Testing the Master Constraint Programme for Loop Quantum Gravity I. General Framework

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Abstract

Recently the Master Constraint Programme for Loop Quantum Gravity (LQG) was proposed as a classically equivalent way to impose the infinite number of Wheeler – DeWitt constraint equations in terms of a single Master Equation. While the proposal has some promising abstract features, it was until now barely tested in known models.

In this series of five papers we fill this gap, thereby adding confidence to the proposal. We consider a wide range of models with increasingly more complicated constraint algebras, beginning with a finite dimensional, Abelean algebra of constraint operators which are linear in the momenta and ending with an infinite dimensional, non-Abelean algebra of constraint operators which closes with structure functions only and which are not even polynomial in the momenta.

In all these models we apply the Master Constraint Programme successfully, however, the full flexibility of the method must be exploited in order to complete our task. This shows that the Master Constraint Programme has a wide range of applicability but that there are many, physically interesting subtleties that must be taken care of in doing so. In particular, as we will see, that we can possibly construct a Master Constraint Operator for a non – linear, that is, *interacting* Quantum Field Theory underlines the strength of the background independent formulation of LQG.

In this first paper we prepare the analysis of our test models by outlining the general framework of the Master Constraint Programme. The models themselves will be studied in the remaining four papers. As a side result we develop the Direct Integral Decomposition (DID) Programme for solving quantum constraints as an alternative to Refined Algebraic Quantization (RAQ).

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Contents

1 Introduction

The satisfactory implementation of the quantum dynamics of Loop Quantum Gravity (LQG) (see e.g. the recent reviews [1] and the forthcoming books [2, 3]) remains the major unresolved problem before reliable and falsifiable quantum gravity predictions can be made. While there has been progress in the formulation of the quantum dynamics [4], there remain problems to be resolved before the proposal can be called satisfactory. These problems have to do with the semi-classical limit of the theory and, related to this, the correct implementation of Dirac's algebra of initial value constraints, consisting of the spatial diffeomorphism constraints $C_a(x)$ and the Hamiltonian constraints $C(x)$ respectively. This algebra, sometimes called the **Hypersurface Deformation Algebra** or **Dirac Algebra** $\mathfrak{D}$, has the following structure

$$\begin{aligned} \{\vec{C}(\vec{N}),\vec{C}(\vec{N}')\} &= \kappa\vec{C}(\mathcal{L}_{\vec{N}}\vec{N}') \\ \{\vec{C}(\vec{N}),C(N')\} &= \kappa C(\mathcal{L}_{\vec{N}}N') \\ \{C(N),C(N')\} &= \kappa\vec{C}([dNN'-NdN']q^{-1}) \end{aligned} \tag{1.1}$$

Here κ is the gravitational coupling constant, q the spatial metric of the leaves of Σ_t of a foliation of the spacetime manifold $M\cong\mathbb{R}\times\sigma$, $\mathcal{L}$ denotes the Lie derivative and we have smeared the constraints properly with test functions, that is, $\vec{C}(\vec{N})=\int_\sigma d^3xN^aC_a,\;\; C(N)=\int_\sigma d^3xNC$. Notice that the appearance of the **structure function** q^{-1} appearing in the last relation of (1.1) displays $\mathfrak{D}$ as an algebra which is not an (infinite dimensional) Lie algebra. This makes the representation theory of (1.1) so much more comlicated than that for infinite dimensional Lie (Super-)Algebras that there is almost nothing known about its representation theory. This looks like bad news from the outset for any canonical theory of quantum gravity, such as LQG, which must seek to provide an honest representation of (1.1).

There is another algebra $\mathfrak{A}$ in canonical quantum gravity which plays a central role, the algebra of kinematical (i.e. not gauge invariant) observables which is to separate the points of the classical phase space so that more complicated composite functions can be expressed in terms of (limits of) them. In LQG a very natural choice is given by the holonomy – flux algebra generated by the relations

$$
\begin{aligned}
\{A(e), A(e')\} &= 0 \\
\{E_f(S), E_{f'}(S')\} &= 0 \\
\{E_f(S), A(e)\} &= \kappa f^j(S \cap e) A(e_1) \tau_j A(e_2)
\end{aligned}
\tag{1.2}
$$

where

$$
A(e) = \mathcal{P} \exp(\int_e A), \;\; E_f(S) = \int_S f^j(*E_j) \tag{1.3}
$$

Here we have displayed only the generic cases $S \cap S' = \emptyset$, $e = e_1 \circ e_2; e_1 \cap e_2 = e \cap S$, τ_j is a basis for $su(2)$, $*E$ is the background metric independent two form dual to the vector density E^a_j and A denotes an $SU(2)$ connection. The group $\text{Diff}(\sigma)$ of spatial diffeomorphisms of σ acts by a group of automorphisms

$$
\alpha : \; \text{Diff}(\sigma) \to \text{Aut}(\mathfrak{A}); \; \varphi \mapsto \alpha_\varphi \tag{1.4}
$$

where

$$
\alpha_\varphi(A(e)) = A(\varphi(e)), \; \alpha_\varphi(E_f(S)) = E_{f \circ \varphi^{-1}}(\varphi(S)) \tag{1.5}
$$

In view of the fact that we want to ultimately construct a physical Hilbert space of solutions to the spatial diffeomorphism constraint and the Hamiltonian constraint it is desirable to have at our disposal a cyclic and spatially diffeomorphism invariant representation of $\mathfrak{A}$. This is best described by a (half) regular, positive linear functional ω on the C^*-algebra $\mathfrak{A}$ of the corresponding Weyl elements satisfying $\omega \circ \alpha_\varphi = \omega$ for all $\varphi \in \text{Diff}(\sigma)$. The corresponding representation is then the GNS representation corresponding to ω. The theory of spatially diffeomorphism invariant representations of $\mathfrak{A}$ has been analyzed in detail in [5] with the surprising result that there is only one such representation, namely the Ashtekar – Isham – Lewandowski representation [6] that has been used exclusively in LQG for a decade already, thereby being justified in retrospect.

