The Phoenix Project: Master Constraint Programme for Loop Quantum Gravity

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Abstract

The Hamiltonian constraint remains the major unsolved problem in Loop Quantum Gravity (LQG). Seven years ago a mathematically consistent candidate Hamiltonian constraint has been proposed but there are still several unsettled questions which concern the algebra of commutators among smeared Hamiltonian constraints which must be faced in order to make progress.

In this paper we propose a solution to this set of problems based on the so-called **Master Constraint** which combines the smeared Hamiltonian constraints for all smearing functions into a single constraint. If certain mathematical conditions, which still have to be proved, hold, then not only the problems with the commutator algebra could disappear, also chances are good that one can control the solution space and the (quantum) Dirac observables of LQG. Even a decision on whether the theory has the correct classical limit and a connection with the path integral (or spin foam) formulation could be in reach.

While these are exciting possibilities, we should warn the reader from the outset that, since the proposal is, to the best of our knowledge, completely new and has been barely tested in solvable models, there might be caveats which we are presently unaware of and render the whole **Master Constraint Programme** obsolete. Thus, this paper should really be viewed as a proposal only, rather than a presentation of hard results, which however we intend to supply in future submissions.

1 Introduction

The quantum dynamics has been the most difficult technical and conceptual problem for quantum gravity ever since. This is also true for Loop Quantum Gravity (LQG) (see [1] for recent reviews). Seven years ago, for the first time a mathematically well-defined Hamiltonian constraint operator has been proposed [2, 3, 4, 5, 6, 7, 8, 9] for LQG which is a candidate for the definition of the quantum dynamics of the gravitational field and all known (standard model) matter. That this is possible at all is quite surprising because the Hamiltonian constraint of classical General Relativity (GR) is a highly non-polynomial function on phase space and the corresponding operator should therefore be plagued with UV singularities even more serious than for interacting, ordinary Quantum Field Theory. In fact, it should be at this point where the non-renormalizability of perturbative quantum (super)gravity is faced in LQG [10]. That this does not happen is a direct consequence of the background independence of LQG which is built in at a fundamental level and therefore requires a non-perturbative definition of the theory in a representation [11, 12, 13, 14] which is fundamentally different from the usual background dependent Fock representations.

Despite this success, immediately after the the appearance of [2, 3, 4, 5, 6, 7, 8, 9] three papers [15, 16, 17] were published which criticized the proposal by doubting the correctness of the

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classical limit of the Hamiltonian constraint operator. In broad terms, what these papers point out is that, while the algebra of commutators among smeared Hamiltonian constraint operators is anomaly free in the mathematical sense (i.e. does not not lead to inconsistencies), it does not manifestly reproduce the classical Poisson algebra among the smeared Hamiltonian constraint functions. While the arguments put forward are inconclusive (e.g. the direct translation of the techniques used in the full theory work extremely well in Loop Quantum Cosmology [18]) these three papers raised a serious issue and presumably discouraged almost all researchers in the field to work on an improvement of these questions. In fact, except for two papers [19] there has been no publication on possible modifications of the Hamiltonian constraint proposed. Rather, the combination of [2, 3, 4] with path integral techniques [20] and ideas from topological quantum field theory [21] gave rise to the so-called spin foam reformulation of LQG [22] (see e.g. [23] for a recent review). Most of the activity in LQG over the past five years has focussed on spin foam models, partly because the hope was that spin foam models, which are defined rather independently of the Hamiltonian framework, circumvent the potential problems pointed out in [15, 16, 17]. However, the problem reappears as was shown in recent contributions [24] which seem to indicate that the whole virtue of the spin foam formulation, its manifestly covariant character, does not survive quantization.

One way out could be to look at constraint quantization from an entirely new point of view [25] which proves useful also in discrete formulations of classical GR, that is, numerical GR. While being a fascinating possibility, such a procedure would be a rather drastic step in the sense that it would render most results of LQG obtained so far obsolete.

In this paper we propose a new, more modest, method to **cut the Gordic Knot** which we will describe in detail in what follows. Namely we introduce the **Phoenix Project** which aims at *reviving interest in the quantization of the Hamiltonian Constraint.* However, before the reader proceeds we would like to express a word of warning:
So far this is really only a proposal. While there are many promising features as we will see, many mathematical issues, mostly functional analytic in nature, are not yet worked out completely. Moreover, the proposal is, to the best of our knowledge, completely new and thus has been barely tested in solvable models. Hence, there might be possible pitfalls which we are simply unaware of at present and which turn the whole programme obsolete. On the other hand there are so many mathematical facts which work together harmonically that it would be a pity if not at least part of our idea is useful. It is for this reason that we dare to publish this paper although the proposal is still premature. This should be kept in mind for waht follows.

The origin of the potential problems pointed out in [15, 16, 17] can all be traced back to simple facts about the constraint algebra:

1. The (smeared) Hamiltonian constraint is not a spatially diffeomorphism invariant function.
2. The algebra of (smeared) Hamiltonian constraints does not close, it is proportional to a spatial diffeomorphism constraint.
3. The coefficient of proportionality is not a constant, it is a non-trivial function on phase space whence the constraint algebra is open in the BRST sense.

These phrases are summarized in the well-known formulas (Dirac or hpersurface deformation algebra)

$$\begin{aligned}
\{\vec{C}(\vec{N}),\vec{C}(\vec{N}')\} &= \kappa\vec{C}(\mathcal{L}_{\vec{N}}\vec{N}') \\
\{\vec{C}(\vec{N}),C(N')\} &= \kappa C(\mathcal{L}_{\vec{N}}N') \\
\{C(N),C(N')\} &= \kappa\int_\sigma d^3x(N_{,a}N'-NN'_{,a})(x)q^{ab}(x)C_b(x)
\end{aligned}$$

where $C(N)=\int_\sigma d^3xN(x)C(x)$ is the smeared Hamiltonian constraint, C_b is the spatial diffeomorphism constraint, $\vec{C}(\vec{N}) = \int_\sigma d^3x N^a(x) C_a(x)$ is the smeared spatial diffeomorphism constraint, q^{ab} is the inverse spatial metric tensor, N, N', N^a, N'^a are smearing functions on the spatial three-manifold σ and κ is the gravitational constant.

This is actually the source of a whole bunch of difficulties which make the regularization of the Hamiltonian constraint a delicate issue if one wants to simultaneously avoid an inconsistency of the constraint algebra. Notice that due to the third relation the Dirac algebra is fantastically much more complicated than any infinite dimensional Lie (Super)algebra. Moreover, while the Hamiltonian constraint of [2, 3, 4] uses spatial diffeomorphism invariance in an important way in order to remove the regulator in the quantization procedure, the resulting operator does not act on spatially diffeomorphism invariant states (it maps diffeomorphim invariant states to those which are not) thus preventing us from using the Hilbert space of spatially diffeomorphism states constructed in [26].

The observation of this paper is that all of this would disappear if it would be possible to reformulate the Hamiltonian constraint in such a way that it is equivalent to the original formulation but such that it becomes a spatially diffeomorphism invariant function with an honest constraint Lie algebra. There is a natural candidate, namely

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

We call it the **Master Constraint** corresponding to the infinite number of constraints $C(x),\ x \in \sigma$ because, due to positivity of the integrand, the **Master Equation** $\mathbf{M} = 0$ is equivalent with $C(x) = 0\ \ \forall x \in \sigma$ since $C(x)$ is real valued. (One could also consider higher, positive powers of $C(x)$ but quadratic powers are the simplest). The factor $1/\sqrt{\det(q)}$ has been incorporated in order to make the integrand a scalar density of weight one (remember that $C(x)$ is a density of weight one). This guarantees 1) that $\mathbf{M}$ is a spatially diffeomorphism invariant quantity and 2) that $\mathbf{M}$ has a chance to survive quantization [7].

Why did one not think of such a quantity before ? In fact, related ideas have been expressed already: In [27] the authors did construct an *infinite number* of modified Hamiltonian constraints $\mathbf{K}(x)$, rather than a *single* **Master Constraint**, which have an Abelean algebra among themselves. One can show that none of these **Kuchař Densities** $\mathbf{K}(x)$ is simulataneously 1) a density of weight one, 2) a polynomial in $C(x)$ and 3) positive definite. Rather, they are algebraic aggregates built from $C(x)^2$ and $C(x)^2 - (q^{ab}C_aC_b)(x)$. If it is not a polynomial, then it will be not differentiable on the constraint surface and if it is not a density of weight one then it cannot be quantized background independently. Thus from this point of view, $\mathbf{M}$ is an improvement, since clearly $\{\mathbf{M}, C_a(x)\} = \{\mathbf{M}, \mathbf{M}\} = 0$, moreover the number of constraints is drastically reduced. But still there is an a priori problem with $\mathbf{M}$ which prevented the author from considering it seriously much earlier: On the constraint surface $\mathbf{M} = 0$ we obviously have $\{O, \mathbf{M}\} = 0$ for *any* differentiable function O on the phase space. This is a problem because (weak) Dirac observables for first class constraints such as $C(x) = 0$ are selected precisely by the condition $\{O, C(x)\} = 0$ for all $x \in \sigma$ on the constraint surface. Thus the **Master Constraint** seems to fail to detect Dirac observables with respect to the original set of Hamiltonian constraints $C(x) = 0,\ x \in \sigma$.

The rather trivial, but yet important observation is that this is *not the case*: We will prove that an at least twice differentiable function O on phase space is a weak Dirac observable with respect to all Hamiltonian constraints $C(x) = 0,\ x \in \sigma$ if and only if it satisfies the single **Master Equation**

$$\{O, \{O, \mathbf{M}\}\}_{\mathbf{M}=0} = 0$$

The price we have to pay in order to replace the infinite number of linear (in O) conditions $\{O, C(x)\}_{\mathbf{M}=0} = 0,\ x \in \sigma$ by this single **Master Equation** is that it becomes a non-linear condition on O. This is a mild price to pay in view of having only a single equation to solve. Now from the theory of differential equations one knows that non-linear partial differential equations (such as the Hamilton-Jacobi equation) are often easier to solve if one transforms them first into a system of linear (ordinary, in the case of Hamilton's equations,) partial differential equations and one might think that in order to find solutions to the **Master Equation** one has to go back to the original infinite system of conditions. However, also this is not the case: As we will show, one can explicitly solve the **Master Condition** for the subset of *strong* Dirac observables by using **Ergodic Theory Methods**.

Hence, the **Master Constraint** seems to be quite useful at the classical level. How about the quantum theory ? It is here where things become even more beautiful: Several facts *work together harmonically*:

i) *Spatially Diffeomorphism Invariant States*
The complete space of solutions to the spatial diffeomorphism constraints $C_a(x) = 0,\ x \in \sigma$ has already been found long ago in [26] and even was equipped with a natural inner product induced from that of the kinematical Hilbert space $\mathcal{H}_{Kin}$ of solutions to the Gauss constraint. However, there is no chance to define the Hamiltonian constraint operators corresponding to $C(x)$ (densely) on $\mathcal{H}_{Diff}$ because the Hamiltonian constraint operators do not preserve $\mathcal{H}_{Diff}$. The Hamiltonian constraints $C(x)$ therefore had to be defined on $\mathcal{H}_{Kin}$ but this involves the axiom of choice and thus introduces a huge quantization ambiguity [3]. Moreover, removal of the regulator of the regulated constraint operator is possible only in an unusual operator topology which involves diffeomorphism invariant distributions.

However, $\mathbf{M}$ is spatially diffeomorphism invariant and therefore *can be defined on* $\mathcal{H}_{Diff}$. Therefore, we are finally able to **exploit the full power of the results obtained in [26]**! Hence the ambiguity mentioned disappears, the convergence of the regulated operator is the standard weak operator topology of $\mathcal{H}_{Diff}$, the whole quantization becomes much cleaner. Yet, all the steps carried out in [2, 3, 4, 5, 6, 7, 8] still play an important role for the quantization of $\mathbf{M}$, so these efforts were not in vain at all.

ii) *Physical States and Physical Inner Product*
What we are a priori constructing is actually not an operator corresponding to $\mathbf{M}$ but rather only a (spatially diffeomorphism invariant) quadratic form $Q_{\mathbf{M}}$ on $\mathcal{H}_{Diff}$. That is, we are able to compute the matrix elements of the would-be operator $\widehat{\mathbf{M}}$. For most practical purposes this is enough, however, things become even nicer if $Q_{\mathbf{M}}$ really is induced by an actual operator on $\mathcal{H}_{Diff}$. Now *by construction the quadratic form* $Q_{\mathbf{M}}$ *is positive.* However, for semi-bounded quadratic forms, of which the positive ones are a subset, general theorems in functional analysis guarantee that there is a unique, positive, self-adjoint operator $\widehat{\mathbf{M}}$ whose matrix elements reproduce $Q_{\mathbf{M}}$, provided that the quadratic form is closable. Now, although we do not have a full proof yet, since $Q_{\mathbf{M}}$ is not some random positive quadratic form but actually comes from a positive function on the phase space, chances are good that a closed extension exists.

Let us assume that this is actually the case. Now in contrast to $\mathcal{H}_{Kin}$ the Hilbert space $\mathcal{H}_{Diff}$ *is separable.* (This is not a priori the case but can be achieved by a minor modification of the procedure in [26]). It is, in general, only for *separable* Hilbert spaces that the following theorem holds: There is a direct integral decomposition of $\mathcal{H}_{Diff}$ corresponding to the self-adjoint operator $\widehat{\mathbf{M}}$ into Hilbert spaces $\mathcal{H}^{\oplus}_{Diff}(\lambda),\ \lambda \in \mathbb{R}$ such that the action of $\widehat{\mathbf{M}}$ on $\mathcal{H}^{\oplus}_{Diff}(\lambda)$ reduces to multiplication by λ. Hence, *the physical Hilbert space* is simply given by $\mathcal{H}_{Phys} = \mathcal{H}^{\oplus}_{Diff}(0)$. Notice that this Hilbert space *automatically comes with its own physical inner product* which is induced by that of $\mathcal{H}_{Diff}$ (which in turn is induced by that of $\mathcal{H}_{Kin}$). So we would have shown automatically existence of $\mathcal{H}_{Phys}$, however, it is not a priori clear if it is sufficiently large (contains enough semiclassical states). That is, while the constraint algebra with respect to $\widehat{\mathbf{M}}$ has been trivialized, operator ordering choices still will play an important role in the sense that they will have influence on the size of $\mathcal{H}_{Phys}$. Hence, the issue of **anomaly freeness** has been transformed into the issue of **the size of** $\mathcal{H}_{Phys}$. Hence it seems that nothing has been gained, but this is not true: The **Master Constraint Method** allows us to postpone operator issues until the very end of the analysis with the advantage that there are no additional mathematical obstacles along the way.

iii) *Strong Quantum Dirac Observables*
Again, if a self-adjoint operator $\widehat{\mathbf{M}}$ exists, then we can construct the weakly continuous one-parameter unitary groups $t \mapsto \hat{U}(t)$ generated by it. Let $\hat{O}_{Diff}$ be a bounded, self-adjoint operator on $\mathcal{H}_{Diff}$, say one of the spectral projections of a normal operator on $\mathcal{H}_{Diff}$. Suppose that

$$[\hat{O}] := \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt\, \hat{U}(t)\, \hat{O}_{Diff}\, \hat{U}(t)^{-1}$$

converges in the uniform operator topology to a bounded, symmetric operator on $\mathcal{H}_{Diff}$ (and can thus be extended to a self-adjoint operator there). Then (the spectral projections of) $[\hat{O}]$ commute(s) with (the spectral projections of) $\widehat{\mathbf{M}}$, hence it leaves $\mathcal{H}_{Phys}$ invariant and induces a bounded, symmetric, hence self adjoint operator $\hat{O}_{Phys}$ there. Then this *ergodic mean technique* would be a simple tool in order to construct *strong quantum Dirac Observables* with the correct (induced) adjountness relations.

In summary, we feel that 1. **Diffeomorphism Invariance of $\mathbf{M}$**, 2. **Positivity of $\mathbf{M}$** and 3. **Separability** of $\mathcal{H}_{Diff}$ work together harmonically and provide us with powerful functional analytic tools which are not at our disposal when working with the Hamiltonian constraints.

This finishes the introduction. This is the first of a series of papers in which we will analyze the functional analytic properties of the **Master Constraint Operator** and hopefully complete all the missing steps in our programme. This first paper just aims at sketching the broad outlines of that programme, more details will follow in subsequent submissions. We have made an effort to keep the number of formulas and theorems at a minimum while keeping the paper self-contained so that also theoretical and mathematical physicists with a surfacial knowledge of LQG can access the paper. More details and proofs for the experts will hopefully follow in future submissions.

The article breaks up into the following sections.

