$ defined by (we drop the factors $1/(2\pi)$ as the physical inner product is

defined only up to a scale)

$$\begin{aligned}
\langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}} &:= \langle \psi, \eta(\psi') \rangle_{\text{kin}} \\
&= \int [d\phi] \int [dQ] \overline{\psi(\phi, Q)} [\eta(\psi')](\phi, Q) \\
&= \int [d\phi] \int [dQ] \overline{\psi(\phi, Q)} V(\phi) [\eta'(\psi')](Q) \\
&= \int [d\phi] \langle \psi(\phi, \cdot), V(\phi) \eta'(\psi') \rangle_{L_2(dQ)} \\
&= \langle \int [d\phi] V(\phi)^{-1} \psi(\phi, \cdot), \eta'(\psi') \rangle_{L_2(dQ)} \\
&= \langle \eta'(\psi), \eta'(\psi') \rangle_{L_2(dQ)} \tag{4.25}
\end{aligned}$$

where $\eta'(\psi)$ was defined in (4.15). This calculation demonstrates that the physical Hilbert space can be identified with the Hilbert space $\mathcal{H}_{\text{red}} := L_2(dQ)$ which we obtained also in the reduced phase space approach. The identification is established by

$$W : \mathcal{H}_{\text{red}} \rightarrow \mathcal{H}_{\text{phys}} \quad \Psi(Q) \mapsto V(\phi)\Psi(Q) \tag{4.26}$$

$\mathcal{H}_{\text{phys}}$ can also be recognised as the (closure of the) set of equivalence classes of vectors in \mathcal{H}_{kin} where $\psi \sim \psi'$ iff $\eta'(\psi) = \eta'(\psi')$ are the same $L_2(dQ)$ functions. Notice that η' is not a projector, $[\eta']^2$ is ill defined.

It is worthy pointing out the importance of the knowledge of the map (4.26): Often one only knows a path integral expression for $\langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}}$ in terms of the boundary states ψ, ψ' which, however, lack any physical interpretation, they are not gauge invariant. The vectors $\eta(\psi)$ are gauge invariant, however, the path integral expression which we will also derive below is not in terms of $\eta(\psi)$ but in terms of ψ , $\eta(\psi)$ is often not known explicitly. In the case considered here, $\eta(\psi)$ is known explicitly: Neglecting about the details of the domains of the maps we have $\eta(\mathcal{H}_{\text{kin}}) = W(\mathcal{H}_{\text{red}})$ and since W just operates by a unitary operator with a specific ϕ dependence, all the non trivial physical information is contained in \mathcal{H}_{red} .

To make the link with the path integral formulation now does not require much further work. For any $\Psi, \Psi' \in \mathcal{H}_{\text{red}}$ pick $\psi, \psi' \in \mathcal{H}_{\text{kin}}$ with $\eta'(\psi) = \Psi$, $\eta'(\psi') = \Psi'$. Any such Ψ is generated from the cyclic vacuum vector Ω (a ground state vector under the time evolution, i.e. a stationary vector under $H_{\text{red}}(t)$ for some fixed value of t ; in the case of a conservative system, the choice of this t is irrelevant) by operating with (limits of) polynomials f of the operators Q^A . On the other hand, from the point of view of $\mathcal{H}_{\text{phys}}$ the operators Q^A are ill defined because they are not gauge invariant, or in other words $Q^A \eta(\psi)$ is not annihilated by the F'_μ . The following operators, however, preserve $\mathcal{H}_{\text{phys}}$

$$\tilde{Q}^A = [\exp(i\beta^\mu F'_\mu) Q^A \exp(-i\beta^\mu F'_\mu)]_{\beta=\phi} \tag{4.27}$$

which is the quantisation of the corresponding classical formula (2.23) upon replacing $\{F'_\mu, Q^A\}_{(n)}$ by $[F'_\mu, Q^A]_{(n)}/i^n$. To show that $[F'_\mu, \tilde{Q}^A] = 0$ we notice that since $[\pi_\mu, Q^A] = 0$ we have with the definition of $V(\beta)$ (4.4)

$$\begin{aligned}
\tilde{Q}^A &= [\exp(i\beta^\mu F'_\mu) e^{-i\beta^\mu \pi_\mu} Q^A e^{i\beta^\mu \pi_\mu} \exp(-i\beta^\mu F'_\mu)]_{\beta=\phi} \\
&= V(\phi) Q^A V(\phi)^{-1} \tag{4.28}
\end{aligned}$$

Notice that \tilde{Q}^A is self-adjoint on $\mathcal{H}_{\text{phys}}$ if Q^A is on \mathcal{H}_{red} . Since any physical state is of the form $V(\phi)\Psi(Q)$ it is obvious that \tilde{Q}^A preserves $\mathcal{H}_{\text{phys}}$ by theorem 4.1. We conclude

$$\langle \Psi, \Psi' \rangle_{\text{red}} = \langle \Omega, f(Q)^\dagger f'(Q) \Omega \rangle_{\text{red}} = \langle W\Psi, W\Psi' \rangle_{\text{phys}} = \langle W\Omega, f(\tilde{Q})^\dagger f'(\tilde{Q}) W\Omega \rangle_{\text{phys}} \tag{4.29}$$