Since the positive linear functional ω is spatially diffeomorphism invariant, general theorems from algebraic QFT [7] tell us that we have a unitary representation of $\text{Diff}(\sigma)$ on the GNS Hilbert space $\mathcal{H}_\omega$ defined by $U(\varphi)\pi_\omega(a)\Omega_\omega = \pi_\omega(\alpha_\varphi(a))\Omega_\omega$ where Ω_ω is the cyclic GNS vacuum and π_ω the GNS representation. It turns out [8] that this representation is necessarily such that the one parameter unitary groups $t \mapsto \varphi^{\vec{N}}_t$, where $\varphi^{\vec{N}}_t$ denotes the diffeomorphisms generated by the integral curves of the vector field $\vec{N}$, *are not weakly continuous*. By Stone's theorem, this means that the self-adjoint operator corresponding to $\vec{C}(\vec{N})$ does not exist. This fact presents a major obstacle in representing the third relation in (1.1) which requires the infinitesimal generator (even smeared with operator valued structure functions) on the right hand side. The first two relations in (1.1) can be written in the quantum theory in terms of finite diffeomorphisms via

$$
U(\varphi)U(\varphi') = U(\varphi \circ \varphi'), \;\; U(\varphi)\hat{C}(N)U(\varphi)^{-1} = \hat{C}(\varphi(N)) \tag{1.6}
$$

but not so the third relation in (1.1). Namly, the third relation prevents us from exponentiating the Hamitonian constraints themselves which do not form (together with the spatial diffeomorphism constraints) a Lie Algebra due to appearance of the structure functions.

Another major obstacle is that while the spatial diffeomorphisms form a subalgebra of $\mathfrak{D}$, they do not form an ideal. Now it turns out that in the representation $\mathcal{H}_\omega$ the Hamiltonian constraints $\hat{C}(N)$ can be defined only by exploiting their dual action on the space of solutions to the spatial diffeomorphism constraint $\mathcal{H}_{Diff}$ [8]. However, since spatial diffeomorphisms do not form an ideal, one cannot define the operators directly on $\mathcal{H}_{Diff}$ itself since this space is not preserved. More precisely: A regularized Hamiltonian constraint was defined on $\mathcal{H}_{Kin} := \mathcal{H}_\omega$ and the regulator could be removed using an operator topology which exploits the structure of $\mathcal{H}_{Diff}$. A resulting limit operator exists by the axiom of choice but there is a huge regularization ambiguity. The commutator of two Hamiltonian constraint operators is non-vanishing but annihilates diffeomorphism invariant states which is precisely what the third relation in (1.1) should translate into in the quantum theory if there is no anomaly. Although these methods have been tested successfully in several models (see e.g. the fifth reference in [4] or [9]), the status of the Hamiltonian constraint is not entirely satisfactory. For instance, the right hand side of the commutator does not obviously look like the quantization of the right hand side of the third equation in (1.1) so that one can doubt the correctness of the semiclassical limit of the theory. One could argue that this is because even in the classical theory it is a non trivial calculation which transforms the Poisson bracket of two Hamiltonian constraints into the right hand side of the third line of (1.1) and that in a semiclassical calculation this can be recovered because there one can essentially replace operators and commutators by classical functions and Poisson brackets. However, nobody has shown that so far. Furthermore, the regularization ambiguities are bothersome although they will disappear on the physical Hilbert space which is the joint kernel of all the constraints. Therefore the overall situation is far from being satisfactory.

One could summarize this by saying that the representation theory of the kinematical algebra $\mathfrak{A}$ and the hypersurface deformation algebra $\mathfrak{D}$ are incompatible and what has been done in [4] is the best what can be achieved in the present setup. In order to make progress, the logical way out is to replace either $\mathfrak{A}$ or $\mathfrak{D}$ by a classically equivalent algebra such that their representation theories do become compatible.

The Master Constraint Programme [10] is a proposal for precisely doing that, it replaces the complicated algebra $\mathfrak{D}$ by the much simpler Master Constraint Algebra $\mathfrak{M}$. Namely, instead of the infinitely many Hamiltonian constraints $C(x) = 0,\ x \in \sigma$ we define the single Master Constraint

$$\mathbf{M} = \frac{1}{2} \int_\sigma d^3x \, \frac{C(x)^2}{\sqrt{\det(q)}(x)} \tag{1.7}$$

where q_{ab} denotes the spatial metric constructed from E^a_j via $\det(q) q^{ab} = E^a_j E^b_k \delta^{jk}$. The vanishing of all the infinitely many Hamiltonian constraints is obviously equivalent to the single Master Equation $\mathbf{M} = 0$. Now squaring a constraint as displayed in (1.7) looks like a rather drastic step to do in view of the following fact: A weak Dirac Observable O is determined by the infinite number of relations $\{C(x), O\}_{\mathbf{M}=0} = 0,\ x \in \sigma$. However, the condition $\{\mathbf{M}, O\}_{\mathbf{M}=0} = 0$ is obviously trivially satisfied for any O so that the Master Constraint seems to fail detecting weak Dirac observables. However, this is not the case, it is easy to see that the single Master Relation

$$\{\{\mathbf{M}, O\}, O\}_{\mathbf{M}=0} = 0 \tag{1.8}$$

is completely equivalent to the infinite number of relations $\{C(x), O\}_{\mathbf{M}=0} = 0,\ x \in \sigma$. Therefore the Master Constraint encodes sufficient information in order to perform the constraint analysis.