In section two we compare the **Master Constraint Programme** applied to General Relativity with the original Hamiltonian Constraint Programme of [2, 3, 4, 5, 6, 7, 8, 9], stressing its various advantages and improvements. This section just states the results without derivations.

In section three we will develop the **Master Constraint Programme** for a general constrained Quantum Field Theory, the details of General Relativity will not be important for that section.

In sections four and five we sketch the construction of a quadratic form $Q_{\mathbf{M}}$ for General Relativity where all the LQG techniques developed in [2, 3, 4, 5, 6, 7, 8, 9] will be exploited. More precisely, in section four we describe a graph-changing quadratic form on the diffeomorphism invariant Hilbert space which builds directly on the techniques of [2, 3, 4, 5, 6, 7, 8, 9] while in section five we propose an alternative, non-graph-changing quantization of the **Master Constraint** which has the advantage of resulting directly in a positive, diffeomorphism invariant operator on the kinematical Hilbert space $\mathcal{H}_{Kin}$ (and thus has the Friedrichs extension as distinguished self-adjoint extension). This operator can then be induced on $\mathcal{H}_{Diff}$ and thus sidesteps the quadratic form construction of section four. Moreover, it should be possible to verify its classical limit directly with the methods of [28, 29, 30, 31, 32, 33, 34]. We feel, that this latter implementation of the **Master Constraint** is less fundamental than the one of section four, because it involves an ad hoc quantization step. Yet, it adds to the faith of the more fundamental quantization since it is only a modest modification thereof and can be tested with currently developed coherent states techniques. In any case it results in a much simpler operator and therefore can be easier accessed by analytical methods.

Finally, in section six we mention directions for further research. The most important one is presumably that the **Master Constraint Programme**, at least in th sense of section five, allows for a straightforward connection with the spin foam approach of LQG, that is, a **Path Integral Formulation**. Namely, the **Master Constraint** can be considered as a **true Hamiltonian**. The difference with usual quantum gauge theory is then, besides background independence, that we are just interested in the kernel of that Hamiltonian. This means that our path integral is not a transition amplitude but rather a generalized projector in the sense of refined algebraic quantization. Nevertheless, the usual Feynman-Kac like techniques can be employed in order to give, hopefully, a rigorous construction of the path integral.
Another point to mention is that the **Master Constraint Technique** could be extended to take care also of the spatial diffeomorphism group. This is maybe even preferred by those who do not believe in the relevance of the spatial diffeomorphism group down to the Planck scale. Moreover, when doing this we can actually do Hamiltonian (or Lagrangean when using the path integral) **Lattice LQG** (rather than continuum LQG) [35] without having to be bothered by the fact that the lattice breaks spatial diffeomorphism invariance. Spatial diffeomorphism invariance still plays a role, but only on large scales, and the **Master Constraint** allows us to take care of this new sense of spatial diffeomorphism invariance on any lattice. Finally, with a new sense of spatial diffeomorphisms, possibly room is made to have new kinematical representations of LQG other than the one currently used [13, 14].

In the appendix we review the notion of Rigging Maps and Rigged Hilbert spaces and display the connection with the direct integral method used in the main part of this paper. Knowledge of this background material is not essential in order to read the paper.

2 The Master Constraint Programme versus the Hamiltonian Constraint Quantization Programme for General Relativity

The purpose of this section is to describe the **Master Constraint Programme** when applied to general Relativity. In order to appreciate its advantages and its technical and conceptual improvements over the original Hamiltonian constraint quantization programe, it is helpful to recall the quantization of the Hamiltonian constraint developed in [2, 3, 4, 5, 6, 7, 8, 9] which can be sketched by the following steps:

1. *Cotriad Regularization*
   In order to achieve UV finiteness one had to make sense out of a co-triad operator corresponding to to e_a^j where $e_a^j e_b^k \delta_{jk} = q_{ab}$ is the spatial metric tensor. Since e_a^j is not a polynomial in the elementary phase space coordinates (A_a^j, E_j^a) consisting of an $SU(2)$ connection A and a canonically conjugate $\mathrm{Ad}_{SU(2)}$-covariant vector density E of weight one, this could be achieved by writing the co-triad in the form $e_a^j = \{A_a^j, V\}$ where $V = \int d^3x \sqrt{\det(q)}$ is the volume functional.

2. *Connection Regularization*
   Since the connection operator corresponding to A is not defined on the Hilbert space one had to write the Poisson bracket in the form $\epsilon\{A, V\} = h_{e_\epsilon}(A)\{h_{e_\epsilon}(A)^{-1}, V\}$ where $h_\epsilon(A)$ denotes the holonomy of A along a path e_ϵ of parameter length ϵ. Similarly one had to write the curvature F of A in the form $2\epsilon^2 F = h_{\alpha_\epsilon}(A) - h_{\alpha_\epsilon}(A)^{-1}$ where α_ϵ denotes a loop of parameter circumference ϵ.

3. *Triangulation*
   Since the smeared Hamiltonian constraint can be written in the form

   $$C(N) = \int_\sigma d^3x N \mathrm{Tr}(F \wedge e)$$

   where N is a test function, the power ϵ^3 needed in step 2. can be neatly absorbed by the d^3x volume of a (tetrahedral) cell Δ of a triangulation τ of σ. Hence one can write the

Hamiltonian as a pointwise (on phase space) limit $C(N) = \lim_\epsilon C_\epsilon(N)$ where symbolically

$$C_\tau(N) = \sum_{\Delta\in\tau} \mathrm{Tr}([h_{\alpha_\Delta}(A) - h_{\alpha_\Delta}(A)^{-1}]h_{e_\Delta}(A)\{h_{e_\Delta}(A)^{-1}, V\})$$

4. *Quantization of the Regulated Constraint*
   In order to quantize this expression one now replaced all appearing quantities by operators and the Poisson bracket by a commutator divided by $i\hbar$. In addition, in order to arrive at an unambiguous result one had to make the triangulation *state dependent.* That is, the regulated operator is defined on a certain (so-called spin network) basis elements T_s of the Hilbert space in terms of an adapted triangulation τ_s and extended by linearity. This is justified because the Riemann sum that enters the definition of $C_\tau(N)$ converges to $C(N)$ no matter how we refine the triangulation.

5. *Removal of the Regulator*
   To take the infinite refinement limit (or continuum) $\tau \to \sigma$ of the resulting regulated operator $\hat{C}^\dagger_\tau(N)$ is non-trivial because the holonomy operators $\hat{h}_{e_\Delta}$ are not even weakly continuously represented on the Hilbert space, hence the limit cannot exist in the weak operator topology. It turns out that it exists in the, what one could call, *weak Diff* topology* [1]: Let Φ_{Kin} be a dense invariant domain for the (closable) operator $\hat{C}^\dagger_\tau(N)$ on the Hilbert space $\mathcal{H}_{Kin}$ and let $(\Phi^*_{Kin})_{Diff}$ be the set of all spatially diffeomorphism invariant distributions over Φ_{Kin} (equipped with the topology of pointwise convergence). Then $\lim_{\tau\to\sigma} \hat{C}_\tau(N) = \hat{C}(N)$ if and only if for each $\epsilon > 0,\ T_s,\ l \in (\Phi^*_{Kin})_{Diff}$ there exists $\tau_s(\epsilon)$ *independent of* l such that

$$|l([\hat{C}_{\tau_s}(N) - \hat{C}(N)]T_s)| < \epsilon \ \ \forall \ \ \tau_s(\epsilon) \subset \tau_s$$

   That the limit is uniform in l is crucial because it excludes the existence of the limit on spaces larger than $(\Phi^*_{Kin})_{Diff}$ [16, 17] which would be unphysical because the space of solutions to all constraints must obviously be a subset of $(\Phi^*_{Kin})_{Diff}$. Notice that the limit is required refinements of adapted triangulations only.

   What we just said is sometimes paraphrased by saying that "the Hamiltonian constraint is defined only on diffeomorphism invariant states". But this is certainly wrong in the strict sense, the Hamiltonian constraint is not diffeomorphism invariant and thus the dual operator defined by $[\hat{C}(N)'\Psi](f) := \Psi(\hat{C}(N)^\dagger f)$ does not preserve $(\Phi^*_{Kin})_{Diff}$. Rather, in a technically precise sense the constraint is defined on the Hilbert space $\mathcal{H}_{Kin}$ itself. In order to write it down explicitly, one needs to make use of the axiom of choice, $\hat{C}(N)T_s := \hat{C}_{\tau^0_s}(N)T_s$ in the sense that there is an explicit action which is defined up to a diffeomorphism and the choice $s \mapsto \tau^0_s$ involved corresponds to the choice of a diffeomorphism. One does not need to worry about this choice since it is irrelevant on the space of full solutions which is in particular a subset of $(\Phi^*_{Kin})_{Diff}$.

6. *Quantum Dirac Algebra*
   We may now compute the commutator $[\hat{C}(N), \hat{C}(N')]$ on Φ_{Kin} corresponding to the Poisson bracket $\{C(N), C(N')\}$ which is proportional to the spatial diffeomorphism constraint C_a. This commutator turns out to be non-vanishing on Φ_{Kin} as it should be, however, $\Psi([\hat{C}(N), \hat{C}(N')]f) = 0$ for all $f \in \Phi_{Kin}, \Psi \in (\Phi^*_{Kin})_{Diff}$. This is precisely how we would expect it in the absence of an anomaly. Note that this is sometimes paraphrased by "The algebra of Hamiltonian Constraints is Abelean". But this is clearly wrong in the strict sense, the commutator is defined on Φ_{Kin}, where it does not vanish, and not on $(\Phi^*_{Kin})_{Diff}$. On the other hand, the right hand side of the commutator on Φ_{Kin} does not obviously resemble the quantization of the classical expression $\int d^3x(NN'_{,a} - N_{,a}N')q^{ab}C_b$ so there are doubts, expressed in [15, 16, 17] whether the quantization of $C(N)$ produces the correct quantum dynamics. Notice, however, that this is not surprising because in order to write the classical Poisson bracket $\{C(N), C(N')\}$ in the form $\int d^3x(NN'_{,a} - N_{,a}N')q^{ab}C_b$ one must perform integrations by parts, use non-linear differential geometric identities, reorder

terms etc., which are manipulations all of which are very difficult to perform at the quantum level. Moreover, it is possible to quantize the expression $\int d^3x(NN'_{,a} - N_{,a}N')q^{ab}V_b$ directly [5] and its dual annihilates $(\Phi^*_{Kin})_{Diff}$ as well.

In summary: There is certainly no mathematical inconsistency but there are doubts on the correct classical limit of the theory. Notice, however, that aspects of the Hamiltonian constraint quantization has been successfully tested in model systems [4, 18].

7. *Classical Limit*
   In order to improve on this one could try to prove the correctness of the Hamiltonian constraint by computing its expectation value in coherent states for non-Abelean gauge theories [28, 29, 30, 31, 32, 33] because then the manipulations just mentioned can be performed for the function valued (rather than operator valued) expectation values. However, the problem with such an approach is that coherent states which would suitable for doing this would naturally be elements of the full distributional dual Φ^*_{Kin} of Φ_{Kin} as has been shown in [34, 36]. However, Φ^*_{Kin}, in contrast to $(\Phi_{Kin})^*_{Diff}$, does not carry a (natural) inner product, so that expectation values cannot be computed. The technical reason for why the non-distributional states constructed in [28, 29, 30, 31, 32, 33, 34] are insufficient to compute the classical limit is that they are designed 1) for a representation which supports the non-Abelean holonomy-flux algebra [13, 14] and 2) for operators only which leave invariant the graph on which a given spin network state is supported, however, the Hamiltonian constraint does not naturally have this latter property.

The **Master Constraint Approach** now improves on these issues as follows:

1.+2.+3. *Cotriad Regularization, Connection Regularization and Triangulation*
   These three steps are essentially unchanged.

4. *Quantization of the Regulated Constraint*
   It is here where things become most interesting: In contrast to $\hat{C}(N)$ which had to be quantized on Φ_{Kin} since $\hat{C}(N)$ does not preserve diffeomorphism invariant states, we can quantize $\mathbf{M}$ directly on $(\Phi^*_{Kin})_{Diff}$, *thus being able to use the full power of the results derived in [26]*. We can sketch the procedure as follows: There is an anti-linear map $\eta: \Phi_{Kin} \to (\Phi^*_{Kin})_{Diff}$ constructed in [26] the image of which is dense in the Hilbert space $\mathcal{H}_{Diff}$ of diffeomorphism invariant states which carries the inner product $<\eta(f), \eta(f')>_{Diff} := \eta(f')[f]$ where the right hand side denotes the action of the distribution $\eta(f')$ on the element $f \in \Phi_{Kin}$. We now point-split $\mathbf{M}$ as follows

$$\mathbf{M} = \lim_{\substack{\tau\to\sigma \\ \epsilon\to 0}} \sum_{\Delta,\Delta'} [\int_\Delta d^3x (\frac{C}{\sqrt[4]{\det(q)}})(x)][\int_{\Delta'} d^3y \phi_\epsilon(x,y) (\frac{C}{\sqrt[4]{\det(q)}})(y)]$$

   where $\phi_\epsilon(x,y)$ is any point splitting function converging to the $\delta-$distribution in the sense of tempered distributions and Δ, Δ' are cells of the triangulation. Exploiting that $<.,.>_{Diff}$ has a complete orthonormal basis $\eta(b_I)$ for some $b_I \in \Phi_{Kin}$ where I belongs to some index set $\mathcal{I}$, we try to define the *quadratic form* on (a suitable form domain of) $\mathcal{H}_{Diff}$ by

$$Q_{\mathbf{M}}(\eta(f), \eta(f')) := \lim_{\substack{\tau\to\sigma \\ \epsilon\to 0}} \sum_{I\in\mathcal{I}} \int_\sigma d^3x \int_\sigma d^3y\; \phi_\epsilon(x,y)\; \overline{\eta(f)[\widehat{\frac{C}{\sqrt[4]{\det(q)}}}(x) b_I]}\; \eta(f')[\widehat{\frac{C}{\sqrt[4]{\det(q)}}}(y) b_I]$$

   Now it turns out that because we were careful enough to keep the integrand of $\mathbf{M}$ a density of weight one, the limit $\epsilon \to 0$ can be taken with essentially the same methods as those developed in [2, 3, 4, 5, 6]. The operator valued distributions that appear in that expression involve a loop derivative, however, since we are working with diffeomorphism invariant states, *we never have to take the derivative, we just need to take loop differentials*! This is in contrast to [37] and again related to the density weight one.

5. *Removal of the Regulator*
   Now by the same methods as in [2, 3, 4] one can remove the triangulation dependence. Diffeomorphism invariance ensures that the limit does not depend on the representative index set $\mathcal{I}$ (the map η is many to one).

   In summary, we end up with a quadratic form $Q_{\mathbf{M}}$ on $\mathcal{H}_{Diff}$ which by inspection is *positive*, hence semibounded. Now, if we can prove that the form is closed, then there is a unique positive, self-adjoint operator $\widehat{\mathbf{M}}$ such that

$$Q_{\mathbf{M}}(\eta(f),\eta(f')) =< \eta(f), \widehat{\mathbf{M}}\, \eta(f') >_{Diff}$$

   Notice that this operator is automatically densely defined and closed on $\mathcal{H}_{Diff}$, so we really have pushed the constraint analysis one level up from $\mathcal{H}_{Kin}$. Notice that not every semibounded quadratic form is closable (in contrast to symmetric operators) and therefore whether or not $Q_{\mathbf{M}}$ is closable is a non-trivial and crucial open question which we are going to address in a subsequent publication [44].

6. *Quantum Dirac Algebra*
   There is no constraint algebra any more, the issue of mathematical consistency (anomaly freeness) is trivialized. However, the issue of physical consistency is not answered yet in the sense that operator ordering choices will have influence on the size of the physical Hilbert space and thus on the number of semiclassical states, see below.

7. *Classical Limit*
   Since no semiclassical states have been constructed yet on $\mathcal{H}_{Diff}$ we cannot decide whether the **Master Constraint Operator** $\widehat{\mathbf{M}}$, if it exists, has the correct classical limit. However, the fact that there is significantly less quantization ambiguity involved than for the Hamiltonian constraints $C(x)$ themselves adds some faith to it. Moreover, the issues of 7. above could improve on the level of $\mathcal{H}_{Diff}$ for two reasons: First of all, $\mathcal{H}_{Diff}$ in contrast to Φ^*_{Kin} *does* carry an inner product. Secondly, when adopting the viewpoint of section 4.3, the Hilbert space $\mathcal{H}_{Diff}$ is separable and hence coherent states are not distributional but rather honest elements of $\mathcal{H}_{Diff}$. Finally, there is a less ambitious programme which we outline in section 5 where $\widehat{\mathbf{M}}$ exists as a diffeomorphism invariant operator on $\mathcal{H}_{Kin}$ and where one can indeed try to answer the question about the correctness of the classical limit with existing semiclassical tools. The reason for why this procedure is less favoured is that it is an ad hoc modification of the action of the operator in such a way that it leaves the graph of a spin network on which the operator acts invariant. On the other hand, the modification is not very drastic and therefore supports our more fundamental version of the **Master Constraint Operator**.