We see that the physical scalar product can be directly related to the reduced Hilbert space inner product. Now we just need to relate the latter to the n-point functions already derived in the previous section. But this is easy: Evidently (4.29) is a finite linear combination of monomials of the form

$$\langle \Omega, Q^{A_1} \dots Q^{A_n} \Omega \rangle_{\text{red}} \tag{4.30}$$

which is the coincidence limit of an n-point function

$$\lim_{t_1, \dots, t_n \rightarrow t} \langle \Omega, Q^{A_1}(t_1) \dots Q^{A_n}(t_n) \Omega \rangle_{\text{red}} \quad (4.31)$$

for arbitrary t . In interacting Wightman QFT's it is expected that such equal time correlators are too singular [11]. On the other hand, if the theory can be canonically quantised at all then such limits must exist as otherwise the notion of equal time commutation relations is meaningless and therefore presumably violates at least one of the Wightman axioms, e.g. the uniqueness of the vacuum. In any case, we derived a path integral formula for the right hand side of (4.31) in terms of a path integral for the generating functional.

There is also a more direct derivation for a path integral formula for $\langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}}$ for which, however, the relation to the reduced phase space path integral is less clear. On the other hand that alternative derivation makes the connection to the Master constraint path integral clearer. We will thus display it here for completeness. We start from the definition of the rigging map (4.1), choose some arbitrary but fixed reference vector Ω_0 and normalise the physical inner product by asking that the norm of $\eta(\psi)$ be unity. Thus we have to divide (4.1) by a constant up to which the inner product is anyway undetermined and obtain

$$\langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}} = \frac{\int [d\beta] \langle \psi, e^{i\beta^\mu F'_\mu} \psi' \rangle_{\text{kin}}}{\int [d\beta] \langle \Omega_0, e^{i\beta^\mu F'_\mu} \Omega_0 \rangle_{\text{kin}}} \quad (4.32)$$

Notice that (4.32) is not a path integral over β , it is just an integral at fixed time of the Lagrange multipliers β^μ . In order to introduce a path integral of Lagrange multipliers we introduce an arbitrary time parameter T which we will eventually send to ∞ and multiply both numerator and denominator of (4.32) by the infinite constant

$$C = \int [D\lambda] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t)\right) \quad (4.33)$$

which is a path integral over paths $t \mapsto \lambda(t)$, $t \in [-T, T]$. By shifting the integration variable $\lambda(t) = \lambda'(t) - \frac{1}{2T}\beta$ for any constant path $\beta/(2T)$ we see that C can also be written

$$C = \int [D\lambda] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t) - \beta^\mu\right) \quad (4.34)$$

where β is arbitrary. Inserting this into (4.32) and interchanging the $[D\lambda]$, $[d\beta]$ integrals we obtain

$$\begin{aligned} \langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}} &= \frac{\int [d\beta] \langle \psi, e^{i\beta^\mu F'_\mu} \psi' \rangle_{\text{kin}} \left[\int [D\lambda] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t) - \beta^\mu\right) \right]}{\int [d\beta] \langle \Omega_0, e^{i\beta^\mu F'_\mu} \Omega_0 \rangle_{\text{kin}} \left[\int [D\lambda] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t) - \beta^\mu\right) \right]} \\ &= \frac{\int [D\lambda] \langle \psi, e^{i\int_{-T}^T dt \lambda^\mu(t) F'_\mu} \psi' \rangle_{\text{kin}} \left[\int [d\beta] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t) - \beta^\mu\right) \right]}{\int [D\lambda] \langle \Omega_0, e^{i\int_{-T}^T dt \lambda^\mu(t) F'_\mu} \Omega_0 \rangle_{\text{kin}} \left[\int [d\beta] \prod_\mu \delta\left(\int_{-T}^T dt \lambda^\mu(t) - \beta^\mu\right) \right]} \\ &= \frac{\int [D\lambda] \langle \psi, e^{i\int_{-T}^T dt \lambda^\mu(t) F'_\mu} \psi' \rangle_{\text{kin}}}{\int [D\lambda] \langle \Omega_0, e^{i\int_{-T}^T dt \lambda^\mu(t) F'_\mu} \Omega_0 \rangle_{\text{kin}}} \end{aligned} \quad (4.35)$$

By writing

$$\left[\int_{-T}^T dt \lambda^\mu(t) \right] F'_\mu = \lim_{N \rightarrow \infty} \frac{1}{2N} \sum_{n=-N}^{N-1} \lambda^\mu(nT/N) F'_\mu \quad (4.36)$$

we finally obtain using the usual skeletonisation techniques

$$\langle \eta(\psi), \eta(\psi') \rangle = \frac{\int [DQ DP D\phi D\pi D\lambda] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) e^{i \int_{-T}^T dt P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu - \lambda^\mu F'_\mu(Q, P, \phi, \pi)}}{\int [DQ DP D\phi D\pi D\lambda] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) e^{i \int_{-T}^T dt P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu - \lambda^\mu F'_\mu(Q, P, \phi, \pi)}} \quad (4.37)$$

Notice that all canonical coordinates and Lagrange multipliers are integrated over paths in time in the interval $[-T, T]$ and that the operator F'_μ has been replaced by the classical function in (4.36). In this expression the parameter T is arbitrary and we can take $T \rightarrow \infty$.