The point is now the following simplified constraint algebra, called the Master Constraint Algebra $\mathfrak{M}$

$$\begin{aligned} \{\vec{C}(\vec{N}), \vec{C}(\vec{N})\} &= \kappa \vec{C}(\mathcal{L}_{\vec{N}} \vec{N}') \\ \{\vec{C}(\vec{N}), \mathbf{M}\} &= 0 \\ \{\mathbf{M}, \mathbf{M}\} &= 0 \end{aligned} \tag{1.9}$$

In other words, since we have carefully divided by $\sqrt{\det(q)}$ in (1.7), the integrand is a density of weight one and hence the integral is spatially diffeomorphism invariant. Thus now spatial diffeomorphisms do form an ideal in the Master Constraint Algebra and whence the Master Constraint Operator must preserve $\mathcal{H}_{Diff}$. This is precisely what we wanted in order to remove the regularization ambiguities mentioned above. Furthermore, the difficult third relation in (1.1) is replaced by the simple third relation in (1.9) which is a tremendous simplification because structure functions are avoided. Hence we do have a chance to make progress with the representation theory of the Master Constraint Algebra $\mathfrak{M}$.

Of course, squaring a constraint in QFT is dangerous also from the perspective of the worsened ultraviolet behaviour of the corresponding operator and hence the Master Constraint Programme has to be performed with due care. Moreover, the factor ordering problem will be now much more complex and different orderings may very well drastically change the size of the physical Hilbert space. It is here where anomalies in the usual framework will manifest themselves, hence nothing is "swept under the rug". However, as we will see in the next section, the Master Constraint Programme has a chance to at least complete the canonical quantization programme to the very end, **with no further mathematical obstructions on the way**. Whether the resulting theory is satisfactory then depends solely on the question whether the final physical Hilbert space contains a sufficient number of semiclassical states in order to have the original classical theory as its classical limit.

Hence the Master Constraint Programme is so far only a proposal and is far from granted to be successful. It is the purpose of this series of papers to demonstrate by means of a selected list of models that the Master Constraint Programme is flexible enough in order to deal successfully with a large number of subtleties, in particular, anomalies, ultraviolet divergences etc. It also offers an alternative to the group averaging programme, also called Refined Algebraic Quantization (RAQ), [11] from which it differs in two important aspects: First of all, RAQ needs as an additional input the selection of a dense and invariant domain for all the constraint operators, equipped with a finer topology than that of the Hilbert space into which it is embedded. On the other hand the Master Constraint Programme only uses standard spectral theory for normal operators on a Hilbert space in order to arrive at a direct integral decomposition (DID) of the Hilbert space. The physical Hilbert space is then the induced zero eigenvalue "subspace". That subspace is however only known up to structures of measure zero and in order to fix the remaining ambiguities, additional physical input is needed, namely that the induced Hilbert space carries a self adjoint representation of the Dirac observables. We will show however that, even without using further physical input, the amount of ambiguity for DID is smaller than for RAQ. The second difference is that RAQ, at least so far, cannot rigorously deal with constraint algebras which involve non-trivial structure functions since the group averaging really requires an honest (Lie) group structure. In contrast, the Master Constraint Programme does not draw an essential distinction between the case with structure constants and structure functions respectively. Finally the Master Constraint Programme is very flexible in the sense that for a given set of constraints there is an infinite number of associated Master Constraint functionals which are classically all equivalent but which have different quantizations. One can exploit that freedom in order to avoid, e.g., ultraviolet problems and factor ordering problems as we will see.

The present paper is organized as follows:

In section two we briefly review the Master Constraint Programme from [10] for a general theory.

Section three develops the general theory of the direct integral decomposition (DID) method for solving quantum constraints. Most of this is standard spectral theory for possibly unbounded self – adjoint operators and will be familiar to experts. More precisely, we recall the spectral theorem for unbounded self – adjoint operators in its projection valued measure and functional calculus form, give the abstract definition of a direct integral, display the direct integral resolution of the spectral projections of self – adjoint operators (functional model), recall how to split a Hilbert space into a direct sum such that the respective restrictions of the operator has pure point or continuous spectrum (which will be important for our applications), connect direct integral representations with constraint quantization, derive the explicit action of strong Dirac observables on the physical Hilbert space and finally compare RAQ and DID methods.

In section four we describe, for readers not interested in these mathematical details displayed in section three, a brief algorithm for how to arrive at the physical Hilbert space given a self adjoint constraint operator by the Direct Integral Decomposition Technique (DID). Reading that section will be sufficient for readers who are just interested in the application of the formalism.

We conclude in section five and anticipate some of the results of our companion papers [27, 28, 29, 30].

2 Review of the Master Constraint Programme

We briefly review the Master Constraint Programme. For more details the reader is referred to [10].

Let be given a phase space $\mathcal{M}$ with real valued, first class constraint functions $C_I(y): \mathcal{M} \to \mathbb{R};\ m \mapsto [C_I(y)](m)$ on $\mathcal{M}$. Here we let take $I \in \mathcal{I}$ take discrete values while $y \in Y$ belongs to some continuous index set. To be more specific, Y is supposed to be a measurable space and we choose a measure ν on Y. Then we consider the fiducial Hilbert space $\mathfrak{h} := L_2(X, d\mu)^{|\mathcal{I}|}$ with inner product

$$< u, v >_{\mathfrak{h}} = \int_Y d\nu(x) \sum_{I \in \mathcal{I}} \overline{u_I(y)} v_I(y) \tag{2.1}$$

Finally we choose a positive – operator valued function $\mathcal{M} \to \mathcal{L}_+(\mathfrak{h});\ m \mapsto K(m)$ where $\mathcal{L}_+(\mathfrak{h})$ denotes the cone of positive linear operators on $\mathfrak{h}$.