In addition to these technical improvements of [2, 3, 4, 5, 6, 7], the **Master Constraint Operator**, 1. if it exists and 2. if the issue about its classical limit can be settled, also possibly provides conceptual advantages because *it has a chance to complete the technical steps of the Canonical Quantization Programme:*

i. *Solution of all Quantum Constraints*
   Since by construction $\widehat{\mathbf{M}}$ is a self-adjoint operator we can solve the **Master Constraint** in the following, at least conceptually simple, way which rests on the assumption that $\mathcal{H}_{Diff}$ *is separable*, that is, the index set $\mathcal{I}$ has countable cardinality. Now as is well known [38] the Hilbert space is not a priori separable because there are continuous moduli associated with intersecting knot classes with vertices of valence higher than four. It turns out that there is a simple way to remove those moduli by performing an additional averaging in the definition of the (rigging) map η mentioned above. This should not affect the classical limit of the theory because this modification is immaterial for vertices of valence four or lower which are the ones that are most important in semiclassical considerations of lattice gauge theories (essentially because they are sufficient to construct dual triangulations). If

one is satisfied with heuristic considerations then we can use Rigging Map techniques to solve the constraint which formally work also in the non-separable case, see the appendix.

Thus, if $\mathcal{H}_{Diff}$ is separable, then we can construct the direct integral representation of $\mathcal{H}_{Diff}$ associated with the self-adjoint operator $\widehat{\mathbf{M}}$, that is,

$$\mathcal{H}_{Diff} = \int_{\mathbb{R}}^{\oplus} d\mu(\lambda) \mathcal{H}_{Diff}^{\oplus}(\lambda)$$

where μ is a positive probability measure on μ. Notice that the scalar product on the individual $\mathcal{H}_{Diff}^{\oplus}(\lambda)$ and the measure μ are uniquely induced by that on $\mathcal{H}_{Diff}$ up to unitary equivalence. Since $\widehat{\mathbf{M}}$ acts on the Hilbert space $\mathcal{H}_{Diff}^{\oplus}(\lambda)$ by multiplication with λ it follows that

$$\mathcal{H}_{Phys} := \mathcal{H}^{\oplus}(0)$$

is the physical Hilbert space and a crucial open question to be answered is whether it is large enough (has a sufficient number of semiclassical solutions).

ii. *Quantum Dirac Observables*
Let $\hat{O}_{Diff}$ be a bounded self adjoint operator on $\mathcal{H}_{Diff}$, for instance a spectral projection of the volume operator corresponding to the total volume of σ. Since the **Master Constraint Operator** is self-adjoint, we may construct the strongly continuous one-parameter family of unitarities $\hat{U}(t) = \exp(it\widehat{\mathbf{M}})$. Then, if the uniform limit exists, the operator

$$[\hat{O}_{Diff}] := \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt\, \hat{U(t)}\, \hat{O}_{Diff}\, \hat{U}(t)^{-1}$$

commutes with the **Master Constraint**, hence provides a strong Dirac observable, preserves $\mathcal{H}_{Phys}$ and induces a bounded self-adjoint operator $\hat{O}_{Phys}$ there.

Should all of these steps go through we would still be left with conceptual issues such as interpretational ones, the reconstruction problem etc., see e.g. [39], as well as practical ones (actually computing things). However, at least on the technical side (i.e. rigorous existence) the steps outlined above look very promising because they involve standard functional analytic questions which are well posed and should have a definite answer. They are much cleaner than the ones involved in the Hamiltonian Constraint Quantization programme. Let us list those questions once more:

Task A *Closure of Quadratic Form*
Show that the quadratic form $Q_{\mathbf{M}}$ is closable. This is an important task because it is not granted by abstract theorems that this is possible. Once the existence of the closure is established then it is only a practical problem to compute the unique positive, self-adjoint operator $\widehat{\mathbf{M}}$ to which it corresponds.

Task B *Spectral Analysis of* $\widehat{\mathbf{M}}$
Derive a direct integral representation of the Hilbert space $\mathcal{H}_{Diff}$ corresponding to $\widehat{\mathbf{M}}$. Also this is only a practical problem once we have made $\mathcal{H}_{Diff}$ separable by the additional averaging described below. The corresponding physical Hilbert space is then simply $\mathcal{H}_{Phys} = \mathcal{H}_{Diff}^{\oplus}(0)$. Show that it is "large enough", that is, contains a sufficient number of physical, semiclassical states.

Task C *Quantum Dirac Observables*
Find out for which diffeomorphism invariant, bounded, self-adjoint operators $\hat{O}_{Diff}$ the corresponding ergodic mean $[\hat{O}_{Diff}]$ converges (in the uniform operator topology induced by the topology of $\mathcal{H}_{Diff}$). Then compute the induced operator $\hat{O}_{Phys}$ on $\mathcal{H}_{Phys}$ which is automatically self adjoint.

Task D *Spatially Diffeomorphism Invariant Coherent States*
Construct semiclassical, spatially diffeomorphism invariant states, maybe by applying the map η to the states constructed in [28, 29, 30, 31, 32, 33, 34], and compute expectation values and fluctuations of the **Master Constraint Operator**. Show that these quantities coincide with the expectetd classical values up to $\hbar$ corrections. This is the second most important step because the existence of suitable semiclassical states, at the spatially diffeomorphism invariant level is not a priori granted. Once this step is established, we would have shown that the classical limit of $\widehat{\mathbf{M}}$ is the correct one and therefore the quantization really qualifies as quantum field theory of GR. Notice that this task can be carried out even before we show that $Q_{\mathbf{M}}$ is closable.

3 Elements of the Master Constraint Programme

In this section we will describe in more detail the basic ideas of the **Master Constraint Programme** for a general theory. Presumably elements of that idea are scattered over the vast literature on constraint quantization but to the best knowledge of the author these elements have not been combined into the form that we need here which is why we included this section. Also we believe that one can state the results outlined below in much broader contexts and it is very well possible that hard theorems already exist in the literature that state them more precisely than we do here. The author would be very interested to learn about the existence of such results.

3.1 Classical Theory

We begin with a general symplectic manifold $(\mathcal{M},\ \{.,.\})$ which may be infinite dimensional. Here $\mathcal{M}$ is a differentiable manifold modelled on a Banach space (phase space) and the (strong) symplectic structure is defined in terms of a Poisson bracket $\{.,.\}$ on $C^\infty(\mathcal{M}) \times C^\infty(\mathcal{M})$. Furthermore, we are given a set of constraint functions $C_J,\ J \in \mathcal{J}$ where the index set $\mathcal{J}$ may involve discrete and continuous labels. For the sake of definiteness and because it is the most interesting case in field theory, suppose that $\mathcal{J} = D \times X$ where D is a discrete label set and X is a topological space. Hence we may write $J = (j, x)$ and $C_J = C_j(x)$. Without loss of generality we assume that all constraints are real-valued and first class, replace the Poisson bracket by the corresponding Dirac bracket in order to remove potentially present second class constraints if necessary.

Let μ be a positive measure on the Borel $\sigma-$algebra of X and for each $x \in X;\ j,k \in D$ let be given a positive definite "metric" function $g^{jk}(x) \in C^\infty(\mathcal{M})$. We will now state some more or less obvious results which we, however, could not find anywhere in the literature.

Lemma 3.1.
The constraint hypersurface $\mathcal{C}$ of $\mathcal{M}$ defined by

$$\mathcal{C} := \{m \in \mathcal{M};\ \ C_J(m) = 0 \ \ \textit{for}\ \mu - a.a.\ \ J \in \mathcal{J}\} \tag{3.1}$$

can be equivalently defined by

$$\mathcal{C} = \{m \in \mathcal{M};\ \ \mathbf{M}(m) = 0\} \qquad \textbf{(Master Condition)} \tag{3.2}$$

where

$$\mathbf{M} := \frac{1}{2}\int_X d\mu(x) \sum_{j,k\in D} q^{jk}(x) C_j(x) C_k(x) \tag{3.3}$$

is the called **Master Constraint** *associated with C_J, μ, g.*

The proof is trivial. If, as usually the case in applications, the functions $C_J(m), g(m)$ are smooth in X for each $m \in \mathcal{M}$ then the "almost all" restriction can be neglected.

Let us recall the notion of a Dirac observable.

Definition 3.1.
i)
A function $O \in C^\infty(\mathcal{M})$ is called a weak Dirac observable provided that

$$\{O, C(N)\}_{|\mathcal{C}} = 0 \tag{3.4}$$

for all test functions (smooth of compact support) N^j and where

$$C(N) = \int_X d\mu(x)\; N^j(x) C_j(x) \tag{3.5}$$

The set of all weak Dirac observables is denoted by $\mathcal{O}_w$.
ii)
A function $O \in C^\infty(\mathcal{M})$ is called an ultrastrong Dirac observable provided that

$$\{O, C(N)\} \equiv 0 \tag{3.6}$$

for all test functions (smooth of compact support) N^j. The set of all ultrastrong Dirac observables is denoted by $\mathcal{O}_u$.

Obviously every ultrastrong Dirac observable is a weak Dirac observable. The following simple theorem is crucial for the validity of the **Master Constraint Proposal**.

Theorem 3.1.
A function $O \in C^\infty(\mathcal{M})$ is a weak Dirac Observable if and only if

$$\{O, \{O, \mathbf{M}\}\}_{\mathbf{M}=0} = 0 \qquad \textbf{(Master Equation)} \tag{3.7}$$

Proof of theorem 3.1:
The proof is so trivial that we almost do not dare to call this result a theorem:

Since O is certainly twice differentiable by assumption we easily compute (formally, to be made precise using the topology of $\mathcal{M}$)

$$\begin{aligned} \{O, \{O, \mathbf{M}\}\} &= \int_X d\mu(x)\; [g^{jk}(x)\{O, C_j(x)\}\{O, C_k(x)\} + g^{jk}(x)\{O, \{\{O, C_j(x)\}\}C_k(x) \\ &+ \{O, g^{jk}(x)\}\{O, C_j(x)\}C_k(x) + \frac{1}{2}\{O, \{O, g^{jk}(x)\}\}C_j(x)C_k(x)] \end{aligned} \tag{3.8}$$

Restricting this expression to the constraint surface $\mathcal{C}$ is equivalent, according to lemma 3.1, to setting $\mathbf{M} = 0$ hence

$$\{O, \{O, \mathbf{M}\}\}_{\mathbf{M}=0} = \int_X d\mu(x)\; g^{jk}(x)\{O, C_j(x)\}_{|\mathcal{C}}\{O, C_k(x)\}_{|\mathcal{C}} \tag{3.9}$$

Since g is positive definite this is equivalent with

$$\{O, C_j(x)\}_{|\mathcal{C}} = 0 \text{ for a.a. } x \in X \tag{3.10}$$

hence this is equivalent with

$$\{O, C(N)\}_{|\mathcal{C}} = 0 \tag{3.11}$$

for all smooth test functions of compact support.
□
Obviously the theorem also holds under the weaker assumption that O is at least twice differentiable.

The characterization of weak Dirac observables as shown in theorem 3.1 motivates the following definition.

Definition 3.2.
A function $O \in C^\infty(\mathcal{M})$ is called strong Dirac Observable if

$$\{O, \mathbf{M}\} \equiv 0 \tag{3.12}$$

The set of all strong Dirac observables is denoted by $\mathcal{O}_s$.

The inclusion $\mathcal{O}_s \subset \mathcal{O}_w$ is obvious. Notice that restriction to twice differentiable functions does not harm the validity of this inclusion. However, whether every ultrastrong Dirac observable is also a strong one is less clear as one can easily check and presumably there do exist counterexamples. We will not be concerned with this in what follows.

Definition 3.3.
Let $O \in C_b^\infty(\mathcal{M})$ be a bounded function on $\mathcal{M}$ (in sup-norm) and let $\chi_{\mathbf{M}}$ be the Hamiltonian vector field of $\mathbf{M}$ (which is uniquely determined because our symplectic structure is strong by assumption). The **ergodic mean** *of O, if it exists, is defined by the pointwise (on $\mathcal{M}$) limit*

$$[O] := \mathbf{P}^{\mathbf{M}} \cdot O := \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt\; e^{t\mathcal{L}_{\chi_{\mathbf{M}}}} O \tag{3.13}$$

It is clear that the operator $\mathbf{P}^{\mathbf{M}} :\ C_b(\mathcal{M}) \to C_b(\mathcal{M})$ is (formally) a projection because the operators

$$\alpha_t^{\mathbf{M}} := e^{t\mathcal{L}_{\chi_{\mathbf{M}}}} \tag{3.14}$$

are unitary on the Hilbert space $L_2(\mathcal{M}, d\Omega)$ where Ω is the (formal) Liouville measure on $\mathcal{M}$. Notice that the one-parameter family of symplectomorphisms (3.14) defines an inner automorphism on the Poisson algebra $C^\infty(\mathcal{M})$.

The usefulness of the notion of a strong Dirac observable is stressed by the following result.

Theorem 3.2.
Suppose that $[O]$ is still at least in $C_b^2(\mathcal{M})$. Then, under the assumptions spelled out in the proof, $[O] \in \mathcal{O}_s$.

Notice that the requirement that $[O]$ is at least twice differentiable is crucial, otherwise $[O]$ is not granted to be an element of $\mathcal{O}_w$ even if it has vanishing first Poisson bracket with $\mathbf{M}$ everywhere on $\mathcal{M}$.
Proof of theorem 3.2:
Let

$$[O]_T := \frac{1}{2T} \int_{-T}^{T} dt\; e^{t\mathcal{L}_{\chi_{\mathbf{M}}}} O \tag{3.15}$$

Provided we may interchange the integral with the Poisson bracket we have

$$\{[O]_T, \mathbf{M}\} = \frac{1}{2T} \int_{-T}^{T} dt\; \frac{d}{dt} e^{t\mathcal{L}_{\chi_{\mathbf{M}}}} O = \frac{e^{T\mathcal{L}_{\chi_{\mathbf{M}}}} - e^{-T\mathcal{L}_{\chi_{\mathbf{M}}}}}{2T} O \tag{3.16}$$

Since O is bounded (in sup-norm) on $\mathcal{M}$ by assumption, so is $e^{\pm T\mathcal{L}_{\chi_{\mathbf{M}}}} O$, hence

$$\lim_{T\to\infty} \{[O]_T, \mathbf{M}\} = 0 \tag{3.17}$$

Thus, provided that we may interchange the limit $T \to \infty$ with the Poisson bracket, we get $\{[O], \mathbf{M}\} = 0$.
$\Box$
Sufficient conditions for the existence assumptions and the allowedness to interchange the opertions indicated in the proof are examined in [42]. The restriction of the ergodic mean to bounded functions is thus motivated by the proof of this theorem. On the other hand, in order that $[O] \neq 0$ it is necessary that the evolution $\alpha_t^{\mathbf{M}}(O)$ does not decay (in sup-norm) as $t \to \infty$ but rather stays bounded away from zero.

Hence the ergodic mean technique provides a *guideline for explicitly constructing Dirac Observables*. It would be nice to have an equally powerful technique at our disposal which immediately constructs functions which satisfy the more general non-linear condition (3.7) but we could not find one yet. Notice that, formally, we can carry out the integral in (3.13) by using the power expansion, valid for smooth O

$$\alpha_t^{\mathbf{M}}(O) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \{O, \mathbf{M}\}_{(n)} \tag{3.18}$$

where the the multiple Poisson bracket is inductively defined by $\{O, \mathbf{M}\}_{(0)} = O,\ \{O, \mathbf{M}\}_{(n+1)} = \{\{O, \mathbf{M}\}_{(n)}, \mathbf{M}\}$. Hence, formally

$$[O]_T = \sum_{n=0}^{\infty} \frac{T^{2n}}{(2n+1)!} \{O, \mathbf{M}\}_{(2n)} \tag{3.19}$$

However, the series is at best asymptotic and the limit $T \to \infty$ can be taken only after resummation of the series. Thus the presentation (3.19) is useless, we need a perturbative definition of $[O]$ which is practically more useful with more control on convergence issues. Maybe some of the ideas of [40] can be exploited. This leads us to the **theory of dynamical systems, integrable systems, the theory of invariants and ergodic theory** [41]. Aspects of this are currently under investigation and will be published elsewhere [42].