In order to invoke the gauge fixing conditions $G_\mu = \tau^\mu(t) - \phi^\mu$ we will make use of the Fadeev – Popov procedure: Let $\alpha_{\gamma(t)} = \exp(\gamma^\mu(t)\{F'_\mu(t), \cdot\})$ where $F'_\mu(t) = F'_\mu(u(t))$ is the constraint on the copy of the phase space at time t and $u(t) = (Q(t), P(t), \phi(t), \pi(t))$. Then $\alpha_{\gamma(t)}(G^\mu(t)) = G^\mu(t) + \gamma^\mu(t)$ so that in this case trivially

$$\int [D\gamma] \prod_{t,\mu} \delta(\alpha_{\gamma(t)}(G^\mu(t))) = 1 \quad (4.38)$$

We multiply both numerator and denominator of (4.37) by this unity. Assuming $\lim_{T \rightarrow \infty} \gamma(\pm T) = 0$ the kinetic term in the exponential of (4.37) is invariant (being a symplectic potential), F'_μ is invariant due to the Abelianess and the Liouville measure at time t is invariant under the canonical transformations $\alpha_{\gamma(t)}$. Thus after a change of variables from $u \rightarrow \alpha_{\gamma}(u)$ and since $[\alpha_{\gamma}(G)](u) = G(\alpha_{\gamma}(u))$ nothing depends on γ anymore and the integral over $D\gamma$ can be dropped. We obtain

$$\langle \eta(\psi), \eta(\psi') \rangle = \frac{\int [DQ DP D\phi D\pi] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) \delta[F'] \delta[G] e^{i \int_{-T}^T dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu]} \int [DQ DP D\phi D\pi] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) \delta[F'] \delta[G] e^{i \int_{-T}^T dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu]} \quad (4.39)$$

where we have also integrated over λ .

Finally, in order to invoke the second class constraints in the form $z_\Sigma = (x^\sigma, y_\sigma) = 0$ we simply insert a $\delta[z]$ distribution and integrate over z . This yields

$$\langle \eta(\psi), \eta(\psi') \rangle = \frac{\int [DQ DP D\phi D\pi Dx Dy] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) \delta[F'] \delta[G] \delta[z] e^{i \int_{-T}^T dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu + y_\sigma \dot{x}^\sigma]} \int [DQ DP D\phi D\pi Dx Dy] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) \delta[F'] \delta[G] \delta[z] e^{i \int_{-T}^T dt [P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu + y_\sigma \dot{x}^\sigma]} \quad (4.40)$$

Next we observe that $\det(\{F', G\}), \det(\{z, z\})$ are constant in the system of coordinates chosen so we can multiply numerator and denominator of (4.40) by these constants. As established in section 3, the expression

$$\delta[F'] \delta[G] \delta[z] |\det(\{F', G\})| \sqrt{\det(\{z, z\})} \quad (4.41)$$

is invariant under any mapping $(F', G, z) \mapsto (F, G', S)$ as long as both triples reduce to the same gauge cut of the same constraint surface. We may therefore restore the original first and second class constraints F, S while keeping $G = G'$ provided we keep the determinant factors in (4.41). Finally we can restore the original system of coordinates q^a, p_a which arise from $(q'^a, p'_a) := (Q^A, P_A), (\phi^\mu, \pi_\mu), (x^\sigma, y_\sigma)$ by a canonical transformation α because the symplectic potential in the exponent of (4.40) as well as the Liouville measure remain invariant and the Poisson brackets are simply expressed in the new coordinates, e.g.

$$\{S, S\}(q', p') = \{S, S\}(\alpha(q, p)) = \{S \circ \alpha, S \circ \alpha\}(q, p) \quad (4.42)$$

(by S we denote the original S expressed in whatever canonical coordinates). Accordingly

$$\langle \eta(\psi), \eta(\psi') \rangle = \frac{\int [Dq Dp] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) \delta[F] \delta[G] \delta[S] |\det(\{F, G\})| \sqrt{\det(\{S, S\})} e^{i \int_{-T}^T dt p_a \dot{q}^a} \int [Dq Dp] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) \delta[F] \delta[G] \delta[S] |\det(\{F, G\})| \sqrt{\det(\{S, S\})} e^{i \int_{-T}^T dt p_a \dot{q}^a} \quad (4.43)$$

Notice that due to the gauge fixing condition $G(t) = \tau(t) - \phi(t)$ the integral over ϕ is anyway concentrated at the fixed path $\tau(t)$ so that it is allowed to assume that ψ, ψ', Ω are actually independent of ϕ . In this sense the final result (4.43) precisely agrees with (3.70) with the understanding that ψ, ψ' in (4.43) can be generated from the generating functional (3.70) by suitable functional differentiation with respect to the current j at $j = 0$ at coincident points of time $\pm T$ in the limit $T \rightarrow \infty$.