Definition 2.1.
The Master Constraint *for the system of constraints $m \mapsto [C_I(x)](m)$ corresponding to the choice ν of a measure on Y and the operator valued function $m \mapsto K(m)$ is defined by*

$$\mathbf{M}(m) = \frac{1}{2} < C(m), K(m) \cdot C(m) >_{\mathfrak{h}} \tag{2.2}$$

Of course ν, K must be chosen in such a way that (2.2) converges and that it defines a differentiable function on $\mathcal{M}$, but apart from that the definition of a Master Constraint allows a great deal of flexibility which we will exploit in the examples to be discussed. It is clear that the infinite number of constraint equations $C_I(y) = 0$ for a.a. $y \in Y$ and all $I \in \mathcal{I}$ is equivalent with the single Master Equation $\mathbf{M} = 0$ so that classically all admissable choices of ν, K are equivalent.

Notice that we have explicitly allowed $\mathcal{M}$ to be infinite dimensional. In case that we have only a finite dimensional phase space, simply drop the structures y, Y, ν from the construction.

We compute for any function $O \in C^2(\mathcal{M})$ that

$$\{\{O, \mathbf{M}\}, O\}_{\mathbf{M}=0} = [< \{O, C\}, K \cdot \{O, C\} >_{\mathfrak{h}}]_{\mathbf{M}=0} \tag{2.3}$$

hence the Master Relation $\{\{O, \mathbf{M}\}, O\}_{\mathbf{M}=0} = 0$ is equivalent with $\{O, C_I(y)\}_{\mathbf{M}=0} = 0$ for a.a. $y \in Y$ and $I \in \mathcal{I}$. Among the set of all weak Dirac observables satisfying the Master Relation the strong Dirac observables form a subset. These are those twice differentiable functions on $\mathcal{M}$ satisfying $\{O, \mathbf{M}\} \equiv 0$ identically[1] on all of $\mathcal{M}$. They can be found as follows: Let $t \mapsto \alpha_t^{\mathbf{M}}$ be the one-parameter group of automorphisms of $\mathcal{M}$ defined by time evolution with respect to $\mathbf{M}$. Then the **ergodic mean** of $O \in C^\infty(\mathcal{M})$

$$[O] := \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} dt\ \alpha_t^{\mathbf{M}}(O) \tag{2.4}$$

[1] Notice that this does not automatically imply that $\{O, C_I(y)\} = 0$ identically for all y, I, however, it implies $\{O, C_I(y)\}_{\widehat{\mathbf{M}}=0} = 0$.

has a good chance to be a strong Dirac observable if twice differentiable as one can see by formally commuting the integral with the Poisson bracket with respect to $\mathbf{M}$. In order that the limit in (2.5) is non-trivial, the integral must actually diverge. Using l' Hospital's theorem we therefore find that if (2.4) converges and the integral diverges (the limit being an expression of the form ∞/∞) then it equals

$$[O] := \lim_{T\to\infty} \frac{1}{2}[\alpha^{\mathbf{M}}_T(O) + \alpha^{\mathbf{M}}_{-T}(O)] \tag{2.5}$$

which is a great simplification because, while one can often compute the time evolution $\alpha^{\mathbf{M}}_t$ for a bounded function O (for bounded functions the integral will typically diverge linearly in T so that the limit exists), doing the integral is impossible in most cases. Hence we see that the Master Constraint Programme even provides some insight into the structure of the classical Dirac observables for the system under consideration.

Now we come to the quantum theory. We assume that a judicious choice of ν, K has resulted in a positive, self-adjoint operator $\widehat{\mathbf{M}}$ on some kinematical Hilbert space $\mathcal{H}_{Kin}$ which we assume to be separable. Following (a slight modification of) a proposal due to Klauder [12], if zero is not in the spectrum of $\widehat{\mathbf{M}}$ then compute the finite, positive number $\lambda_0 := \inf(\sigma(\widehat{\mathbf{M}}))$ and redefine $\widehat{\mathbf{M}}$ by $\widehat{\mathbf{M}} - \lambda_0 \mathrm{id}_{\mathcal{H}_{Kin}}$. Here we assume that λ_0 vanishes in the $\hbar \to 0$ limit so that the modified operator still qualifies as a quantization of $\mathbf{M}$. This is justified in all examples encountered so far where λ_0 is usually related to some reordering of the operator. More generally, it might be necessary to subtract a "normal ordering operator" $\hat{\lambda}_0$ (so that the resulting operator is still positive) which is supposed to vanish in the $\hbar \to 0$ limit. See e.g. [18] for an example where free quantum fields are coupled to gravity which could be looked at as a model with second class constraints in analogy to the scond example in [27] and the usual infinite normal ordering constant becomes a densely defined operator. Hence in what follows we assume w.l.g. that $0 \in \sigma(\widehat{\mathbf{M}})$.