A couple of remarks are in order before we turn to the quantum theory:
1.
When applying the above theory to LQG at the diffeomorphism invariant level one should start the classical description from the diffeomorphism invariant phase space. This is defined by considering all diffeomorphism invariant functions on the kinematical phase space as its (over)coordinatization and by using the Poisson bracket between diffeomorphism invariant functions induced by the kinematical Poisson bracket as the diffeomorphism invariant Poisson bracket between those functions.
2.
The automorphisms $\alpha_t^{\mathbf{M}}$ do not only preserve the constraint hypersurface $\mathcal{C}$, they also preserve *every individual point* $m \in \mathcal{C}$ because $\{O, \mathbf{M}\}_{\mathbf{M}=0} = 0$ for any $O \in C^\infty(\mathcal{M})$. In other words, the Hamiltonian vector field $\chi_{\mathbf{M}}$ is not only tangential to $\mathcal{C}$ as it is the case for first class constraints, it vanishes identically on $\mathcal{C}$. Imagine a foliation of $\mathcal{M}$ by leaves $\mathcal{M}_t = \{m \in \mathcal{M};\ \mathbf{M}(m) = t\}$ where $\mathcal{M}_0 = \mathcal{C}$. If $\mathbf{M}$ is an least once differentiable function on $\mathcal{M}$ determined by first class constraints as we assumed then in an open neighbourhood of $\mathcal{C}$ the vector field $\chi_{\mathbf{M}}$ will be tangential to the corresponding leaf but non-vanishing there. This is dangerous because it means that the automorphisms $\alpha_t^{\mathbf{M}}$ for $t \neq 0$ are non-trivial and thus the ergodic mean $[O]$ could be discontinuous precisely in any neighbourhood of $\mathcal{C}$, hence it is not differentiable there and thus does not qualify as a strong Dirac observable. Investigations in simple models show that this indeed happens. In fact, experience with dynamical systems reveals that typical observables (integrals of motion generated by the "Hamiltonian" $\mathbf{M}$) generated by an ergodic mean are rather discontinuous functions on $\mathcal{M}$ even if the system is completely integrable [43].

However, there is a simple procedure to repair this: Consider only the values of $[O]$ restricted to a set of the form $\mathcal{M} - \mathcal{U}$ where $\mathcal{U}$ is any open neighbourhood of $\mathcal{C}$. If $[O]$ is at least C^2 there, extend to all of $\mathcal{M}$ in an at least C^2 fashion. The resulting new observable $[O]'$ coincides with $[O]$ except on $\mathcal{C}$, is C^2 and satisfies $\{[O]', \mathbf{M}\} \equiv 0$ hence defines an element of $\mathcal{O}_w$.
3.
One could avoid these subtleties by generalizing the concept of a strong Dirac observable as follows:

Definition 3.4.
Let $\alpha_t^{\mathbf{M}}$ be the one-parameter family of automorphisms (symplectic isometries) generated by the Hamiltonian vector field $\chi_{\mathbf{M}}$ of the **Master Constraint**. *Then a (not necessarily continuous) function on $\mathcal{M}$ is called a generalized strong Dirac observable provided that*

$$\alpha_t^{\mathbf{M}}(O) = O \tag{3.20}$$

for all $t \in \mathbb{R}$.

Notice that definitions 3.4 and 3.2 are certainly not eqivalent. On the other hand, with this weaker notion the above discontinuity problems disappear and the proof of theorem 3.2 holds under weaker assumptions because now limits and integrals commute under weaker assumptions with the operation $\alpha_t^{\mathbf{M}}$. Also in quantum theory definition 3.4 is easier to deal with because

it changes the focus from the unbounded, self-adjoint operator $\mathbf{M}$ to the bounded, unitary operators $\exp(it\widehat{\mathbf{M}})$ which avoids domain questions, see below.
4.
In summary, the ergodic mean $[O]$ of O is a **candidate** for an element of $\mathcal{O}_s$. In order to check whether it really is it is sufficient that it be twice differentiable and $\{O, \mathbf{M}\} \equiv 0$. Similarly, in the quantum theory one must check whether the **candidate** operator $[\hat{O}]$ of (3.24) has commuting spectral projections with those of $\widehat{\mathbf{M}}$ since in general only then $[[\hat{O}], \widehat{\mathbf{M}}] \equiv 0$ identically. There is no differentiability condition to be checked, however, since the quantum analogue of Poisson brackets, namely commutators between bounded spectral projections, always make sense. In that sense the quantum theory is better behaved.

3.2 Quantum Theory

Let us now come to quantization which is actually just a straightforward transcription of the above structure from functions to operators. Suppose that we managed to find a representation of the Poisson algebra as an algebra $\widehat{\mathcal{O}}$ of operators on a *separable* Hilbert space $\mathcal{H}_{Kin}$ and that, in particular, the **Master Constraint $\mathbf{M}$** is represented as a *positive, self-adjoint* operator $\widehat{\mathbf{M}}$. We therefore can construct the weakly continuous, one-parameter family of unitary operators

$$\hat{U}(t) = e^{it\widehat{\mathbf{M}}} \tag{3.21}$$

We then have a representation of the automorphisms $\alpha_t^{\mathbf{M}}$ of $\mathcal{O}$ as inner automorphisms on $\widehat{\mathcal{O}}$ according to

$$\hat{\alpha}_t^{\mathbf{M}}(\hat{O}) = \hat{U}(t)\hat{O}\hat{U}(t)^{-1} \tag{3.22}$$

Definition 3.5. *A strong,* **generalized** *quantum Dirac observable is defined as a self-adjoint element $\hat{O} \in \widehat{\mathcal{O}}$ such that*

$$\hat{\alpha}_t^{\mathbf{M}}(\hat{O}) = \hat{O} \tag{3.23}$$

for all $t \in \mathbb{R}$. A (genuine) strong quantum Dirac Observable is such that the spectral projections of $\hat{O}$ and $\widehat{\mathbf{M}}$ commute.

Candidates of the set $\mathcal{O}_s$ of strong quantum Dirac Observables can be constructed using the ergodic mean of bounded operators $\hat{O}$ (in the uniform operator norm induced by the topology of $\mathcal{H}_{Kin}$)

$$[\hat{O}] = \lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} dt \; \hat{\alpha}_t^{\mathbf{M}}(\hat{O}) \tag{3.24}$$

Notice that no domain questions arise. The direct translation of (3.7) is more difficult since it cannot be easily written in terms of the bounded operators $\hat{U}(t)$, hence domain questions arise:

Definition 3.6. *Let Φ_{Kin} be a common, dense, invariant domain for the self adjoint operators $\hat{O}, \widehat{\mathbf{M}}$ and let $(\Phi^*_{Kin})_{Phys}$ be the subspace of the space Φ^*_{Kin} of algebraic distributions over Φ_{Kin} satisfying $l(\widehat{\mathbf{M}} f) = 0$ for any $f \in \Phi_{Kin}$. Then $\hat{O}$ is a weak quantum Dirac Observable provided that*

$$l([\hat{O}, [\hat{O}, \widehat{\mathbf{M}}]] f) = 0 \text{ for all } f \in \Phi_{Kin},\; l \in (\Phi^*_{Kin})_{Phys} \tag{3.25}$$

Obviously any strong quantum Dirac observable is a weak one. A more precise examination between the notions of strong and weak quantum Dirac observables will be performed in [42].

As shown in the appendix, there is a one to one correspondence between $l_\psi \in (\Phi^*_{Kin})_{Phys}$ (defined below) and solutions to the quantum constraint, i.e physical states $\psi \in \mathcal{H}_{Phys}$, heuristically given by $l_\psi =< \delta(\widehat{\mathbf{M}})\psi, . >_{Kin}$. The precise construction of physical states is conceptually straightforward: Since $\mathcal{H}_{Kin}$ is separable by assumption, as is well-known, [64] it can be represented as a direct integral of separable Hilbert spaces $\mathcal{H}^{\oplus}_{Kin}(\lambda),\ \lambda \in \mathbb{R}$, subordinate to $\widehat{\mathbf{M}}$ according to

$$\mathcal{H}_{Kin} = \int_{\mathbb{R}}^{\oplus} d\nu(\lambda)\; \mathcal{H}^{\oplus}_{Kin}(\lambda) \tag{3.26}$$

that is, any element $\psi \in \mathcal{H}_{Kin}$ can be thought of as a collection $(\psi(\lambda))_{\lambda\in\mathbb{R}}$ where $\psi(\lambda) \in \mathcal{H}^{\oplus}_{Kin}(\lambda)$ such that

$$||\psi||^2 = \int_{\mathbb{R}} d\nu(\lambda)\ ||\psi(\lambda)||^2_{\mathcal{H}^{\oplus}_{Kin}(\lambda)} \tag{3.27}$$

converges (the functions $\lambda \mapsto ||\psi(\lambda)||^2_{\mathcal{H}^{\oplus}_{Kin}(\lambda)}$ are measurable in particular). The operator $\widehat{\mathbf{M}}$ is represented on $\mathcal{H}^{\oplus}_{Kin}(\lambda)$ as multiplication by λ, $\widehat{\mathbf{M}}(\psi(\lambda))_{\lambda\in\mathbb{R}} = (\lambda\psi(\lambda))_{\lambda\in\mathbb{R}}$ whenever $\psi \in \mathrm{dom}(\widehat{\mathbf{M}})$. The measure ν and the Hilbert spaces $\mathcal{H}^{\oplus}_{Kin}(\lambda)$ are not uniquely determined but different choices give rise to unitarily equivalent representations. Given such a choice, the scalar product on $\mathcal{H}^{\oplus}_{Kin}(\lambda)$ is uniquely determined by that on $\mathcal{H}_{Kin}$. It follows:

Definition 3.7. *The physical Hilbert space is given by*

$$\mathcal{H}_{Phys} := \mathcal{H}^{\oplus}_{Kin}(0) \tag{3.28}$$

Notice that $\mathcal{H}_{Phys}$ comes automatically with a physical inner product, that is, we have simultaneously constructed the full solution space and an inner product on it. Moreover, one can show that if $\hat{O}_{Inv}$ is a strong self-adjoint quantum Dirac observable, more precisely, if the spectral projections of the operators $\hat{O}_{Inv}, \widehat{\mathbf{M}}$ commute, then $\hat{O}_{Inv}$ can be represented as a collection $(\hat{O}_{Inv}(\lambda))_{\lambda\in\mathbb{R}}$ of symmetric operators $\hat{O}_{Inv}(\lambda)$ on the individual $\mathcal{H}^{\oplus}_{Kin}(\lambda)$. If $\hat{O}_{Inv}$ is also bounded then $\hat{O}_{Inv}(\lambda)$ is even self-adjoint there. Thus $\hat{O}_{Inv}(0)$ preserves $\mathcal{H}_{Phys}$ and the adjointness relations from $\mathcal{H}_{Kin}$ are transferred to $\mathcal{H}_{Phys}$. Candidates for $\hat{O}_{Inv}$ are, of course, the $[\hat{O}]$ of (3.24).

Remarks:
1.
At the classical level, the immediate criticism about the **Master Constraint Proposal** is that it seems to fail to detect weak Dirac observables since it has vanishing Poisson brackets with every function O on the constraint surface. This criticism is wiped out by theorem 3.1.

At the quantum level there is a related criticism: How can it be that the *multitude* of quantum constraints $\hat{C}_J$ have the same number of solutions as the the *single* **Quantum Master Constraint** $\widehat{\mathbf{M}}$? The answer lies in the functional analytic details: As long as we are just looking for solutions of the single equation $\widehat{\mathbf{M}}\,\psi = 0$ without caring to which space it belongs, then it has zillions of solutions which are not solutions of the many equations $\hat{C}_J\psi = 0$. However, the requirement that those solutions be normalizable with respect to the inner product induced, e.g. by the direct integral representation or the Rigging Map construction, rules out those extra solutions as one can explicitly verify in solvable models. Alternatively, when constructing the physical inner product by requiring that a complete number of (strong) Dirac observables (including the operators $\hat{C}_J$) be represented as self-adjoint operators on $\mathcal{H}_{Phys}$, one finds out, in solvable models, that the solution space must be reduced to the simultaneous one of all constraints. We will come back to this issue in [42].
2.
We have restricted ourselves here to first class constraints for simplicity. But the **Master Constraint Programme** can also deal with second class constraints on the classical level. On the quantum level, as solvable models reveal, one has to be careful with the ordering of the operator as otherwise there might be no solutions at all [42].
3.
We have assumed the separability of the Hilbert space because it implies an existence theorem about the physical Hilbert space. At an heuristic level, without rigorous proofs, one can live with the Rigging Map construction, recalled in the appendix, which does not assume separability of the Hilbert space. For instance, these heuristics worked quite well for the spatial diffeomorphism constraint in [26].
4.
The constraint algebra of the **Master Constraint Operator** is trivial even if the constraint algebra of the original first class constraints C_J is not. This seems strange at first because the usual operator constraint quantization $\hat{C}_J$ needs to be supplemented by a discussion of anomaly

freeness. There is no contradiction because a non-anomalous operator ordering of the $\hat{C}_J$, if any, should enlarge the physical Hilbert space of the corresponding **Master Constraint Operator**, heuristically given by $\widehat{\mathbf{M}} = \sum_J \hat{C}_J^\dagger \hat{C}_J$ where the adjoint is with respect to $\mathcal{H}_{Kin}$. Since only a non-anomalous constraint algebra usually results in a sufficiently large $\mathcal{H}_{Phys}$ (sufficient number of semiclassical states), the issue of anomaly freeness has been merely translated into the size of $\mathcal{H}_{Phys}$. However, while physically nothing has been gained (as it should not) by the **Master Constraint Programme**, mathematically it has the huge advantage that it lets us carry out the quantization programme until the very end, with the verification of the correct semiclassical limit as the only and final non-trivial consistency check while simplifying the solution of the constraints and the construction of Dirac observables.

4 The Master Constraint Operator for General Relativity: 1. Graph-Changing Version

The purpose of this section is to sketch the quantization of the **Master Constraint** for General Relativity. Many more details will follow in subsequent submissions [44]. We assume the reader to be familiar with LQG at an at least introductory level and follow the notation of the first reference of [1].

4.1 Classical Preliminaries

By $C(x)$ we mean, of course, the Lorentzian Hamiltonian constraint of General Relativity plus all known matter in four spacetime dimensions. For the introductory purposes of this paper we will restrict ourselves to the purely geometrical piece because it entails already the essential features of the new quantization that we are about to introduce. Thus in what follows, $C(x)$ will mean that gravitational part only.

As shown in [2, 3], the smeared constraint $C(N)$ can be written in the following form

$$\begin{aligned} C(N) &= C(N) + [\beta^2 + 1] T(N) \\ C_E(N) &= \frac{1}{\kappa} \int_\sigma N \mathrm{Tr}(F \wedge e) \\ T(N) &= \frac{1}{\kappa} \int_\sigma N \mathrm{Tr}(K \wedge K \wedge e) \end{aligned} \tag{4.1}$$

where κ is the gravitational constant. The $SU(2)-$valued one-forms e and K respectively are related to the intrinsic metric q_{ab} and the extrinsic curvature K_{ab} of the ADM formulation respectively by the formulas

$$q_{ab} = \delta_{jk} e_a^j e_b^k, \;\; K_{ab} = K^j_{(a} e^k_{b)} \delta_{jk} \tag{4.2}$$

so e_a^j is nothing else than the cotriad. The Ashtekar – Barbero variables [45] of the connection formulation of General Relativity are the canonically conjugate pair

$$A_a^j = \Gamma_a^j + \beta K_a^j, \;\; E_j^a = \det(e) e_j^a / \beta \tag{4.3}$$

where Γ is the spin connection of e and β is called the Immirzi parameter [46].

In order to quantize the **Master Constraint** corresponding to (4.1) we proceed as in [2, 3] and use the **key identities**

$$\begin{aligned} e_a^j(x) &= -\frac{2}{\kappa\beta} \{A_a^j(x), V(R_x)\} \\ K_a^j(x) &= -\frac{1}{\kappa\beta} \{A_a^j(x), \{C_E(1), V\}\} \\ V(R_x) &= \int_\sigma \chi_{R_x}(y) d^3y \sqrt{\det(q)}(y) \\ C_E(1) &= C_E(N)_{|N=1} \end{aligned} \tag{4.4}$$

The quantity $V(R_x)$ is the volume of the of the open region R_x which is completely arbitrary, the only condition being that $x \in R_x$. On the other hand, V is the total volume of σ which diverges when σ is not compact but this is unproblematic since V appears only inside a Poisson bracket (its functional derivative is well-defined). The logic behind (4.4) is that $V(R)$ has a well-defined quantization $\hat{V}(R)$ for any region R on the kinematical Hilbert space $\mathcal{H}_{Kin}$ of LQG [47]. Thus, if we replace Poisson brackets by commutators divided by $i\hbar$ then we may be able to first quantize $C_E(x)$ and then $T(x)$.