5 Master Constraint Path Integral

The Master Constraint Programme (MCP) was originally designed precisely in order to be able to cope with gauge systems whose classical first class constraint algebra involves structure functions [16] and for which therefore group averaging techniques do not work. It is true that locally the first class constraints F can be replaced by equivalent ones whose algebra is Abelian and we have made heavy use of that fact in the two previous sections. However, for the case of interest, namely General Relativity, in vacuum the Abelian constraints are rather non local on the spatial manifold, algebraically difficult to deal with and not explicitly known even classically [42]. Even with standard matter this is true. It is for this reason that in [10, 33] non standard matter (Brown – Kuchař Dust [43]) was used in order to achieve the Abelianisation in a local form and such that the resulting expressions remain practically manageable. The MCP does not rely on Abelianisation and thus is both more global (on phase space) in character and does not require any special type of matter. In principle it does not even require that the constraints are quantised without anomalies and even second class constraints can be treated by the MCP [16]. Since the Master Constraint is a weighted sum of squares of the first class constraints, we expect that its kernel is empty when the constraints are not quantised without anomalies. In that case one could consider the Hilbert “subspace” corresponding to the lowest “eigenvalue” as the suitable substitute for the anomaly free situation. See [16] for further discussion. In that sense the MCP may be considered as a much more flexible approach to constrained systems with structure functions.

While for a wide range of models the MCP has been tested versus the more traditional operator constraint method [16], its equivalence with the latter is so far lacking. On the one hand, the equivalence seems to be obvious since both the Master constraint and the individual constraints are supposed to define the same (common) kernel. On the other hand, the equivalence is rather not obvious because the formulae for defining the physical inner product or equivalently the rigging map are totally different. For the individual constraints in Abelianised form the rigging map is defined in (4.1) while for the MCP it is heuristically defined by¹⁹

$$\eta_M : \mathcal{H}_{\text{kin}} \rightarrow \mathcal{H}_{\text{phys}}^M; \psi \mapsto \int_{\mathbb{R}} \frac{dt}{2\pi} e^{itM} \psi \quad (5.1)$$

where the Master constraint is defined by

$$M = \sum_{\mu, \nu} F_{\mu}^{\dagger} K_{\mu\nu} F_{\nu} \quad (5.2)$$

The symmetric (possibly operator valued) matrix K should be so chosen such that M is positive and such that it arises from a classically positive definite matrix valued function on phase space. There is great flexibility in the choice of K and while all (sufficiently differentiable) positive definite classical matrices are equivalent, in quantum theory this flexibility must be exploited in order to arrive at well defined master Constraint Operators [16]. Normally we require that F_{μ} is quantised as a self adjoint operator but in the case of structure functions this must be relaxed [16] which is why we included the adjoint in (5.2).

The task of the present section is to connect with the results of the previous two sections. Those sections made use of the Abelian constraints F'_{μ} and we will therefore use those in order to build our Master Constraint. We assume as in sections 3 and 4 that F'_{μ} is self – adjoint since the F'_{μ} are supposed to be quantised without anomalies. As in the previous section we choose a reference vector Ω_0 and define the Master Constraint physical inner product by

$$\langle \eta_M(\psi), \eta_M(\psi') \rangle_{\text{phys}}^M := \frac{\int_{\mathbb{R}} dt \langle \psi, e^{itM} \psi' \rangle_{\text{kin}}}{\int_{\mathbb{R}} dt \langle \Omega_0, e^{itM} \Omega_0 \rangle_{\text{kin}}} \quad (5.3)$$

To see that (4.1) and (5.3) formally coincide, recall [4] that for any self – adjoint operator A on a (separable²⁰) Hilbert

¹⁹Again there are subtle domain issues which we neglect here and moreover one should switch to a direct integral representation of \mathcal{H}_{kin} subordinate to M ; see [16] for details.