Under these circumstances we can **completely solve the** Quantum Master Constraint Equation $\widehat{\mathbf{M}} = 0$ **and explicitly provide the physical Hilbert space and its physical inner product**. Namely, as it is well known [14] the Hilbert space $\mathcal{H}_{Kin}$ is unitarily equivalent to a direct integral

$$\mathcal{H}_{Kin} \cong \int^{\oplus}_{\mathbb{R}^+} d\mu(x)\; \mathcal{H}^{\oplus}_{Kin}(x) \tag{2.6}$$

where μ is a so-called spectral measure and $\mathcal{H}^{\oplus}_{Kin}(x)$ is a separable Hilbert space with inner product induced from $\mathcal{H}_{Kin}$. This simply follows from spectral theory. The operator $\widehat{\mathbf{M}}$ acts on $\mathcal{H}^{\oplus}_{Kin}(x)$ by multiplication by x, hence the physical Hilbert space is simply given by

$$\mathcal{H}_{Phys} = \mathcal{H}^{\oplus}_{Kin}(0) \tag{2.7}$$

Strong Quantum Dirac Observables can be constructed in analogy to (2.4), (2.5), namely for a given bounded operator on $\mathcal{H}_{Kin}$ we define, if the uniform limit exists

$$\widehat{[O]} := \lim_{T\to\infty} \frac{1}{2}[U(T)\hat{O}U(T)^{-1} + U(T)^{-1}\hat{O}U(T)] \tag{2.8}$$

where

$$U(t) = e^{it\widehat{\mathbf{M}}} \tag{2.9}$$

is the unitary evolution operator corresponding to the self-adjoint $\widehat{\mathbf{M}}$ via Stone's theorem. One must check whether the spectral projections of the bounded operator (2.8) commute with those of $\widehat{\mathbf{M}}$ but if they do then $\widehat{[O]}$ defines a strong quantum Dirac observable. Notice, however, that in the case of interest (structure functions) strong Dirac observables are not very interesting and weak Dirac observables can only be constructed by using (2.8) by using judicious $\hat{O}$ (it has to be invariant under all constraints but one). For a systematic procedure to construct weak Dirac classical and quantum observables see [13].

This concludes our sketch of the general theory. We will now describe precisely how to arrive at (2.6) and (2.7). In particular, there are certain choices to be made and we will state precisely how physical predictions will depend on those choices. The result is that the presentation of (2.6) is actually unique (up to unitary equivalence) but (2.7) can be fixed only by using additional physical input. We will outline in detail what that input is in order to make (2.7) essentially as unique as it can possibly be. Readers not interested in those details who just want to apply DID can skip the next section and jump immediately to section 4 where we summarize our findings.

3 General Framework for the Master Constraint Programme

The Master Constraint Programme makes extensive use of the spectral theory for self − adjoint operators, their invariants up to unitary equivalence and their functional models, that is, the realization as multiplication operators on a direct integral Hilbert space. This theory is of course well known in mathematical physics but we feel that it is worthwhile reviewing it here so that one has a compact account of the relevant theory together with the essential proofs at one's disposal. The proofs are also instructive because one actually learns how the method works in detail. Specialists can safely skip this section, except for section 3.5 where the direct integral decomposition (DID) theory is connected with constraint quantization and section 3.7 where DID is compared with RAQ. Practitioners not interested in the mathematical details can immediately jump to section four where we simply summarize in algorithmic form the contents of this section.

This section is subdivided as follows:

First of all we recall the spectral theorem for self − adjoint operators and how to construct the associated projection valued measures (p.v.m.).

Next we define direct integral Hilbert spaces and their associated p.v.m. These could also be called bundles of Hilbert spaces with fibres $\mathcal{H}_x$ whose dimension may vary as x varies over a measurable space $(X, \mathcal{B})$ where X is some set (the base) and $\mathcal{B}$ a $\sigma-$algebra[2] over X, together with a measure[3] μ. We require that the $\mathcal{H}_x$ are all separable, that X is $\sigma-$finite (is a countable union of measurable sets each of which has finite μ measure) and that $\mathcal{B}$ is separable[4]. It turns out that direct integrals of Hilbert spaces over the same $(X, \mathcal{B})$ together with their spectral projections are unitarily equivalent if and only if 1. the associated measures are equivalent[5] and 2. the dimension functions $N(x) := \dim(\mathcal{H}_x)$ coincide $\mu-$a.e.[6]

Next we connect the first and second part by showing that for each self − adjoint operator a on a Hilbert space $\mathcal{H}$ we find a direct integral representation for its spectral projections.

[2] A $\sigma-$algebra $\mathcal{B}$ on a set X is a collection of subsets of X which contains X and the empty set $\emptyset$ and is closed under countable unions and intersections. The members $B \in \mathcal{B}$ are called measurable sets.

[3] A measure μ on a measurable space $(X, \mathcal{B})$ is a countably additive, positive set function $\mu:\ \mathcal{B} \to \mathbb{R}^+ \cup \{\infty\}$, that is, if $B_n,\ n = 1, 2, ..$ are mutually disjoint measurable sets then $\mu(\cup_n B_n) = \sum_n \mu(B_n)$.

[4] I.e. there is a countable collection $\mathcal{C}$ of measurable sets in $\mathcal{B}$, called a base, so that for each $B \in \mathcal{B}$ and each $\epsilon > 0$ there is a $B_0 \in \mathcal{C}$ such that $\mu([B - B_0] \cup [B_0 - B]) < \epsilon$.

[5] For two measures μ, ν on $(X, \mathcal{B})$ we say that ν is absolutely continuous with respect to μ if $\mu(B) = 0$ implies $\nu(B) = 0$. Mutually absolutely continuous measures are called eqivalent.

[6] A property holds on X $\mu-$a.e. (almost everywhere) if it is violated at most on measurable sets B of vanishing μ measure, that is, $\mu(B) = 0$.

The role of $(X, \mathcal{B})$ is here taken by $(\sigma(a) \subset \mathbb{R}, \mathcal{B}_{Borel})$ where $\sigma(a)$ denotes the spectrum of a[7] and $\mathcal{B} := \mathcal{B}_{Borel}$ is the natural Borel $\sigma-$algebra on $\mathbb{R}$[8]. Not only will we give a constructive procedure for how to do that, but also we will show that the choices that one has to make within that procedure lead to unitarily equivalent representations. Furthermore, we show that all operators b commuting with a (that is, the corresponding spectral projections commute) are fibre preserving, that is, they induce operators $b(x)$ on all $\mathcal{H}_x$ which are self − adjoint on $\mathcal{H}_x$ if and only if b is self − adjoint.