Inserting (4.4) into (4.1) we obtain

$$\begin{aligned} C_E(N) &= -\frac{2}{\kappa^2\beta}\int_\sigma N\mathrm{Tr}(F\wedge\{A,V\}) \\ T(N) &= -\frac{2}{\kappa^4\beta^3}\int_\sigma N\mathrm{Tr}(\{A,\{C_E(1),V\}\}\wedge\{A,\{C_E(1),V\}\}\wedge\{A,V\}) \end{aligned} \tag{4.5}$$

Correspondingly, the **Master Constraint** can be written in the form

$$\begin{aligned} \mathbf{M} &:= \int_\sigma d^3x \frac{C(x)^2}{\sqrt{\det(q)}(x)} = \int_\sigma d^3x(\frac{C}{\sqrt[4]{\det(q)}})(x)\int_\sigma d^3y\delta(x,y)(\frac{C}{\sqrt[4]{\det(q)}})(y) \qquad (4.6) \\ &= \lim_{\epsilon\to 0}(\frac{2}{\kappa\sqrt{\beta}})^4\int_\sigma d^3x\mathrm{Tr}([F+\frac{\beta^2+1}{(\kappa\beta)^2}\{A,\{C_E(1),V\}\}\wedge\{A,\{C_E(1),V\}\}]\wedge\{A,\sqrt{V_{\epsilon,.}}\})(x)\times \\ &\quad \times\int_\sigma d^3y\chi_\epsilon(x,y)\mathrm{Tr}([F+\frac{\beta^2+1}{(\kappa\beta)^2}\{A,\{C_E(1),V\}\}\wedge\{A,\{C_E(1),V\}\}]\wedge\{A,\sqrt{V_{\epsilon,.}}\})(y) \end{aligned}$$

Here $\chi_\epsilon(x,y)$ is any one-parameter family of, not necessarily smooth, functions such that $\lim_{\epsilon\to 0}\chi_\epsilon(x,y)/\epsilon^3=\delta(x,y)$ and $\chi_\epsilon(x,x)=1$. Moreover,

$$V_{\epsilon,x} := \int_\sigma d^3y\chi_\epsilon(x,y)\sqrt{\det(q)}(y) \tag{4.7}$$

Thus, in the last line of (4.6) we have performed a convenient point split.

Readers familiar with [2, 3, 4, 5, 6, 7, 8, 9] already recognize that the integrands of the two integrals in (4.6) are *precisely* those of [3], the only difference being that the last factor in the wedge product is given by $\{A,\sqrt{V_{\epsilon,.}}\}$ rather than $\{A,V\}$ which comes from the additional factor of $(\sqrt[4]{\det(q)})^{-1}$ in our point-split expression. Thus we proceed exactly as in [3] and introduce a partition $\mathcal{P}$ of σ into cells $\Box$, splitting both integrals into sums $\int_\sigma=\sum_{\Box\in\mathcal{P}}$. Assigning to each cell $\Box$ an interior point $v(\Box)$, in the infinite refinement limit $\mathcal{P}\to\sigma$ in which all the cells collapse to a single point and those points fill all of σ we may replace (4.6) by the limit of the following double Riemann sum

$$\begin{aligned} \mathbf{M} &= \lim_{\epsilon\to 0}\lim_{\mathcal{P}\to\sigma}\sum_{\Box,\Box'\in\mathcal{P}}\chi_\epsilon(v(\Box),v(\Box'))(\frac{2}{\kappa\sqrt{\beta}})^4\times \\ &\quad\times\int_\Box d^3x\mathrm{Tr}([F+\frac{\beta^2+1}{(\kappa\beta)^2}\{A,\{C_E(1),V\}\}\wedge\{A,\{C_E(1),V\}\}]\wedge\{A,\sqrt{V_{\epsilon,.}}\})(x)\times \\ &\quad\times\int_{\Box'} d^3y\mathrm{Tr}([F+\frac{\beta^2+1}{(\kappa\beta)^2}\{A,\{C_E(1),V\}\}\wedge\{A,\{C_E(1),V\}\}]\wedge\{A,\sqrt{V_{\epsilon,.}}\})(y) \end{aligned} \tag{4.8}$$

Notice that the limit of the Riemann sum is independent of the way we refine the partition.

Now the integrals over $\Box,\Box'$ in (4.8) are of the type of functions that can be quantized by the methods of [2, 3, 4, 5, 6, 7, 8, 9]. Before we do that we recall why the limit $\mathcal{P}\to\sigma$ does not exist in the sense of operators on the kinematical Hilbert space and forces us to define the operator (or rather a quadratic form) directly on the diffeomorphism invariant Hilbert space $\mathcal{H}_{Diff}$ [26]. This makes sense for $\mathbf{M}$ in contrast to $C(N)$ since $\mathbf{M}$ is a diffeomorphism invariant function.

4.2 Spatially Diffeomorphism Invariant Operators

Lemma 4.1.
Let Q be a spatially diffeomorphism invariant quadratic form on $\mathcal{H}_{Kin}$ whose form domain contains the smooth cylindrical functions Cyl^∞. Let $Q_{s,s'} := Q(T_s, T_{s'})$ where s denotes a spin network (SNW) label and T_s the corresponding spin network function (SNWF). Then a necessary condition for Q to be the quadratic form of a spatially diffeomorphism invariant operator densely defined on Cyl^∞ is that $Q_{s,s'} = 0$ whenever $\gamma(s) \neq \gamma(s')$ where $\gamma(s)$ denotes the graph label of s.

Proof of lemma 4.1:
Recall the unitary representation $\hat{U}: \text{Diff}^\omega(\sigma) \to \mathcal{B}(\mathcal{H}_{Kin})$ of the group of analytic diffeomorphisms of σ on the kinematical Hilbert space defined by $\hat{U}(\varphi)p_\gamma^* f_\gamma = p_{\varphi(\gamma)}^* f_\gamma$ where p_γ is the restriction of a (generalized) connection $A \in \overline{\mathcal{A}}$ to the edges $e \in E(\gamma)$ and f_γ; $SU(2)^{|E(\gamma)|} \to \mathbb{C}$. A spatially diffeomorphism invariant quadratic form then is defined by $Q(U(\varphi)f, U(\varphi)f') = Q(f, f')$ for all $f, f' \in \text{dom}(Q)$.

Consider any $\gamma(s) \neq \gamma(s')$ where $\gamma(s)$ is the graph underlying the SNW s. Then we find a countably infinite number of analytic diffeomorphisms $\varphi_n,\ n = 0, 1, 2, ..$ such that $T_{s'}$ is invariant but $T_{s_n} = U(\varphi_n)T_s$ are mutually orthogonal spin network states (we have set $\varphi_0 = \text{id}$; interchange s, s' if $T_s = 1$). Suppose now that Q is the quadratic form of a spatially diffeomorphism invariant operator $\hat{O}$ on $\mathcal{H}_{Kin}$, that is, $\hat{U}(\varphi)\hat{O}\hat{U}(\varphi)^{-1} = \hat{O}$ for all $\varphi \in \text{Diff}^\omega(\sigma)$, $Q(f, f') =< f, \hat{O}f' >$, densely defined on Cyl^∞. Then

$$||\hat{O}T_s'||^2 = \sum_s |Q_{s,s'}|^2 \geq \sum_{n=0}^\infty |Q_{s_n,s'}|^2 = |Q_{s,s'}|^2 [\sum_{n=0} 1] \tag{4.9}$$

diverges unless $Q_{s,s'} = 0$.
□
We conclude that diffeomorphism invariant operators which are graph changing cannot exist on $\mathcal{H}_{Kin}$. The only diffeomorphism invariant operators which can be defined on $\mathcal{H}_{Kin}$ must not involve the connection A, they are defined purely in terms of E. The total volume of σ is an example for such an operator. Since $\mathbf{M}$ involves the curvature F of A, the operator $\widehat{\mathbf{M}}$ cannot be defined on $\mathcal{H}_{Kin}$ unless one uses an ad hoc procedure as in section 5. The way out, as noticed in [2, 3, 4], is to define $\widehat{\mathbf{M}}$ not on $\mathcal{H}_{Kin}$ but on $\mathcal{H}_{Diff}$. The effect of this is, roughly speaking, that all the terms in the infinite sum in (4.9) are eqivalent under diffeomorphisms, hence we also need only one of them, whence the infinite sum becomes finite.

4.3 Diffeomorphism Invariant Hilbert Space

Recall the definition of $\mathcal{H}_{Diff}$. A diffeomorphism invariant distribution l is a, not necessarily continuous, linear functional on $\Phi_{Kin} :=\text{Cyl}^\infty$ (that is, an element of Φ_{Kin}^*) such that

$$l(\hat{U}(\varphi)f) = l(f)\ \ \forall\ \ f \in \text{Cyl}^\infty,\ \varphi \in \text{Diff}^\omega(\sigma) \tag{4.10}$$

Since the finite linear span of SNWF's is dense in Cyl^∞ it suffices to define l on the SNWF, hence l can formally be written in the form

$$l(.) = \sum_s l_s < T_s, . >_{Kin} \tag{4.11}$$

for complex valued coefficients which satisfy $l_s = l_{s'}$ whenever $T_{s'} = \hat{U}(\varphi)T_s$ for some diffeomorphism φ. In other words, the coefficients only depend on the orbits

$$[s] = \{s';\ T_{s'} = \hat{U}(\varphi)T_s \text{ for some } \varphi \in \text{Diff}^\omega(\sigma)\} \tag{4.12}$$

Hence the distributions

$$b_{[s]} = \sum_{s' \in [s]} < T_{s'}, . >_{Kin} \tag{4.13}$$

play a distinguished role since

$$l(.) = \sum_{[s]} l_{[s]} b_{[s]} \tag{4.14}$$

The Hilbert space $\mathcal{H}_{Diff}$ is now defined as the completion of the finite linear span of the $b_{[s]}$ in the scalar product obtained by declaring the $b_{[s]}$ to be an orthonormal basis, see [26] for a detailed derivation through the procedure of refined algebraic quantization (group avaraging) [63]. More explicitly, the scalar product $< .,. >_{Diff}$ is defined on the basis elements by

$$< b_{[s]}, b_{[s']} >_{Diff} = \overline{b_{[s]}(T_{s'})} = b_{[s']}(T_s) = \chi_{[s]}(s') = \delta_{[s],[s']} \tag{4.15}$$

and extended by sesquilinearity to the finite linear span of the $b_{[s]}$.

In this paper we will actually modify the Hilbert space $\mathcal{H}_{Diff}$ as follows: One might think that $\mathcal{H}_{Diff}$ as defined is separable, however, this is not the case: As shown explicitly in [38], since the diffeomorphism group at a given point reduces to $GL_+(3,\mathbb{R})$, for vertices of valence five or higher there are continuous, diffeomorphism invariant parameters associated with such vertices. More precisely, we have the following: Given an $n-$valent vertex v of a graph γ, consider all its $\binom{n}{3}$ triples (e_1, e_2, e_3) of edges incident at it. With each triple we associate a degeneracy type $\tau(e_1, e_2, e_3)$ taking six values depending on whether the tangents of the respective edges at v are 0) linearly independent, 1) co-planar but no two tangents are co-linear, 2a) co-planar and precisely one pair of tangents is co-linear but the corresponding edges are not analytic continuations of each other, 2b) co-planar and precisely one pair of tangents is co-linear where the corresponding edges are analytic continuations of each other, 3a) co-linear but for no pair the corresponding edges are analytic continuations of each other, 3b) co-linear and precisely for one pair the corresponding edges are analytic continuations of each other. Notice that an analytic diffeomorphism or a reparameterization cannot change the degenaracy type of any triple. We could refine the classification of degeneracy types by considering also the derivatives of the edges of order $1 < k < \infty$ (we just considered $k = 1, \infty$) in which case we would associate more discrete diffeomorphism invariant information with a vertex of valence n but for our purposes this will sufficent. By the degeneracy type of a graph we will mean the collection of degeneracy types of each of the triples of all vertices.

Given a SNW s with $\gamma(s) = \gamma$ we now mean by $\{s\}$ the set of all s' such that $[s]$ and $[s']$ differ at most by a different value of continuous moduli but not by a degeneracy type for any triple of edges for any vertex. In other words, $s = s'$ whenever $\gamma(s), \gamma(s')$ are *ambient isotopic* up to the degeneracy type. That is, $\gamma(s)$ can be deformed into $\gamma(s')$ by a smooth one-parameter family of analytic maps $f_t : \sigma \to \sigma,\ t \in [0,1]$ with analytic inverse such that $f_0(\gamma(s)) = \gamma(s),\ f_1(\gamma(s)) = \gamma(s')$ without changing the degeneracy type of $\gamma(s)$. If $\gamma(s)$ has at most four-valent vertices then $\{s\} = [s]$ but otherwise these two classes are different. The class $\{s\}$ depends only on discrete labels and if we define

$$b_{\{s\}}(.) = \sum_{s' \in \{s\}} < T_{s'}, . >_{Kin} \tag{4.16}$$

and

$$< b_{\{s\}}, b_{\{s'\}} >_{Diff} := \overline{b_{\{s\}}(T_{s'})} = b_{\{s'\}}(T_s) = \chi_{\{s\}}(s') = \delta_{\{s\},\{s'\}} \tag{4.17}$$

then $\mathcal{H}_{Diff}$ becomes separable. The passage from (4.14), (4.15) (diffeomorphism invariant states) to (4.16), (4.17) (ambient isotopy modulo degeneracy type invariant states) may seem as a drastic step because ambient isotopy is not induced by the symmetry group. On the other hand, for graphs with at most four valent vertices, which are the most important ones for semi-classical considerations since the dual graph of any simplicial cellular decomposition of a manifold is four-valent, there is no difference. Moreover, any $b_{\{s\}}$ is a (possibly uncountably infinite) linear combination over of the $b_{[s]}$ by summing over the corresponding continuous moduli. There might be other ways to get rid of the non-separabilty, for example by introducing a measure on the *Teichmüller*-like space of continuous moduli, but this goes beyond the scope of the present paper.

4.4 Regularization and Quantization of the Master Constraint

We now have recalled all the tools to quantize $\mathbf{M}$ itself. As we have explained in detail, this will be possible only on $\mathcal{H}_{Diff}$. Moreover, we must construct an operator $\widehat{\mathbf{M}}$ (or rather a dual operator $\widehat{\mathbf{M}}'$ on $\mathcal{H}_{Diff}$) which is positive in order that it really enforces the constraint $C(x) = 0$ for all $x \in \sigma$. The following strategy allows us to guarantee this by construction:

At given $\epsilon, \mathcal{P}$ the basic building blocks of (4.8) are the integrals

$$C_{\epsilon,\mathcal{P}}(\square) = \int_\square d^3x \mathrm{Tr}([F + \frac{\beta^2+1}{(\kappa\beta)^2}\{A, \{C_E(1), V\}\} \wedge \{A, \{C_E(1), V\}\}] \wedge \{A, \sqrt{V_{\epsilon,.}}\})(x) \quad (4.18)$$

In [3] the following strategy for the quantization of operators of the type of (4.18) was developed:

1. *Regulated Operator on* $\mathcal{H}_{Kin}$
   Replacing Poisson brackets by commutators divided by $i\hbar$ and functions by their corresponding operators, we obtain a regulated operator $\hat{C}^\dagger_{\epsilon,\mathcal{P}}(\square)$ which, together with its adjoint, is densely defined on the invariant domain Φ_{Kin} :=Cyl$^\infty$.

2. *Dual Reguated Operator on* Φ^*_{Kin}
   Let Φ^*_{Kin} be the algebraic dual of Φ_{Kin}, then we may define a dual regulated operator $\hat{C}'_{\epsilon,\mathcal{P}}(\square)$ on Φ^*_{Kin} by the formula

$$(\hat{C}'_{\epsilon,\mathcal{P}}(\square)l)[f] := l[\hat{C}^\dagger_{\epsilon,\mathcal{P}}(\square)f] \quad (4.19)$$

3. *Taking* $\epsilon \to 0$
   One regularization step is to interchange the limits in (4.8), hence we take $\epsilon \to 0$ at finite $\mathcal{P}$. This enforces that the douple sum collapses to a single one since $\lim_{\epsilon\to 0} \chi_\epsilon(v(\square), v(\square')) = \delta_{\square,\square'}$, moreover, due to the particulars of the volume operator also the limit $\epsilon \to 0$ of $\hat{C}'_{\epsilon,\mathcal{P}}(\square)$ exists in the topology of pointwise convergence on Φ^*_{Kin}, resulting in $\hat{C}'_{\mathcal{P}}(\square)$.