²⁰In LQG the Hilbert space is not separable but the operator M preserves the separable subspaces into which the Hilbert space decomposes

space there exists a unitary transformation (generalised Fourier transform)

$$U : \mathcal{H} \rightarrow \mathcal{H}^\oplus := \int_{\text{spec}(A)} d\mu(\lambda) \mathcal{H}_\lambda^\oplus; \quad \psi \mapsto (\tilde{\psi}(\lambda))_{\lambda \in \text{spec}(A)} \quad (5.4)$$

from \mathcal{H} to a direct integral of Hilbert spaces $\mathcal{H}_\lambda^\oplus$ (possibly with different dimensions for each λ but in a measurable way, hence more general than a Hilbert bundle) with respect to a probability measure μ on the spectrum $\text{spec}(A)$ of A . Here $\tilde{\psi}(\lambda) \in \mathcal{H}_\lambda^\oplus$. The correspondence between the inner products is

$$\langle \psi, \psi' \rangle_{\mathcal{H}} = \langle \tilde{\psi}, \tilde{\psi}' \rangle_{\mathcal{H}^\oplus} := \int_{\text{spec}(A)} d\mu(\lambda) \langle \tilde{\psi}(\lambda), \tilde{\psi}'(\lambda) \rangle_{\mathcal{H}_\lambda^\oplus} \quad (5.5)$$

The point of this spectral decomposition is that $[UAU^{-1}\tilde{\psi}](\lambda) = \lambda\tilde{\psi}(\lambda)$, i.e. A acts by multiplication by λ on $\mathcal{H}_\lambda^\oplus$. If (the spectral projections of) two self – adjoint operators A, B commute then UBU^{-1} preserves $\mathcal{H}_\lambda^\oplus$ and we may apply the just quoted theorem which then tells us that there exists a joint probability measure $d\mu(\lambda_A, \lambda_B)$ on the joint spectrum $\text{spec}(\{A, B\}) = \text{spec}(A) \times \text{spec}(B)$ of A, B and a representation of \mathcal{H} as a direct integral of Hilbert spaces $\mathcal{H}_{\lambda_A, \lambda_B}^\oplus$ on which A, B respectively act by multiplication by λ_A, λ_B respectively.

Iterating like that we obtain the statement that for a (countable) family of mutually commuting self – adjoint operators F'_μ there exists a unitary operator U from \mathcal{H}_{kin} to \mathcal{H}^\oplus which is the direct integral with respect to a measure μ on the joint spectrum of the F'_μ of Hilbert spaces $\mathcal{H}_{\{\lambda_\mu\}_\mu}^\oplus$ on which $UF'_\mu U^{-1}$ acts by multiplication by λ_μ . This is the key to link (5.3) and (4.1). Namely we formally obtain for (4.1)

$$\begin{aligned} \langle \eta(\psi), \eta(\psi') \rangle_{\text{phys}} &= \frac{\int [d\beta] \langle \psi, e^{i\beta^\mu F'_\mu} \psi' \rangle_{\text{kin}}}{\int [d\beta] \langle \Omega_0, e^{i\beta^\mu F'_\mu} \Omega_0 \rangle_{\text{kin}}} \\ &= \frac{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\psi}(\{\lambda\}), \tilde{\psi}'(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^\oplus} [\int [d\beta] e^{i\beta^\mu \lambda_\mu}]}{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\Omega}_0(\{\lambda\}), \tilde{\Omega}_0(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^\oplus} [\int [d\beta] e^{i\beta^\mu \lambda_\mu}]} \\ &= \frac{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\psi}(\{\lambda\}), \tilde{\psi}'(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^\oplus} \delta(\{\lambda\})}{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\Omega}_0(\{\lambda\}), \tilde{\Omega}_0(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^\oplus} \delta(\{\lambda\})} \\ &= \frac{\rho(\{0\}) \langle \tilde{\psi}(\{0\}), \tilde{\psi}'(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^\oplus}}{\rho(\{0\}) \langle \tilde{\Omega}_0(\{0\}), \tilde{\Omega}_0(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^\oplus}} \\ &= \frac{\langle \tilde{\psi}(\{0\}), \tilde{\psi}'(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^\oplus}}{\langle \tilde{\Omega}_0(\{0\}), \tilde{\Omega}_0(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^\oplus}} \quad (5.6) \end{aligned}$$

where formally $d\mu(\{\lambda\}) =: \rho(\{\lambda\})[d\lambda]$. Notice that $\rho(\{\lambda\})$ can have distributional contributions if the spectrum has a pure point part, see [16, 25]. Of course there are measure theoretic issues such as: if 0 lies in the continuous spectrum of some F'_μ then $\{0\}$ has μ measure zero and $\mathcal{H}_{\{0\}}^\oplus$ is not well defined without further assumptions spelled out in [16]. For the purposes of this paper we take a formal attitude and simply let the formal cancelation of the $\rho(\{0\})$ in numerator and denominator of (5.6) take place as indicated. For a more careful definition see [25].