Then we have to connect this with constraint quantization. If zero belongs to the spectrum of a then we would like to choose $\mathcal{H}_{phys} := \mathcal{H}_{x=0}$ as the physical Hilbert space selected by the constraint $a = 0$. However, here we have to add physical input since the set $\{x\}$ is of $\mu-$measure zero provided that x is not in the pure point spectrum of a. Hence, if $x = 0$ does not lie in the point spectrum then we are free to set $\mathcal{H}_x = \{0\}$ without affecting the unitary equivalence with the direct integral representation. Moreover, if $x = 0$ is an eigenvalue embedded into the continuous spectrum then the direct integral Hilbert space $\mathcal{H}_{x=0}$ is granted to correspond to the zero eigenvectors only while generalized eigenvectors corresponding to the continuous spectrum are easily missed. Both features are of course unacceptable and we demonstrate how to repair this by adding an additional requirement which is motivated by the concrete physical examples studied so far where our procedure gives the correct results. In order to do this properly we have to connect this with the measure theoretic origin of the pure point and continuous spectrum respectively which we briefly recall as well.

Next we show explicitly how the direct integral decomposition (DID) automatically leads to an induced self-adjoint representation on the physical Hilbert space of strong self adjoint Dirac observable operators.

Last but not least we establish how DID relates to the programme of refined algebraic quantization (RAQ). Notice that RAQ has actually two implementations: A heuristic version, called group averaging, and a rigorous version, using Rigged Hilbert Spaces. We show that there is no universally applicable group averaging procedure and that the theory of Rigged Hilbert Spaces uses more structural input than DID needs. Moreover, DID can deal with structure functions in contrast to RAQ.

Our exposition is based on relevant parts of [14, 20, 22] which should be consulted for further information.

3.1 Spectral Theorem, Projection Valued Measures, Spectral Projections, Functional Calculus

Definition 3.1.
Let $(X, \mathcal{B})$ be a measurable space and $\mathcal{H}$ a Hilbert space. A function E from $\mathcal{B}$ into the set of projection operators on $\mathcal{H}$ is called a projection valued measure (p.v.m.) provided it satisfies
1. $E(\cup_{n=1}^\infty B_n) = \sum_{n=1}^\infty E(B_n)$ *for mutually disjoint* $B_n \in \mathcal{B}$.
2. $E(X) = 1_{\mathcal{H}}$

From the projection property $E(B)^2 = E(B)$ one easily derives $E(B_1)E(B_2) = E(B_1 \cap B_2)$, $E(\emptyset) = 0$ and $E(B_1) \leq E(B_2)$ for $B_1 \subset B_2$ where for two projections $P_1 \leq P_2$ means that $P_1\mathcal{H} \subset P_2\mathcal{H}$.

[7]The spectrum of a densely defined and closable (the adjoint $a^\dagger$ is also densely defined) operator a on a Hilbert space $\mathcal{H}$ is the set of complex numbers λ such that $a - \lambda 1_{\mathcal{H}}$ does not have a bounded inverse. For self-adjoint operators (that is, a and $a^\dagger$ have the same domain of definition and $a = a^\dagger$) the spectrum is a subset of the real line.

[8]This is the smallest $\sigma-$algebra containing all the open sets of $\mathbb{R}$ with respect to its natural metric topology.

Given a p.v.m. E and a unit vector $\Omega \in \mathcal{H}$ we define the spectral measure

$$\mu_\Omega(B) :=< \Omega, E(B)\Omega >_{\mathcal{H}} =: \int_B d\mu_\Omega(x) \tag{3.1}$$

That this defines indeed a positive, normalized, $\sigma-$additive set function is easily verified from definition 3.1. Using the polarization identity

$$\begin{aligned} < \Omega_1, E(B)\Omega_2 > &= \frac{1}{4}[< (\Omega_1 + \Omega_2), E(B)(\Omega_1 + \Omega_2) > - < (\Omega_1 - \Omega_2), E(B)(\Omega_1 - \Omega_2) > \\ &\quad -i < (\Omega_1 + i\Omega_2), E(B)(\Omega_1 + i\Omega_2) > +i < (\Omega_1 - i\Omega_2), E(B)(\Omega_1 - i\Omega_2) >] \end{aligned} \tag{3.2}$$

we may define the complex measures $\mu_{\Omega_1,\Omega_2}(B) =< \Omega_1, E(B)\Omega_2 >$ as well.

Given a measurable complex valued function[9] f on X we may approximate it pointwise by simple functions of the form $f_N(x) = \sum_{n=1}^N z_n \chi_{B_n}(x)$ where χ_B denotes the chracteristic function of the set $B \in \mathcal{B}$ and $z_n \in \mathbb{C}$ (that is, we find a sequence such that $\lim_{N\to\infty} f_N(x) = f(x)$ where the rate of convergence may depend on x, see e.g. [21]). Associate to f_N the operator $f_N(E) := \sum_{n=1}^N z_n E(B_n)$. Then

$$< \Omega_1, f_N(E)\Omega_2 >= \sum_{n=1}^N z_n < \Omega_1, E(B_n)\Omega_2 >= \sum_{n=1}^N z_n \int_X \chi_{B_n}(x) d\mu_{\Omega_1,\Omega_2}(x) = \int_X f_N(x) d\mu_{\Omega_1,\Omega_2}(x) \tag{3.3}$$

Passing to the limit[10] we find

$$< \Omega_1, f(E)\Omega_2 >= \int_X f(x) d\mu_{\Omega_1,\Omega_2}(x) \tag{3.4}$$

for every measurable function f. By using the the notation

$$d\mu_{\Omega_1,\Omega_2}(x) =: d < \Omega_1, E(x)\Omega_2 >=:< \Omega_1, dE(x)\Omega_2 > \tag{3.5}$$

one writes (3.4) often in the form

$$f(E) = \int_X f(x) dE(x) \tag{3.6}$$

whose precise meaning is given by (3.4).