4. *Refinement Limit*
   The limit $\mathcal{P} \to \sigma$ does not exist in the topology of pointwise convergence on all of Φ^*_{Kin} but on the subspace $(\Phi^*_{Kin})_{Diff}$ of diffeomorphism invariant distributions. The limit defines an element of Φ^*_{Kin} again but it is not an element of $(\Phi^*_{Kin})_{Diff}$, hence it does not leave that space invariant.

In [3] these steps were used in order to define a smeared Hamiltonian constraint operator densely defined on Φ_{Kin} by introducing a new kind of operator topology which involves $(\Phi^*_{Kin})_{Diff}$. The definition of the resulting operator involves the axiom of choice, hence it exists but cannot be written down explicitly, only its dual action on $(\Phi^*_{Kin})_{Diff}$ can be written explicitly. It is at this point that we use a different strategy. Namely we propose the following heuristic expression for a quadratic form

$$Q_{\mathbf{M}}(l, l') := \lim_{\mathcal{P}\to\sigma} \sum_{\square\in\mathcal{P}} (\frac{2}{\kappa\sqrt{\beta}})^4 < \hat{C}'_{\mathcal{P}}(\square)l, \hat{C}'_{\mathcal{P}}(\square)l' >_{Diff} \quad (4.20)$$

on the dense subspace of $\mathcal{H}_{Diff}$ defined by the finite linear span of the $b_{\{s\}}$.

The immediate problem with (4.20) is that the objects $\hat{C}'_{\mathcal{P}}(\square)l$ are elements of Φ^*_{Kin} but in general not of $(\Phi^*_{Kin})_{Diff}$, hence the scalar product on $\mathcal{H}_{Diff}$ in the last line of (4.20) is ill-defined. However, as we will show in detail in [44], the scalar product *does* become well-defined in the limit $\mathcal{P} \to \sigma$ for the same reason that the classical expression (4.8) becomes diffeomorphism invariant only in the limit $\mathcal{P} \to \sigma$. The precise proof of this fact is lengthy and goes beyond the scope of the present paper, hence we will restrict ourselves here to a heuristic derivation which provides a shortcut to the final formula. (Alternatively, one may view the procedure below as *part of the of the regularization*).

The shortcut is based on a **resolution of identity trick**:
Making use of the fact that the $b_{\{s\}}$ form an orthonormal basis of $\mathcal{H}_{Diff}$ and pretending that the $\hat{C}'_{\mathcal{P}}(\Box)l$ are elements of $\mathcal{H}_{Diff}$ we can insert an identity

$$Q_{\mathbf{M}}(l,l') := \lim_{\mathcal{P}\to\sigma} \sum_{\Box\in\mathcal{P}} (\frac{2}{\kappa\sqrt{\beta}})^4 \sum_{\{s\}} \quad < \hat{C}'_{\mathcal{P}}(\Box)l, b_{\{s\}} >_{Diff} \quad < b_{\{s\}}, \hat{C}'_{\mathcal{P}}(\Box)l' >_{Diff} \tag{4.21}$$

Still pretending that the $\hat{C}'_{\mathcal{P}}(\Box)l$ are elements of $\mathcal{H}_{Diff}$ we may now use the definition of the scalar product on $\mathcal{H}_{Diff}$ and arrive at the, now meaningful, expression

$$Q_{\mathbf{M}}(l,l') := \sum_{\{s\}} \lim_{\mathcal{P}\to\sigma} \sum_{\Box\in\mathcal{P}} (\frac{2}{\kappa\sqrt{\beta}})^4 \;\; (\hat{C}'_{\mathcal{P}}(\Box)l)[T_{s_0(\{s\})}] \;\; \overline{(\hat{C}'_{\mathcal{P}}(\Box)l')[T_{s_0(\{s\})}]} \tag{4.22}$$

where we have chosen suitable representatives $s_0(\{s\}) \in \{s\}$ and have interchanged the sum $\sum_{\{s\}}$ with the limit $\mathcal{P}\to\sigma$ which is again part of the regularization. Now one of the properties of the operators $\hat{C}'_{\mathcal{P}}(\Box)$ that were proved in [3] is that the dependence of $(\hat{C}'_{\mathcal{P}}(\Box)l)[T_{s_0(\{s\})}]$ on the representative $s_0(\{s\})$ reduces to the question of how many vertices of $\gamma(s_0(\{s\}))$ of which vertex type are contained in $\Box$. For each vertex contained in $\Box$ we obtain a contribution which no longer depends on the representative but only on the diffeomorphism class of the vertex (or the ambient isotopy class up to the degenracy type), that is, its vertex type. Let us write this as

$$(\hat{C}'_{\mathcal{P}}(\Box)l)[T_{s_0(\{s\})}] = \sum_{v\in V(\gamma(s_0(\{s\})))\cap\Box} (\hat{C}'_{\mathcal{P}}(v)l)[T_{s_0(\{s\})}] \tag{4.23}$$

where, thanks to the diffeomorphism (or ambient isotopy up to degeneracy) invariance of l the numbers $(\hat{C}'_{\mathcal{P}}(v)l)[T_{s_0(\{s\})}]$ depend only on the vertex type of v and are, in this sense, diffeomorphism (or ambient isotopy up to degeneracy type) invariant.

Now, in the limit $\mathcal{P}\to\infty$ it is clear that no matter how that limit is reached and no matter which representative was chosen, each $\Box$ contains at most one vertex of $\gamma(s_0(\{s\}))$. Moreover, recall that by definition in [3] the partition is refined depending on $s_0(\{s\})$ in such a way that its topology is constant in the neighbourhood of any vertex of $\gamma(s_0(\{s\}))$ for sufficiently fine partition. This state dependent regularization is justified by the fact that the classical Riemann sum converges to the same integral no matter how the partition is refined. More precisely, the state dependent refinement limit is such that eventually for each vertex $v\in V(\gamma(s_0(\{s\}))$ there is precisely one cell $\Box_v$ which contains v as an interior point and the partition is refined in such a way that $\Box_v\to\{v\}$ while it is arbitrary for any cell which does not contain a vertex.

It follows that for each class $\{s\}$ and any representative $s_0(\{s\})$ the partition $\mathcal{P}$ will eventually be so fine that the numbers

$$(\hat{C}'_{\mathcal{P}}(\Box_v)l)[T_{s_0(\{s\})}] =: (\hat{C}'_{\mathcal{P}}(v)l)[T_{s_0(\{s\})}] \tag{4.24}$$

do not change any more as $\Box_v\to\{v\}$. Hence (4.22) can eventually be written in the form

$$\begin{aligned}
Q_{\mathbf{M}}(l,l') &= \sum_{\{s\}} \lim_{\mathcal{P}\to\sigma} \sum_{v\in V(\gamma(s_0(\{s\})))} (\frac{2}{\kappa\sqrt{\beta}})^4 \;\; (\hat{C}'_{\mathcal{P}}(\Box_v)l)[T_{s_0(\{s\})}] \;\; \overline{(\hat{C}'_{\mathcal{P}}(\Box_v)l')[T_{s_0(\{s\})}]} \\
&= \sum_{\{s\}} \lim_{\mathcal{P}\to\sigma} \sum_{v\in V(\gamma(s_0(\{s\})))} (\frac{2}{\kappa\sqrt{\beta}})^4 \;\; (\hat{C}'_{\mathcal{P}}(v)l)[T_{s_0(\{s\})}] \;\; \overline{(\hat{C}'_{\mathcal{P}}(v)l')[T_{s_0(\{s\})}]} \\
&= \sum_{\{s\}} \sum_{v\in V(\gamma(s_0(\{s\})))} (\frac{2}{\kappa\sqrt{\beta}})^4 \;\; (\hat{C}'_{\mathcal{P}}(v)l)[T_{s_0(\{s\})}] \;\; \overline{(\hat{C}'_{\mathcal{P}}(v)l')[T_{s_0(\{s\})}]}
\end{aligned} \tag{4.25}$$

where in the last line we could finally take the limit $\mathcal{P}\to\sigma$. The beauty of (4.22) is that it really is independent of the choice of the representative $s_0(\{s\})$ because for any representative we get the same number of vertices of each vertex type, hence the sum of the contributions does not change under change of representative. Thus, the **axiom of choice is no longer necessary to compute (4.25).**

The quadratic form (4.25) is positive by inspection and since, in the sense we just described, it comes from an operator, chances a good that it can be closed and hence determines a unique self-adjoint operator $\widehat{\mathbf{M}}$ on $\mathcal{H}_{Diff}$. We will examine this in a future publication [44]. Notice that it is neither necessary nor possible to check whether $Q_{\mathbf{M}}$ defines a spatially diffeomorphism invariant quadratic form since it is already defined on $\mathcal{H}_{Diff}$. We could check this only if we would have a quadratic form on the kinematical Hilbert space $\mathcal{H}_{Kin}$ but, as we explained, this is impossible for a graph changing operator. The only remnant of such a check is the independence of (4.25) of the choice of representatives $s_0(\{s\})$ which we just did.

The expression (4.25), seems to be hard to compute due to the infinite sum $\sum_{\{s\}}$, it even looks divergent. However, this is not the case: Let Φ_{Diff} be the dense (in $\mathcal{H}_{Diff}$) subset of $(\Phi^*_{Kin})_{Diff}$ consisting of the finite linear combinations of the $b_{\{s\}}$. Then for given $l, l' \in \Phi_{Diff}$ there are always only a finite number of terms that contribute to (4.25). This also justifies the interchange of the limit $\mathcal{P} \to \sigma$ and the sum $\sum_{\{s\}}$ performed in (4.25) Hence the dense subspace $\Phi_{Diff} \subset \mathcal{H}_{Diff}$ certainly belongs to the *form domain* of the positive quadratic form $Q_{\mathbf{M}}$. Notice that this reasoning would hold also if we would only stick with the non-separable $\mathcal{H}_{Diff}$, separability is required only for the direct integral decomposition of $\mathcal{H}_{Diff}$.

Remarks:
1.
A serious criticism spelled out in [15] is that the action of the Hamiltonian constraint of [2, 3, 4] is "too local" in the sense that it does not act at the vertices that it creates itself, so in some sense information does not propagate. While this is inconclusive because the constraint certainly acts everywhere, it is still something to worry about. The reason for why the action at those vertices had to be trivial was that otherwise the Hamiltonian constraint would be anomalous. Now the **Master Constraint** is not subject to any non-trivial algebra relations and hence **increases our flexibility in the way it acts at vertices that it creates itself**, thus at least relaxing the worries spleeld out in [15]. In [44] we will come back to this issue.
2.
We have stressed that we would like to prove that $Q_{\mathbf{M}}$ has a closure in order to rigorously grant existence of $\widehat{\mathbf{M}}$. At a heuristic level (group averaging, Rigging Map) one can even live just with the quadratic form: Consider the dense subspace Φ_{Diff} of $\mathcal{H}_{Diff}$ and its algebraic dual Φ^*_{Diff} (not to be confused with the subset $(\Phi^*_{Kin})_{Diff}$ of kinematical algebraic distributions Φ^*_{Kin}). Then typical elements of the physical subspace $(\Phi^*_{Diff})_{Phys}$ of Φ^*_{Diff} will be of the form $l_{Phys} = \sum_{\{s\}} z_{\{s\}} < b_{\{s\}}, . >_{Diff}$ with complex valued coefficients $z_{\{s\}}$ and one would impose the condition

$$(\widehat{\mathbf{M}}' \, l_{Phys})[F] := l_{Phys}[\widehat{\mathbf{M}} \, F] := \sum_{\{s\}} z_{\{s\}} Q_{\mathbf{M}}(b_{\{s\}}, F) = 0 \tag{4.26}$$

for all $F \in \Phi_{Diff}$. Notice that this condition constructs possibly a solution space but not an inner product for which we would need at least a Rigging Map. If there is a subset $\Phi_{Phys} \subset (\Phi^*_{Diff})_{Phys}$ of would-be analytic vectors for $\widehat{\mathbf{M}}$ then one could try to define such a map as

$$\begin{aligned}
&< \eta_{Phys}(F), \eta_{Phys}(F') >_{Phys} := \int_{\mathbb{R}} \frac{dt}{2\pi} < F', e^{it\widehat{\mathbf{M}}} F >_{Diff} \\
:= \quad & \int_{\mathbb{R}} \frac{dt}{2\pi} \sum_{n=0}^{\infty} \frac{(it)^n}{n!} < F', \widehat{\mathbf{M}}^n \, F >_{Diff} \\
:= \quad & \int_{\mathbb{R}} \frac{dt}{2\pi} \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \sum_{\{s_1\},..,\{s_n\}} Q_{\mathbf{M}}(F', b_{\{s_1\}}) Q_{\mathbf{M}}(b_{\{s_1\}}, b_{\{s_2\}})..Q_{\mathbf{M}}(b_{\{s_n\}}, F)
\end{aligned} \tag{4.27}$$

But certainly the existence of these objects is far from granted.

5 The Master Constraint Operator for General Relativity: 2. Non-Graph-Changing Version

As we have explained in detail in section 4.2, a **Master Constraint Operator** which changes the graph underlying a spin-network state is incompatible with a diffeomorphism invariant operator. Now the original motivation [2] for having a graph-changing Hamiltonian constraint was to have an anomaly free constraint algebra among the smeared Hamiltonian constraints $\hat{C}(N)$. This motivation is **void** with respect to $\widehat{\mathbf{M}}$ since there is only one $\widehat{\mathbf{M}}$ so there **cannot be any anomaly** (at most in the sense that $\mathcal{H}_{Phys}$ is too small, that is, has an unsufficient number of semiclassical states). It is therefore worthwhile thinking about about a version of the $\widehat{\mathbf{M}}$ which does not change the graph **and therefore can be defined on the kinematical Hilbert space**. That this is indeed possible, even for diffeomorphism invariant operators which are positive was demonstrated in [49]: Essentially one must define $\widehat{\mathbf{M}}$ in the spin-network basis and for each T_s and each $v \in \gamma(s)$ one must invent a unique diffeomorphism covariant prescription for how to choose loops as **parts of the already existing graph** $\gamma(s)$. In [49] we chose the *minimal loop prescription*:

Definition 5.1.
Given a graph γ and a vertex $v \in V(\gamma)$ and two different edges $e, e' \in E(\gamma)$ starting in v, a loop $\alpha_{\gamma,v,e,e'}$ within γ starting along e and ending along $(e')^{-1}$ is said to be minimal provided that there is no other loop with the same properties and fewer edges of γ traversed.

Notice that the notion of a minimal loop does not refer to a background metric and is obviously covariant. Actually it is a notion of **algebraic graph theory** [50] since it does not refer to any knotting (embedding). Thus, it might be possible to make the quantum dynamics look more combinatorical.

Given the data γ, v, e, e', there may be more than one minimal loop but there is at least one (we consider only closed graphs due to gauge invariance). We denote by $L_{\gamma,v,e,e'}$ the set of minimal loops associated with the data γ, v, e, e' (It might be possible to make $\alpha_{\gamma,v,e,e'}$ unique by asking more properties but we could not think of a prescription which is also covariant). If $L_{\gamma,v,e,e'}$ has more than one element then the corresponding **Master Constraint Operator** averages over the finite number of elements of $L_{\gamma,v,e,e'}$, see [49] for details.

The advantage of having a non-graph changing **Master Constraint Operator** is that one can quantize it directly as a positive operator on $\mathcal{H}_{Kin}$ and check its semi-classical properties by testing it with the semi-classical tools developed in [29, 30, 31, 32, 33, 34], to the best of our knowledge currently the only semi-classical states, in a representation supporting the holonomy – flux algebra, for non-Abelean gauge theories for which semi-classical properties were proved. Notice that the original problems of these states mentioned in [29], namely that they have insufficient semiclassical properties as far as holonomy and area operators are concerned, were resolved in [34]: Indeed, they are designed to display semi-classical properties with respect to operators which come from functions on phase space involving **three-dimensional integrals** over σ rather than one – or two-dimensional integrals, provided they are not graph-changing. Hence they are suitable for our diffeomorphism invariant operators, in particular $\widehat{\mathbf{M}}$, when quantized without changing the graph. That then correct semiclassical expectation values and small fluctuations are indeed obtained has been verified explicitly for diffeomorphism invariant operators for matter QFT's coupled to LQG in the second reference of [49]. Hence we are optimistic that this is possible here as well, especially due to some recent progress concerning the spectral analysis of the volume operator [51]. Details will be published in [52].