On the other hand we have

$$\begin{aligned}
\langle \eta_M(\psi), \eta_M(\psi') \rangle_{\text{phys}}^M &= \frac{\int dt \langle \psi, e^{itM} \psi' \rangle_{\text{kin}}}{\int dt \langle \Omega_0, e^{itM} \Omega_0 \rangle_{\text{kin}}} \\
&= \frac{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\psi}(\{\lambda\}), \tilde{\psi}'(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^{\oplus}} [\int dt e^{it \sum_{\mu,\nu} K^{\mu\nu} \lambda_\mu \lambda_\nu}]}{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\Omega}_0(\{\lambda\}), \tilde{\Omega}_0(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^{\oplus}} [\int dt e^{it \sum_{\mu,\nu} K^{\mu\nu} \lambda_\mu \lambda_\nu}]} \\
&= \frac{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\psi}(\{\lambda\}), \tilde{\psi}'(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^{\oplus}} \delta(\sum_{\mu,\nu} K^{\mu\nu} \lambda_\mu \lambda_\nu)}{\int_{\text{spec}(\{F'\})} d\mu(\{\lambda\}) \langle \tilde{\Omega}_0(\{\lambda\}), \tilde{\Omega}_0(\{\lambda\}) \rangle_{\mathcal{H}_{\{\lambda\}}^{\oplus}} \delta(\sum_{\mu,\nu} K^{\mu\nu} \lambda_\mu \lambda_\nu)} \\
&= \frac{\rho(\{0\}) J(\{0\}) \text{Vol}(S) \langle \tilde{\psi}(\{0\}), \tilde{\psi}'(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^{\oplus}}}{\rho(\{0\}) J(\{0\}) \text{Vol}(S) \langle \tilde{\Omega}_0(\{0\}), \tilde{\Omega}_0(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^{\oplus}}} \\
&= \frac{\langle \tilde{\psi}(\{0\}), \tilde{\psi}'(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^{\oplus}}}{\langle \tilde{\Omega}_0(\{0\}), \tilde{\Omega}_0(\{0\}) \rangle_{\mathcal{H}_{\{0\}}^{\oplus}}} \tag{5.7}
\end{aligned}$$

where $J(\{\lambda\})$ is the Jacobian that arises by switching from $\{\lambda\}$ to polar coordinates adapted to the radius squared $r^2 := \sum_{\mu,\nu} K^{\mu\nu} \lambda_\mu \lambda_\nu$. Of course we have assumed that $K_{\mu\nu}$ is just a complex valued positive definite matrix. $\text{Vol}(S)$ is the volume of the corresponding sphere. For countably many F'_μ the volume of the infinite dimensional sphere vanishes as well as the Jacobian at zero. To justify (5.7) less formally one has to take a limit as the number N of F'_μ approaches infinity so that $\text{Vol}(S^{N-1})$ is finite and one also has to regularise $\delta(M)$ by $\delta(M - \epsilon^2)$ and take $\epsilon \rightarrow 0$ as to make $J(\epsilon)$ finite. See [25] for the details and also (5.10) below for a sketch.

Hence (5.6) and (5.7) agree with each other modulo formal manipulations and thus give rise to the same path integral formulation. Our method of ‘‘proof’’ above used spectral theory. We will now provide a more direct (but also formal) ‘‘proof’’ using only path integral techniques. The idea is the same as at the end of section 4 and was already sketched in [16]. First of all we use the same technique as used between (4.32) and (4.37) in order to write (5.3) as

$$\begin{aligned}
\langle \eta_M(\psi), \eta_M(\psi') \rangle_{\text{phys}}^M &= \frac{\int [D\lambda] \langle \psi, e^{i \int_{-T}^T dt \lambda(t) M} \psi' \rangle_{\text{kin}}}{\int [D\lambda] \langle \Omega_0, e^{i \int_{-T}^T dt \lambda(t) M} \Omega_0 \rangle_{\text{kin}}} \\
&= \frac{\int [DQ DP D\phi D\pi D\lambda] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) e^{i \int_{-T}^T dt [(P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu)(t) - \lambda(t) M(Q(t), P(t), \phi(t), \pi(t))]}]}{\int [DQ DP D\phi D\pi D\lambda] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) e^{i \int_{-T}^T dt [(P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu)(t) - \lambda(t) M(Q(t), P(t), \phi(t), \pi(t))]}]} \\
&= \frac{\int [DQ DP D\phi D\pi] \overline{\psi(Q_T, \phi_T)} \psi'(Q_{-T}, \phi_{-T}) [\prod_{t \in [-T, T]} \delta((M(t)))] e^{i \int_{-T}^T dt [(P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu)(t)]}}{\int [DQ DP D\phi D\pi] \overline{\Omega_0(Q_T, \phi_T)} \Omega_0(Q_{-T}, \phi_{-T}) [\prod_{t \in [-T, T]} \delta((M(t)))] e^{i \int_{-T}^T dt [(P_A \dot{Q}^A + \pi_\mu \dot{\phi}^\mu)(t)]}} \tag{5.8}
\end{aligned}$$

where T is again an arbitrary parameter which we take to ∞ eventually. If in (4.37) we perform the integral over λ then the only difference between (4.37) and (5.8) is that instead of $\delta[F']$ the distribution $\delta[M]$ appears in both numerator and denominator. But clearly the two distributions have the same support $\pi = -h'(\phi, Q, P)$. Let us therefore explicitly do the integral in both (4.37) and (5.8) and compare the results. It suffices to do this at fixed t because both δ distributions factorise over $[-T, T]$. We consider $\delta(M)$ as the limit $N \rightarrow \infty, \epsilon \rightarrow 0$ of

$$\delta_{N,\epsilon}(M) := \delta\left(\sum_{\mu,\nu \leq N} K^{\mu\nu} F'_\mu F'_\nu - \epsilon^2\right) \tag{5.9}$$