Let now a be a, not necessarily bounded, self – adjoint operator on $\mathcal{H}$. This means that 1. a is densely defined on a domain $D(a)$, 2. that it is symmetric, i.e. $D(a) \subset D(a^\dagger)$ and $a^\dagger = a$ on $D(a)$ and that 3. actually $D(a^\dagger) = D(a)$. Here $D(a^\dagger) = \{\psi \in \mathcal{H};\ \sup_{0\neq\psi'\in D(a)} |< \psi, a\psi' > |/||\psi'|| < \infty\}$. Then the famous spectral theorem holds.

Theorem 3.1.
Let a be a self – adjoint operator on a Hilbert space. Then there exists a p.v.m. E on the measurable space $(\mathbb{R}, \mathcal{B}_{Borel})$ such that

$$a = \int_{\mathbb{R}} x\, dE(x) \tag{3.7}$$

where the domain of integration can be restricted to the spectrum $\sigma(a)$.

[9] A function $f : X \to Y$ from a measurable space X to a topological space Y is said to be measurable if the set of points $\{x \in X;\ f(x) \in I\}$ is measurable for every open set $I \subset Y$.

[10] The interchange of the limit and the integral is justified by the Lebesgue dominated convergence theorem, see e.g. [21].

In order to construct E from a we notice that for each measurable, bounded set B the function χ_B has support in a closed, finite interval containing B, therefore it can be approximated pointwise by polynomials due to the Weierstrass theorem. On the other hand, the function x can be approximated arbitrarily well by simple functions of the form $f(x) = \sum_k x_k \chi_{B_k}(x)$ where $\cup_n B_k = \mathbb{R}$ is a collection of disjoint intervals and $x_k \in B_k$. Therefore for Ω_2 in the domain of a^n

$$\begin{aligned}
<\Omega_1, a^n \Omega_2> &= \int x \; d\mu_{\Omega_1, a^{n-1}\Omega_2}(x) \\
&= \lim \sum_{k_1} x_{k_1} <\Omega_1, E(B_{k_1}) a^{n-1} \Omega_2> \\
&= \lim \sum_{k_1} x_{k_1} <E(B_{k_1})\Omega_1, a^{n-1} \Omega_2> \\
&= \lim \sum_{k_1} x_{k_1} \int x \; d\mu_{E(B_{k_1})\Omega_1, a^{n-2}\Omega_2}(x) \\
&= \lim \sum_{k_1, k_2} x_{k_1} x_{k_2} <E(B_{k_2}) E(B_{k_1})\Omega_1, a^{n-2} \Omega_2> \\
&= .. \\
&= \lim \sum_{k_1 .. k_n} x_{k_1} .. x_{k_n} <E(B_{k_1} \cap .. \cap B_{k_n})\Omega_1, \Omega_2> \\
&= \lim \sum_{k} x_k^n <\Omega_1, E(B_k)\Omega_2> \\
&= \int x^n \; d\mu_{\Omega_1, \Omega_2}(x)
\end{aligned} \tag{3.8}$$

We conclude that for every measurable set B

$$<\Omega_1, \chi_B(a)\Omega_2> = \int \chi_B(x) \; d\mu_{\Omega_1, \Omega_2}(x) = <\Omega_1, E(B)\Omega_2> \tag{3.9}$$

for all Ω_1, Ω_2 since $E(B)$ is a bounded operator. Thus

$$E(B) = \chi_B(a) \tag{3.10}$$

are the spectral projections associated with a self – adjoint operator. If we know the representation of a on $\mathcal{H}$ then we have to approximate $\chi_B(a)$ by polynomials and then can construct the $E(B)$. In particular we conclude that for every measurable function and Ω_2 in the domain of $f(a)$

$$<\Omega_1, f(a)\Omega_2> = \int f(x) \; d\mu_{\Omega_1, \Omega_2}(x) \tag{3.11}$$

since $f(E) := f(a)$ if $f(E) = \sum_n z_n E(B_n)$. Formula (3.11) is sometimes referred to as the functional calculus. Combining (3.6) and (3.10) we have

$$\chi_{(-\infty, \lambda]}(a) = \theta(\lambda - a) = E((-\infty, \lambda]) = \int_{-\infty}^{\lambda} dE(x) = E(\lambda) - E(-\infty) = E(\lambda) \tag{3.12}$$

where the integration constant $E(-\infty) = 0$ as follows from the fact that $E((-\infty, -\infty)) = E(\emptyset) = 0$ by definition.

Before we close this section we remark that the spectral theorem holds without making any separability assumptions, that is, it holds also when $\mathcal{H}$ does not have a countable basis.