The disadvantage of a non-graph-changing operator is that it uses a prescription like the above minimal loop prescription as an ad hoc quantization step. While it is motivated by the more fundamental quantization procedure of the previous section and is actually not too drastic a modification thereof for sufficiently fine graphs, the procedure of the previous section should be considered as more fundamental. Maybe one could call the operator as formulated in this section an **effective operator** since it presumably reproduces all semiclassical properties. On the other hand, since it defines a positive self-adjoint operator by construction which is diffeomorphism invariant and presumably has the correct classical limit we can exploit the full power of techniques that comes with $\mathcal{H}_{Diff}$ in order to solve the constraint. Even better than that, since the operators $\widehat{\mathsf{M}}$ and $\hat{U}(\varphi)$ commute for all $\varphi \in \text{Diff}^\omega(\sigma)$ we can even solve the constraint $\widehat{\mathsf{M}}$ at the kinematical level in the subspace $\mathcal{H}_{Kin,\gamma} \subset \mathcal{H}_{Kin}$ spanned by spin network states over the graph γ, for each γ separately. This space is definitely separable and hence we do not need to invoke the additional averaging to produce the states $b_{\{s\}}$ when we solve the spatial diffeomorphism constraint in a second step. (Notice, however, that while $\widehat{\mathsf{M}}$ and $\hat{U}(\varphi)$ commute, one cannot simply map the solutions to $\widehat{\mathsf{M}} = 0$ by the map $\eta(T_s) = b_{\{s\}}$ because η is not really a Rigging map, it is a Rigging map on each sector $\mathcal{H}_{Kin,\{s\}}$, the closure of the finite linear span of the $T_{s'}$, $s' \in \{s\}$ but the averaging weights for each sector are different due to graph symmetries which depend on the spin labels, see [26] for details). Thus, although we work in the continuum, for each graph γ we have to solve essentially a problem in Hamiltonian lattice gauge theory when solving the **Master Constraint** before the spatial diffeomorphism constraint.

6 Further Directions and Connection with Spin Foam Models

We finish the paper with remarks and further ideas about applications of the **Master Constraint Procedure**:

i) **Extended Master Constraint**
Up to now we have treated the spatial diffeomorphism constraint and the Hamiltonian constraint on rather unequal footing: The diffeomorphism constraint was solved in the usual way by imposing $C_a(x) = 0 \; \forall \; x \in \sigma$ while the Hamiltonian constraint was solved by the **Master Constraint Method**. This is of course natural because we already have a close to complete framework for the diffeomorphism constraint [26] so we may leave things as they are with respect to the spatial diffeomorphism constraint. One the other hand it is questional why smooth, even analytic diffeomorphisms should play a fundamental role in LQG which seems to predict a discrete structure at Planck scale as the spectrum of the length, area and volume operators reveal. Hence, one might want to consider a different approach to the solution of the spatial diffeomorphism constraint.

The **Master Constraint Programme** allows us to precisely do that and to treat all constraints on equal footing. Consider the **Extended Master Constraint**

$$\mathsf{M}_E := \frac{1}{2} \int_\sigma d^3x \frac{C(x)^2 + q^{ab}(x) C_a(x) C_b(x)}{\sqrt{det(q)(x)}} \tag{6.1}$$

Obviously $\mathsf{M}_E = 0$ if and only if $C(x) = C_a(x) = 0$ for all $a = 1,2,3;\; x \in \sigma$, hence the general theory of section 3 applies. Notice that while $C_a(x)$ cannot be quantized as the self-adjoint generator of one parameter unitary subgroups of the representation $\hat{U}(\varphi)$ of the spatial diffeomorphism group on $\mathcal{H}_{Kin}$ (since the representation is not strongly continuous), the general theorems of [7] show that (6.1) has a chance to be quantized as a positive self-adjoint operator on $\mathcal{H}_{Diff}$ by the methods of section 4 or on $\mathcal{H}_{Kin}$ by the methods of section 5. Since (6.1) is to *define* $\mathcal{H}_{Phys}$ is a single stroke and to define spatial diffeomorphism invariance in a new way, we do not really have $\text{Diff}^\omega(\sigma)$ any more and thus the method of section 5 is preferred. Moreover, the obstruction mentioned in section 4.2 to having a graph changing diffeomorphism invariant operator on $\mathcal{H}_{Kin}$ is not present any more, again because $\text{Diff}^\omega(\sigma)$ no longer exists at the quantum level although it should be recovered on large scales. Thus $\widehat{\mathsf{M}}_E$ may now be defined as a graph changing operator $\mathcal{H}_{Kin}$. Finally, we even have the flexibility to change $\mathcal{H}_{Kin}$ because the uniqueness theorem [13, 14] that selects the Ashtekar – Isham – Lewandowski representation rests on the presence of the group $\text{Diff}^\omega(\sigma)$.

ii) *True Hamiltonian and Master Action*
Now what it is striking about (6.1) is that it provides a **true Hamiltonian**! Certainly we

are only interested in the subset $\mathbf{M} = 0$ but nevertheless there is now only one constraint functional instead of infinitely many. It allows us to define the **Master Action**

$$\mathbf{W}_T = \frac{1}{\kappa} \int_0^T dt\{(\int_\sigma [\dot{A}_a^j E_j^a + A_t^j C_j]) - \mathbf{M}_E\} \tag{6.2}$$

where $C_j = \mathcal{D}_a E_j^a$ is the Gauss constraint and A_t^j a Lagrange multiplier. Actually we may also absorb the Gauss constraint into the **Master Constraint** giving rise to the **Total Master Constraint**

$$\mathbf{M}_T := \frac{1}{2} \int_\sigma d^3x \frac{C(x)^2 + q^{ab}(x) C_a(x) C_b(x) + \delta^{jk} C_j(x) C_k(x)}{\sqrt{det(q)}(x)} \tag{6.3}$$

which enables us to replace (6.2) by the following expression without Lagrange multipliers

$$\mathbf{W}_{T'} = \frac{1}{\kappa} \int_0^{T'} dt\{(\int_\sigma \dot{A}_a^j E_j^a) - \mathbf{M}_T\} \tag{6.4}$$

Notice that the integrands of both (6.1) and (6.3) are are densities of weight one

The proof that the Ashtekar-Barbero phase space [45] with canonically conjugate coordinates (A_a^j, E_j^a) modulo the the symmetries generated by the Gauss constraint on the constraint surface $C_j(x) = 0,\ x \in \sigma$ is precisely the ADM phase space (see e.g. [1] for a detailed proof) does not refer to any dynamics, hence we may reduce (6.2) and arrive at the **Master Action** in ADM coordinates

$$\mathbf{W}_T = \frac{1}{\kappa} \int_o^T dt\{(\int_\sigma \dot{q}_{ab} P^{ab}) - \mathbf{M}_E\} \tag{6.5}$$

in which there are no constraints anymore and $\mathbf{M}$ is written in terms of the ADM Hamiltonian constraint $C(x)$ and the ADM diffeomorphism constraint $C_a(x)$. The equations of motion for q_{ab} that follow from (6.5) are

$$\dot{q}_{ab} = \frac{1}{\sqrt{det(q)}} [\frac{2P_{ab} - q_{ab} P_c^c}{\sqrt{\det(q)}} C + D_{(a} C_{b)}] \tag{6.6}$$

and can, in principle, be inverted for P^{ab} off the constraint surface $\mathbf{M} = 0$ in order to invert the Legendre transformation. However, since the right hand side of (6.6) contains second spatial derivatives of q_{ab}, P^{ab} and moreover is a polynomial of third order in P^{ab}, the functional $P^{ab} = F^{ab}[q, \partial q, \dot{q}, \partial q, \partial^2 q]$ will be a non-local and non-linear expression, that is, a *non-local higher derivative theory of dynamical, spatial geometry on* σ (∂q denotes spatial derivatives) which is spatially diffeomorphism invariant!

Since, however, the functional F^{ab} can presumably not be extended to $\mathbf{M} = 0$, the Lagrangean formulation of the **Master Action** (6.2) or (6.5) is presumably not very useful for path integral formulations, hence we will stick with (6.2). In fact, since the Gauss constraint can be explicitly solved at the quantum level we can work with the **Extended Master Constraint** (6.1) rather than the **Total Master Constraint** (6.3). Notice also that the Lagrangean formulation of the **Master Action** is unlikely to have a manifestly spacetime covariant interpretation. This is because the group of phase space symmetries generated by the Hamiltonian and Diffeomorphism constraint through their Hamiltonian flow are only very indirectly related to spacetime diffeomorphisms, see [1] for a detailed exposition of this relation.

iii) *Path Integral Formulation and Spin Foams*
The terminology *True Hamiltonian* is a little misleading because we are not really interested in the theory defined by the **Master Action** (6.2). It appears only as an intermediate step in the path integral formulation of the theory. Here we will only sketch how this works, more details will follow in future publications [53]. For simplicity we describe the

construction of the path integral for the **Extended Master Constraint** at the gauge invariant level, one could do it similarly with the *Simple Master Constraint* used in previous sections at the gauge and spatially diffeomorphism invariant level as well, in which case one would use the space $\mathcal{H}_{Diff}$ instead of $\mathcal{H}_{Kin}$ as a starting point.

We assume to be given a self-adjoint **Extended Master Constraint Operator** $\widehat{\mathbf{M}}_E$ on the kinematical Hilbert space $\mathcal{H}_{Kin}$. Since that space is not separable, we cannot follow the direct integral construction to solve the constraint but if $\widehat{\mathbf{M}}_E$ is not graph changing then we can use the direct integral construction on separable subspaces of $\mathcal{H}_{Kin}$, see section 5. In any case, according to the general **Master Constraint Programme** sketched in section 2, the constraint $\widehat{\mathbf{M}} = 0$ can be solved, heuristically, by introducing the Rigging Map (see appendix)

$$\eta: \ \Phi_{Kin} \to (\Phi^*_{Kin})_{Phys}; \ \ f \mapsto \eta(f) := \lim_{T\to\infty} \int_{-T}^{T} \frac{dt}{2\pi} \ < e^{it\widehat{\mathbf{M}}_E} f, . >_{Kin} \tag{6.7}$$

and the physical inner product

$$< \eta(f), \eta(f') >_{Phys} := \eta(f')[f] = \lim_{T\to\infty} \int_{-T}^{T} \frac{dt}{2\pi} \ < e^{it\widehat{\mathbf{M}}_E} f', f >_{Kin} \tag{6.8}$$

where $f, f' \in \Phi_{Kin} = \mathrm{Cyl}^\infty$ are e.g. gauge invariant spin-network states. Notice that (6.8) can formally be written as

$$< \eta(f), \eta(f') >_{Phys} = < f', \delta(\widehat{\mathbf{M}}_E) f >_{Kin} \tag{6.9}$$

and defines a generalized projector which is of course the basic idea behind the RAQ Programme, see [63] and references therein.

Formula (6.9) should be viewed in analogy to [20] which tries to define a generalized projector of the form $\prod_{x\in\sigma} \delta(\hat{C}(x))$ at least formally where $\hat{C}(x)$ is the Hamiltonian constraint of [2, 3, 4]. However, this is quite difficult to turn into a technically clean procedure for several reasons: First of all the $\hat{C}(x)$, while defined on $\mathcal{H}_{Kin}$ are not explicitly known (they are known up to a diffeomorphism; they exist by the axiom of choice). Secondly they are not self-adjoint whence the exponential is defined at most on analytic vectors of $\mathcal{H}_{Kin}$. Thirdly, there is an infinite number of constraints and thus the generalized projector must involve a path integral over a suitable Lagrange multiplier N and one is never sure which measure to choose for such an integral without introducing anomalies. Fourthly and most seriously, the $\hat{C}(x)$ are not mutually commuting and since products of projections define a new projection if and only if the individual projections commute, the formal object $\prod_{x\in\sigma} \delta(\hat{C}(x))$ is not even a (generalized) projection. If one defines it somehow on diffeomorphism invariant states (which might be possible because, while the individual $\hat{C}(x)$ are not diffeomorphism invariant, the product might be up to an (infinite) factor) then that problem could disappear because the commutator of two Hamiltonian constraints annihilates diffeomorphism invariant states [2, 3, 4], however, this would be very hard to prove rigorously. It is probably due to these difficulties and the non-manifest spacetime covariance of the amplititudes computed in [20] for the Euclidean Hamiltonian constraint that the spin foam approach has chosen an alternative route that, however, has no clear connection with Hamiltonian formalism so far.

Our proposal not only removes these four problems it also has the potential to combine the canonical and spin foam programme rigorously:
The ordinary amplitude $< f', e^{it\widehat{\mathbf{M}}_E} f >_{Kin}$ in (6.8) should have a path integral formulation by using a Feynman-Kac formula. More precisely, this amplitude should be defined as the analytic continuation $t \mapsto -it$ of the kernel underlying the **Bounded Contraction Semigroup**

$$t \mapsto e^{-t\widehat{\mathbf{M}}_E}, \ \ t \geq 0 \tag{6.10}$$

relying on the **positivity** of $\widehat{\mathbf{M}}_E$. Now for contraction semi-groups there are powerful tools available, associated with the so-called **Osterwalder – Schrader** reconstruction theorem, that allow to connect the Hamiltonian formulation with the a path integral formulation [54, 55] in terms of a probability measure μ on the space $\overline{\overline{\mathcal{A}}}$ of distributional connection **histories**. Let us suppose that we can actually carry out such a programme then, relying on the usual manipulations, the corresponding path integral should have the form (for $t \geq 0$)

$$< f', e^{it\widehat{\mathbf{M}}_E} f >_{Kin}= \int_{\overline{\overline{\mathcal{A}}}} d\mu(A) \overline{f'(A_t)} f(A_0) = \int_{\overline{\overline{\mathcal{A}}}} d\nu(A) \overline{f'(A_t)} f(A_0) \int_{\overline{\overline{\mathcal{E}}}} d\rho(E) e^{i \mathbf{W}_t(A,E)} \tag{6.11}$$

where A_t denotes the point on the history of connection configurations at "time" t and ν, ρ is some measure on the space of distributional connection and electric field histories $\overline{\overline{\mathcal{A}}}$, $\overline{\overline{\mathcal{E}}}$ respectively, both of which are to be determined (the first equality in (6.11) is rigorous while the second is heuristic but can be given meaning in an UV and IR regularization). The path integral of course is to be understood with the appropriate boundary conditions. Notice that in order to obtain the generalized projection we still have to integrate (6.11) over $t \in \mathbb{R}$ which is the precisely the difference between a transition amplitude and a projection.

In order to get a feeling for what those measures ν, ρ could be, we notice that the framework of coherent states is usually very powerful in order to derive path integrals [56]. Hence we could use, as a trial, the coherent states developed in [29, 30, 31, 32, 33] which have the important overcompleteness property and thus can be used to provide suitable resolutions of unity when skeletonizing $\exp(it\widehat{\mathbf{M}}_E) = \lim_{N\to\infty}[\exp(it\widehat{\mathbf{M}}_E/N)]^N$. But then, at least on a fixed (spacetime) graph, we know that the "measure" $\nu \otimes \rho$ is related to the product of heat kernel measures [57] on non-compact spaces of generalized connections, one for each time step, based on the coherent state transform introduced by Hall [57].

Alternatively, one could use resolutions of unity provided by holonomy and electric field eigenfunctions in which case the heat kernel measures, at each time step, are replaced by the Ashtekar-Lewandowski measure $\nu = \mu_{AL}$ [12] times a discrete counting measure ρ which sums over spin-network labels. Then, when performing the Fourier transform [59] with respect to the Ashtekar-Lewandowski measure from the connection representation to the electric field (or spin-network) representation one obtains amplitudes with pure counting measures, that is, **a spin foam amplitude**. These issues are currently under investigation [53].

iv) *Regge Calculus and Dynamical Triangulations*
This new form of a path integral approach to quantum gravity with a clear connection to the Hamiltonian framework and thus a clear physical interpretation of *what exactly the path integral computes* could also be useful for other path integral formulations of gravity such as Regge calculus [60] and dynamical triangulations [61] because, due to the positivity of $\mathbf{M}_E$ the convergence of the path integral might be improved, the "conformal divergence" could be absent. Of course, the function $\mathbf{M}_E$ has flat directions but hopefully they have small enough measure in order to ensure convergence.

v) *Lattice Quantum Gravity and Supercomputers*
Finally it is worthwhile to point out that while we have been working with the continuum formulation throughout, the **Master Constraint Programme** easily specilizes to a **Lattice Quantum Gravity** version, see e.g. [35]. Namely, we can just restrict the theory, when graph-non-changingly defined, to an arbitrary but fixed graph and study how the theory changes under coarsening of the graph (background independent renormalization [65]). In background dependent theories such as QCD this is done in order to provide a gauge invariant UV and IR cut-off, in LQG, however, this should be viewed rather as a restriction of the UV finite theory to a subset of states and the renormalization is to be understood in the sense of Wilson, hence constructs an effective macroscopic theory from

a given fundamental, microscopic one by integrating out degrees of freedom. On the other hand, on a lattice both background dependent theories and LQG (when the constraints are treated in the usual way in the quantum theory) suffer from the same drawback, namely the destruction of continuum symmetries such as Poincaré invariance for background dependent theories or spatial diffeomorphism invariance for LQG [62]. However, this is no longer the case with the **Master Constraint Programme**: By definition the symmetries follow from the **Master Constraint Operator** and are inherently discrete. They are defined by a single operator and not a multitude of them, hence there are simply no operators which must form an algebra. Notice that on the lattice one can certainly define a discrete version of $\hat{C}_a(x)$ but the corresponding operator algebra does not close, this is different with the **Master Constraint Programme**, the algebra consists of a single operator, hence the algebra trivially closes, it is Abelean.