Let $f = f[\pi]$ be any functional of π_μ , $\mu = 1, \dots, N$. The $N \times N$ submatrix $K_N^{\mu\nu} = K^{\mu\nu}$; $\mu, \nu \leq N$ is also positive definite on the corresponding vector subspace. Hence its square root and inverse is well defined. Thus, by shifting

the integration variable and switching to radial r and polar coordinates φ respectively we obtain with the unit vector $x_\mu/r = n_\mu(\varphi)$

$$\begin{aligned}
& \int_{\mathbb{R}^N} d^N \pi \delta_{N,\epsilon}(M) f(\pi) \\
&= \int_{\mathbb{R}^N} d^N x \delta(x^T K_N x - \epsilon^2) f(-h' + x) \\
&= \frac{1}{\sqrt{\det(K_N)}} \int_{\mathbb{R}^N} d^N x \delta(x^T x - \epsilon^2) f(-h' + K_N^{-1/2} x) \\
&= \frac{1}{\sqrt{\det(K_N)}} \int_{\mathbb{R}_+} r^{N-1} dr \delta(r^2 - \epsilon^2) \int_{S^{N-1}} d\text{Vol}(\varphi) f(-h' + K_N^{-1/2} r n(\varphi)) \\
&= \frac{\epsilon^{N-2}}{2 \sqrt{\det(K_N)}} \int_{S^{N-1}} d\text{Vol}(\varphi) f(-h' + K_N^{-1/2} \epsilon n(\varphi))
\end{aligned} \tag{5.10}$$

In the limit $\epsilon \rightarrow 0$ this approaches

$$\frac{\epsilon^{N-2}}{2 \sqrt{\det(K_N)}} \text{Vol}(S^{N-1}) f(-h') \tag{5.11}$$

and in that sense we may write

$$\delta_{N,\epsilon}(M) = \frac{\epsilon^{N-2}}{2 \sqrt{\det(K_N)}} \text{Vol}(S^{N-1}) \delta_N(F'), \quad \delta_N(F') = \prod_{\mu \leq N} \delta(F'_\mu) \tag{5.12}$$

Since K_N is a phase space independent constant, when inserting (5.12) into (5.8), the prefactor cancels in both numerator and denominator and we arrive at (4.37) in the limit $\epsilon \rightarrow 0$ and $N \rightarrow \infty$.

6 Conclusions and Outlook

The three tasks accomplished in the present paper are:

1. We have demonstrated that within the limits of the formal nature of the manipulations that are usually employed when dealing with path integrals, three canonical quantisation methods, namely the reduced phase space –, the operator constraint and the Master Constraint quantisation all lead to the same path integral formulation for the physical inner product. In order that rigging map techniques can be employed to the operator constraint approach, in the case of structure functions one has to pass to Abelianised constraints.
2. The resulting path integral can be written in terms of the classical Lagrangian from which the classical theory descends. However, the correct measure to be used is not the naive Lebesgue measure on path space, rather this measure must be corrected by factors that depend on the first and second class constraints as well as the gauge fixing condition.
3. The gauge fixing condition is in one to one correspondence with the choice and interpretation of a convenient choice of an algebra of physical observables and a physical Hamiltonian. It is possible to do without gauge fixing conditions provided one finds alternative methods to construct an algebra of Dirac observables. However, the resulting algebra is almost surely algebraically more complicated, more difficult to quantise, lacks an a priori physical interpretation and is not equipped with a preferred physical time evolution. In particular, if one wants to talk about the scattering matrix between physical states, the dependence on the gauge fixing is unavoidable because it determines the physical time evolution of the chosen “basis” of gauge invariant operators.

As we have already stated in the introduction, certainly not all the results and techniques derived and used in the present paper are new, bits and pieces of it are already in the literature. However, we believe we have assembled the material in a new and fruitful way in order to better understand the relations between the four quantisation methods discussed in this paper. Also we think that the mathematical and physical influence of the gauge fixing condition has been described in this paper from a new angle.

As we have seen explicitly, both methods of proof in section 5 actually relied on the fact that the matrix K is a constant function on phase space. However, this is not the case for the concrete Master Constraint for General Relativity studied in [16]. Namely, there one considered an expression of the form

$$M = \int_{\sigma} d^3x \frac{C^2}{\sqrt{\det(q)}} \quad (6.1)$$

where C is the Hamiltonian constraint and q is the intrinsic three metric of the hypersurface σ . The “matrix” $K(x, y) = \delta(x, y) / \sqrt{\det(q)(x)}$ is chosen here in order to make (6.1) invariant under spatial diffeomorphisms and is clearly a non – trivial function on phase space. In view of the analysis of the previous section, rather than the Hamiltonian constraint in its original form C , in the presence of the dust matter one would choose it in the locally equivalent form $C'(x) = \pi(x) + h'(q(x), P(x))$ where q, P are the gravitational degrees of freedom and π is one of the dust momenta. Notice that for this type of matter h' does not depend on the dust configuration fields ϕ and therefore dust deparametrises the system and leads to a conserved physical Hamiltonian. However, also C' is a scalar density and thus to make the corresponding Master constraint spatially diffeomorphism invariant, one would again need a phase space dependent matrix of the type considered above. Thus it appears as if the analysis of the present section does not apply to GR.

However, this is not the case: Namely, the dust offers the possibility to completely abelianise the full constraint algebra including spatial diffeomorphisms. Thus in contrast to the usual situation in which the spatial diffeomorphisms form a subalgebra of the constraint algebra but not an ideal, it is possible to completely solve the spatial diffeomorphism constraint before solving the Hamiltonian constraint. In particular it is possible to perform a canonical transformation to coordinates such that C' only depends on spatially diffeomorphism invariant fields [10]. It is therefore no longer necessary to choose a density weight minus one matrix K . We can simply take an orthonormal basis b_{μ} of $L_2(\sigma, d^3x)$ and consider the $F'_{\mu} := \langle b_{\mu}, C' \rangle$. Then one chooses any phase space independent matrix $K^{\mu\nu}$ subject to certain fall off conditions in index space (typically K should be trace class [16]). The fact that C' has density weight one ensures that C' can be quantised on the unique [44] LQG Hilbert space [45] as was shown explicitly in [33]. That quantisation, however, is most probably too naive in order to guarantee anomaly freeness and must be improved. Yet, since the anomaly is an \hbar correction to the classical result, the relation between the MCP (which also works in the anomalous case) and the path integral formulation derived in the previous section, remains correct in the semiclassical limit. An alternative to working with C' already reduced with respect to the spatial diffeomorphism constraint is to keep the unreduced C' and the unreduced Abelianised spatial diffeomorphism constraints C'_j [10]. The caveat in LQG to quantising the classical generator of spatial diffeomorphisms which arises due to strong discontinuity of the one parameter unitary subgroups of spatial diffeomorphisms on the LQG Hilbert space is circumvented because C'_j is not a density one covector but a density one scalar and thus can be quantised on the LQG Hilbert space [47], albeit it is difficult, similar to C' , to achieve anomaly freeness.

This paper has been the starting point for further analysis. In [21] we have computed the correct measure for the Holst action and have checked explicitly that it is consistent with the analysis of [20] for the Plebanski action. In [25] the relation between the Master Constraint Programme and the operator constraint programme for Abelian and anomaly free constraints and with phase space independent matrix K was analysed with higher mathematical precision at the level of the canonical theory and it is shown that under certain technical assumptions the two methods lead to the same result, thus partly removing the formal character of the analysis of section 5. Finally, in [26] it was

formally checked by using available semiclassical techniques [46] that the Master Constraint Programme for General Relativity leads also to the expected path integral formula up to a local measure factor when one considers phase space dependent matrices K and non – Abelian constraints. However, the results here are less strong (more formal) than in the Abelianised case.

Many further questions arise from the present paper:

Since the Master Constraint can in principle also accommodate (sums of squares of) second class constraints if one subtracts a suitable normal ordering constant [16], one could ask whether the separate treatment of first and second class constraints could be unified and if yes how the corresponding path integral would look like. Secondly, in applications to path integral formulations of LQG one should really take the unavoidable measure factor derived in [21] and following the general theory summarised here seriously and define a corresponding spin foam model. Work is in progress in order to achieve that. Next, due to the measure factor the theory lacks manifest spacetime diffeomorphism invariance. On the other hand it should be manifestly invariant under the gauge transformations generated by the first class constraints which in General Relativity corresponds to the Bergmann – Komar “group” [48] (more precisely it is the enveloping algebra generated by the secondary first class constraints of GR). The two groups are known to coincide when the classical equations of motion hold and this is the reason why the Lagrangian and Hamiltonian descriptions are equivalent classically. However, off shell there is no particular relation between these two “groups” and it is consistent with the classical theory that the spacetime diffeomorphism group is not a symmetry of the quantum theory. In [22] it is further analysed in which sense the Bergmann – Komar group is a symmetry of the Hamiltonian path integral. It seems that the attempt to construct a spacetime covariant path integral of GR has no chance to be derived from a canonical platform which is the only systematic starting point that we have and it would be interesting to understand better the implications of this conclusion. In some sense it is clear that spacetime diffeomorphism invariance is far from sufficient in order to guarantee that one has a correct quantisation of a given classical theory. Many Lagrangians are spacetime diffeomorphism covariant (e.g. higher derivative theories) but all of them have different Hamiltonian constraints (even different numbers of degrees of freedom). The effect of this will show, in particular, in the local measure factor that we have exhibited.

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