The advantage of a lattice version is that it can be easily implemented on a **supercomputer**, not more difficult than for QCD, although there will be new computer routines necessary in order to accomodate the non-polynomial structure of LQG. Notice that the **Extended Master Constraint Programme** on the lattice can be compared to the method of [25] in the sense that there are no (constraint algebraic) consistency problems even when working at the discretized level. However, the two methods are quite different because the **Master Constraint Programme** does not fix any Lagrange multipliers (in fact there are none).

We finish this paper with the same warning as in the introduction: To the best of our knowledge, the **Master Constraint Proposal** is an entirely new idea which has been barely tested in solvable model theories and hence one **must test it in such model situations** in order to gain faith in it, to learn about possible pitfalls etc. It is well possible that we overlooked some important fact which invalidates the whole idea or at least requires non-trivial modifications thereof. The author would like to learn about such obstacles and tests in model theories (for instance it is conceivable that Loop Quantum Cosmology [18] provides a fast and interesting test). On the other hand, we hope to have convinced the reader that the **Phoenix Project**, that is, the **Master Constraint Programme** applied to LQG, is an attractive proposal, designed to hopefully make progress with the quantum dynamics of LQG. Criticism, help and improvements by the reader are most welcome.

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A Direct Integral Decompositions and Rigging Maps

For the benefit of the reader more familiar with the theory of generalized eigenvectors in order to solve constraints, we briefly sketch the connection with the direct integral approach below. We do this for a general theory defined on a Hilbert space $\mathcal{H}_{Kin}$.

Let $\Phi_{Kin} \subset \mathcal{H}_{Kin}$ be a dense subspace equipped with a finer topology than the subspace topology induced from $\mathcal{H}_{Kin}$ and let Φ^*_{Kin} be the algebraic dual of Φ_{Kin} equipped with the topology of pointwise convergence (no continuity assumptions). An element $l \in \Phi^*_{Kin}$ is called a generalized eigenvector with eigenvalue λ with respect to a closable operator $\widehat{\mathbf{M}}$ which together with its adjoint is densely defined on the (invariant) domain Φ_{Kin} provided that

$$\widehat{\mathbf{M}}' l = \lambda l \quad \Leftrightarrow l(\widehat{\mathbf{M}}^\dagger f) = \lambda l(f) \;\; \forall f \in \Phi_{Kin} \tag{A.1}$$

Here $\widehat{\mathbf{M}}'$ is called the dual representation on Φ^*_{Kin}. The subspace of generalized eigenvectors with given eigenvalue λ is denoted by $\Phi^*_{Kin}(\lambda) \subset \Phi^*_{Kin}$ and $(\Phi^*_{Kin})_{Phys} := \Phi^*_{Kin}(0)$ is called the physical subspace.

In this generality the concept of generalized eigenvectors does not require $\mathcal{H}_{Kin}$ to be separable which is an advantage. The disadvantage is that $(\Phi^*_{Kin})_{Phys}$ does not automatically come with an inner product. However, in fortunate cases there is a heuristic procedure known under the name "Rigging Map" [63]. We only consider the case at hand and assume to be given a self-adjoint operator $\widehat{\mathbf{M}}$ on $\mathcal{H}_{Kin}$. The Rigging Map is defined as the antilinear operation

$$\eta: \ \Phi_{Kin} \to \Phi_{Phys} \subset (\Phi^*_{Kin})_{Phys}; \ f \mapsto \int_{\mathbb{R}} dt < \hat{U}(t)f, . >_{Kin} \tag{A.2}$$

where

$$< \eta(f'), \eta(f) >_{Phys} := [\eta(f')](f) = \int_{\mathbb{R}} \frac{dt}{2\pi} < \hat{U}(t)f', f >_{Kin} \tag{A.3}$$

It is clear that (A.2) formally defines a physical generalized eigenvector by displaying the generalized eigenvector condition in the form

$$l(\hat{U}(t)^\dagger f) = 0 \ \ \forall t \in \mathbb{R}, \ \ f \in \Phi_{Kin} \tag{A.4}$$

because the measure dt is translation invariant and $t \mapsto \hat{U}(t) = e^{it\widehat{\mathbf{M}}}$ is a one-parameter unitary group. For the same reason, $< .,. >_{Phys}$ is a sesquilinear form. Now η is said to be a Rigging map provided that the sesquilinear form defined in (A.3) is positive semidefinite (if not definite, divide by the null space and complete) and provided that $\hat{O}'\eta(.) = \eta(\hat{O})$. The latter condition is again easy to verify in our case for a strong Dirac observable (it ensures that $(\hat{O}')^* = (\hat{O}^\dagger)'$ where $(.)^*$ is the adjoint on $\mathcal{H}_{Phys}$, hence adjointness relations are induced from $\mathcal{H}_{Kin}$ to $\mathcal{H}_{phys}$).

In the case that $\mathcal{H}_{Kin}$ is separable we can show that the sesquilinear form $< .,. >_{Phys}$ is actually already positive definite. Choose a direct integral representation of $\mathcal{H}_{Kin}$ with respect to $\widehat{\mathbf{M}}$. Then we know by the spectral theorem that the operator $\hat{U}(t)$ is represented on $\mathcal{H}^\oplus_{Kin}(\lambda)$ by multiplication by $e^{it\lambda}$, hence

$$\begin{aligned}
< \eta(f), \eta(f') >_{Phys} &= \int_{\mathbb{R}} \frac{dt}{2\pi} < \hat{U}(t)f', f > \\
&= \int_{\mathbb{R}} \frac{dt}{2\pi} \int_{\mathbb{R}} d\nu(\lambda) < e^{i\lambda t} f'(\lambda), f(\lambda) >_{\mathcal{H}^\oplus_{Kin}(\lambda)} \\
&= \int_{\mathbb{R}} d\nu(\lambda) \delta_{\mathbb{R}}(\lambda) < f'(\lambda), f(\lambda) >_{\mathcal{H}^\oplus_{Kin}(\lambda)} \\
&= \nu(\delta) < f'(0), f(0) >_{\mathcal{H}^\oplus_{Kin}(0)}
\end{aligned} \tag{A.5}$$

The positive factor of proportionality is given by

$$\nu(\delta) := \lim_{\epsilon \to 0} \nu(\delta_\epsilon) \tag{A.6}$$

where δ_ϵ is any family of smooth (thus measurable) functions converging to the $\delta-$distribution.

The framework of generalized eigenvectors can be connected even more precisely to the direct integral theory in the case at hand, at least when $\mathcal{H}_{Kin}$ is separable, through the theory of *Rigged Hilbert Spaces* [64]:

A Rigged Hilbert space is a Gel'fand triple $\Phi_{Kin} \hookrightarrow \mathcal{H}_{Kin} \hookrightarrow \Phi'_{Kin}$ consisting of a *nuclear space* Φ_{Kin}, its *topological dual* Φ'_{Kin} (continuous linear functionals) and a Hilbert space $\mathcal{H}_{Kin}$. The topologies of Φ_{Kin} and $\mathcal{H}_{Kin}$ are connected as follows:

Definition A.1.

i)

A countably Hilbert space Φ is a complete metric space whose topology is defined by a countable family of Hilbert spaces $\Phi_n, \ n = 1, 2, ..$ whose scalar products $< .,. >_n$ are consistent in the following sense: First of all, Φ_n is the Cauchy completion of Φ in the norm $||.||_n$. Then, for any m, n it is required that if (ϕ_k) is both a $||.||_m$ convergent sequence and an $||.||_n$ Cauchy sequence *in* Φ *then* (ϕ_k) *is also* $||.||_n$ *convergent. We may w.l.g. assume that* $||.||_n \le ||.||_{n+1}$ *on* Φ*. Then the metric on* Φ *is given by*

$$d(\phi, \phi') := \sum_{n=1}^{\infty} 2^{-n} \frac{||\phi - \phi'||_n}{1 + ||\phi - \phi'||_n} \tag{A.7}$$

It is easy to verify that $\Phi = \cap_{n=1}^{\infty} \Phi_n$ *and the inclusion* $\Phi_{n+1} \subset \Phi_n$ *holds.*
ii)
Let Φ' *be the topological dual of* Φ *(continuous linear functionals) and* Φ'_n *the topological dual of* Φ_n*. By the Riesz lemma* Φ'_n *is isometric isomorphic with* Φ_n*, that is, for any* $F \in \Phi'_n$ *there is a unique element* $\phi_F^{(n)} \in \Phi_n$ *such that* $F(\phi) =< \phi_F^{(n)}, \phi >_n$ *for all* $\phi \in \Phi_n$ *and*

$$||F||_{-n} := \sup_{0 \ne \phi \in \Phi_n} \frac{|F(\phi)|}{||\phi||_n} = ||\phi_F^{(n)}||_n \tag{A.8}$$

Hence $\Phi'_n =: \Phi_{-n}$ *can also be thought of as a Hilbert space. Since* $\Phi_{n+1} \subset \Phi_n$ *any* $F \in \Phi'_n$ *is also a linear functional in on* Φ_{n+1} *and due to* $||.||_n \le ||.||_{n+1}$ *it is also continuous. Hence we have the inclusion* $\Phi_{-n} \subset \Phi_{-(n+1)}$ *and it is easy to see that* $\Phi' = \cup_{n=1}^{\infty} \Phi_{-n}$*.*
iii)
A Nuclear space Φ *is a countably Hilbert space such that for each* m *there exists* $n \ge m$ *such that the natural injection*

$$T_{nm};\ \Phi_n \to \Phi_m;\ \psi \mapsto \psi \tag{A.9}$$

is a nuclear (that is, trace class) operator.
iv)
A Rigged Hilbert Space $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$ *is given by a Nuclear Space* Φ *and a Hilbert space* $\mathcal{H}$ *which is the Cauchy completion of* Φ *in yet another scalar product* $< .,. > := < .,. >_0$ *such that if* $\phi_k \to \phi$ *in the topology of* Φ *then also* $\phi_k \to \phi$ *in the topology of* $\mathcal{H}$*. One can show that necessarily* $\Phi_1 \subset \Phi_0 := \mathcal{H} =: \Phi'_0 \subset \Phi'_1$ *and hence we have an integer labelled family of spaces with* $\Phi_{n+1} \subset \Phi_n$*.*

The usefulness of the concept of a Rigged Hilbert space is that, given a **positive** self-adjoint operator $\widehat{\mathsf{M}}$ on a Hilbert space $\mathcal{H}_{Kin}$, a corresponding Rigged Hilbert space is often **naturally provided as follows**:
Let $\mathcal{D}$ be a dense, invariant domain for $\widehat{\mathsf{M}}$, generically some space of smooth functions of compact support. Define positive sesquilinear forms $< .,. >_n$ on $\mathcal{D}$ defined by

$$< \phi, \phi' >_n := \sum_{k=0}^{n} < \phi, (\widehat{\mathsf{M}})^k \phi' > \tag{A.10}$$

It is easy to see that $||.||_n \le ||.||_{n+1}$ and that the corresponding $\Phi_{Kin} = \cap_{n=1}^{\infty} \Phi_n$ (where Φ_n is the $||.||_n$ completion of $\mathcal{D}$) is a dense invariant domain for $\widehat{\mathsf{M}}$ and a countably Hilbert space. Whether it is also a Nuclear Space depends on the operator $\widehat{\mathsf{M}}$, however, it is typically the case when $\widehat{\mathsf{M}}$ is a mixture of derivative and multiplication operators.

Thus, given a positive, s.a. operator $\widehat{\mathsf{M}}$ on a separable Hilbert space $\mathcal{H}_{Kin}$, a nuclear space Φ_{Kin} is often *naturally* provided.

Definition A.2.
Let $\Phi'_{Kin}(\lambda) \subset \Phi'_{Kin}$ *be the subspace of generalized eigenvectors with eigenvalue* λ *in a Rigged Hilbert Space corresponding to a self-adjoint operator* $\widehat{\mathsf{M}}$*. For any* $\phi \in \Phi_{Kin}$ *and* $\lambda \in \mathbb{R}$ *we define an element* $\tilde{\phi}_\lambda \in (\Phi'_{Kin}(\lambda))'$ *by*

$$\tilde{\phi}_\lambda(F_\lambda) := F_\lambda(\phi) \tag{A.11}$$

for all $F_\lambda \in \Phi'_\lambda$*. The map*

$$J:\ \Phi_{Kin} \to \cup_{\lambda \in \mathbb{R}} (\Phi'_{Kin}(\lambda))';\ \phi \mapsto (\tilde{\phi}_\lambda)_{\lambda \in \mathbb{R}} \tag{A.12}$$

is called the generalized spectral resolution of $\phi \in \Phi_{Kin}$*.*

The operator $\widehat{\mathsf{M}}$ *is said to have a complete set of generalized eigenvectors provided that the map* J *in (A.12) is an injection.*

The motivation for this terminology is that J is an injection if and only if $\cup_{\lambda\in\mathbb{R}}\Phi'_\lambda$ separates the points of Φ_{Kin}. We notice that if $J(\phi) = (\tilde{\phi}_\lambda)_{\lambda\in\mathbb{R}}$ is the generalized spectral resolution of $\phi \in \Phi_{Kin}$ with respect to the operator $\widehat{\mathbf{M}}$ then $J(\widehat{\mathbf{M}}\,\phi) = (\lambda\tilde{\phi}_\lambda)_{\lambda\in\mathbb{R}}$ which suggests that there is a relation between the $\tilde{\phi}_\lambda$ and the direct integral representation $\phi = (\phi(\lambda))_{\lambda\in\mathbb{R}}$. This is indeed the case as the following theorem reveals.

Theorem A.1.
A self-adjoint operator $\widehat{\mathbf{M}}$ on a separable Rigged Hilbert space $\Phi_{Kin} \hookrightarrow \mathcal{H}_{Kin} \hookrightarrow \Phi'_{Kin}$ has a complete set of generalized eigenvectors corresponding to real eigenvalues. More precisely:

Let $\mathcal{H}_{Kin} = \int_{\mathbb{R}}^{\oplus} d\nu(\lambda)\ \mathcal{H}^{\oplus}_{Kin}(\lambda)$ be the direct integral representation of $\mathcal{H}_{Kin}$. There is an integer n such that for $\nu-$a.a. $\lambda \in \mathbb{R}$ there is a trace class operator $T_\lambda :\ \Phi_n \to \mathcal{H}^{\oplus}_{Kin}(\lambda)$ which restricts to Φ_{Kin} and maps $\phi \in \Phi_{Kin}$ to its direct integral representation $(\phi(\lambda))_{\lambda\in\mathbb{R}}$. Then the map $J_\lambda :\ \mathcal{H}^{\oplus}_{Kin}(\lambda) \to \Phi'_{Kin}(\lambda)$ defined by $\xi \mapsto F^\xi_\lambda :=< T^\dagger_\lambda\xi, . >_n$ is a continuous, linear injection and its image constitutes an already complete set of generalized eigenvectors for $\widehat{\mathbf{M}}$. Restricting $\Phi'_{Kin}(\lambda)$ to the image of J_λ and identifying ξ, F^ξ_λ, it follows form the Riesz lemma that the identity

$$\tilde{\phi}_\lambda(F^\xi_\lambda) =< \xi, \phi(\lambda) >_{\mathcal{H}^{\oplus}_{Kin}(\lambda)} \tag{A.13}$$

constitutes a one-to-one correspondence between $\tilde{\phi}_\lambda$ and $\phi(\lambda)$. Furthermore, combining J_λ, T_λ we may identify (a dense set of) $\mathcal{H}^{\oplus}_{Kin}(\lambda)$ and (the subset defined by the image under J_λ of) $\Phi'_{Kin}(\lambda)$ by constructing $F^\phi_\lambda := F^{T_\lambda\phi}_\lambda = J_\lambda \circ T_\lambda\phi$.

The crucial part of this theorem is the existence of the nuclear operator T_λ for whose existence proof the machinery of Rigged Hilbert spaces is exploited. Theorem A.1 gives a complete answer concerning the question about the connection between generalized eigenvectors and the direct integral construction in the context of Rigged Hilbert Spaces and furthermore guarantees that the physical Hilbert space $\mathcal{H}_{Phys} := \mathcal{H}^{\oplus}_{Kin}(0) \cong \Phi'_{Kin}(0)$ is as large as mathematically possible, given $\widehat{\mathbf{M}}$. This does not mean, however, that it is as large as physically necessary.

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