3.2 Direct Integrals and Functional Models

Definition 3.2.
Let $(X, \mathcal{B}, \mu)$ be a separable measure space such that X is $\sigma-$finite with respect to μ and let $x \mapsto \mathcal{H}_x$ be an assignment of separable Hilbert spaces such that the function $x \mapsto N(x)$, where $N(x)$ is the countable dimension of $\mathcal{H}_x$, is measurable. It follows that the sets $X_N = \{x \in X;\ N(x) = N\}$, where N denotes any countable cardinality, are measurable. Since Hilbert spaces whose dimensions have the same cardinality are unitarily equivalent we may identify all the $\mathcal{H}_x,\ N(x) = N$ with a single $\mathcal{H}_N = \mathbb{C}^N$ with standard l_2 inner product. We now consider maps

$$\psi:\ X \to \prod_{x\in X} \mathcal{H}_x;\ \ x \mapsto (\psi(x))_{x\in X} \tag{3.13}$$

subject to the following two constraints:
1. The maps $x \mapsto <\psi, \psi(x)>_{\mathcal{H}_N}$ are measurable for all $x \in X_N$ and all $\psi \in \mathcal{H}_N$.
2. If

$$<\psi_1, \psi_2> := \sum_N \int_{X_N} d\mu(x) <\psi_1(x), \psi_2(x)>_{\mathcal{H}_N} \tag{3.14}$$

then $<\psi, \psi> < \infty$.
The completion of the space of maps (3.13) in the inner product (3.14) is called the direct integral of the $\mathcal{H}_x$ with respect to μ and one writes

$$\mathcal{H}^{\oplus}_{\mu,N} = \int_X^{\oplus} d\mu(x)\ \mathcal{H}_x,\quad <\xi_1, \xi_2> = \int_X d\mu(x)\ \ <\xi_1(x), \xi_2(x)>_{\mathcal{H}_x} \tag{3.15}$$

The restriction to $\sigma-$finite measures is due to the fact that otherwise the Radon – Nikodym theorem fails to hold [21]: If ν is a finite positive measure absolutely continuous with respect to a finite positive measure on the same $(X, \mathcal{B})$ then there exists a $\mu-$a.e. positive $L_1(X, d\mu)$ function ρ such that $\nu(B) = \int_B \rho d\mu$. If ν is only $\sigma-$finite and positive then ρ is still positive $\mu-$a.e. but only measurable and not necessarily in $L_1(X, d\mu)$. If ν is not $\sigma-$finite then the Radon – Nikodym theorem is false. In both cases one writes $\rho = d\nu/d\mu$. The Radon – Nikodym theorem will prove crucial in our applications. The significance of separability of $\mathcal{B}$ is that such $\sigma-$algebras can be treated, to arbitrary precision, as if they only had a countable number of elements. This implies that the space $\mathcal{H}^{\oplus}_{\mu,N}$ is also separable: Consider functions e_n with $e_n(x) \in \mathcal{H}_x$ and $e_n(x) = 0$ for $n > N(x)$ such that $< e_n(x), e_m(x) >= \delta_{m,n}$ for $m, n \leq N(x)$ and zero otherwise. For $x \in X_N$ the $e_n(x) = e^N_n$ are constant $\mu - a.e.$ and provide an orthonormal basis on $\mathcal{H}_x = \mathcal{H}_N$. Now fix any $f_0 \in L_2(X, d\mu)$ such that $f_0 \neq 0\ \mu - a.e.$. Then for every measurable B from the assumed countable base the functions $e_{B,n} = f_0\chi_B e_n$ with $e_{B,n}(x) = f_0(x)\chi_B(x)e_n(x)$ are measurable and they obviously lie dense. Since the set of labels (B, n) is countable, the Gram – Schmidt orthonormalization of the $e_{B,n}$ produces a countable basis for $\mathcal{H}^{\oplus}_{\mu,N}$. Separability will also prove important for our applications. In what follows, we will always assume that $(X, \mathcal{B}, \mu)$ is $\sigma-$finite and separable.

Definition 3.3.
Let $\mathcal{H}^{\oplus}_{\mu,N},\ \mathcal{H}^{\oplus}_{\mu,N'}$ be direct integral Hilbert spaces over $(X, \mathcal{B})$. Consider a family of fibre preserving, $\mu-$a.e. bounded operators $T(x) \in \mathcal{B}(\mathcal{H}_x, \mathcal{H}'_x)$. The family is said to be measurable provided that the function $x \mapsto <\psi'(x), T(x)\psi(x)>_{\mathcal{H}'_x}$ is measurable for all $\psi \in \mathcal{H}_{\mu,N},\ \ \psi' \in \mathcal{H}_{\mu,N'}$. For a measurable family of fibre preserving operators one defines

$$<\psi', T\psi>_{\mathcal{H}^{\oplus}_{\mu,N'}} = \int_X d\mu(x)\ \ <\psi'(x), T(x)\psi(x)>_{\mathcal{H}'_x} \tag{3.16}$$

In particular, if $N = N'$ $\mu-$a.e. and $T(x)$ is unitary then T is called a measurable unitarity.

Direct integral Hilbert spaces carry the following natural fibre preserving, measurable operators: Let for $B \in \mathcal{B}$ the operator $F(B)$ be defined by

$$(F(B)\psi)(x) := \chi_B(x)\psi(x) \tag{3.17}$$

Then it is easy to see that F is a p.v.m. and the corresponding spectral measures are

$$d\mu_\psi(x) = ||\psi(x)||^2_{\mathcal{H}_x}\, d\mu(x) \tag{3.18}$$

so μ_ψ is absolutely continuous with respect to μ. For any measurable scalar valued function f the fibre preserving multiplication operator

$$(Q_f\psi)(x) := f(x)\psi(x) \tag{3.19}$$

can be written in the spectral resolution form

$$Q_f = \int_X f(x)\, dF(x) \tag{3.20}$$

The following theorem is the first step towards establishing a uniqueness result, up to unitary equivalence, of a direct integral representation subordinate to a self – adjoint operator. We will denote by $[\mu]$ the equivalence class of all mutually absolutely continuous measures containing the representative μ.

Theorem 3.2.
Suppose that two direct integral Hilbert spaces $\mathcal{H}^\oplus_{\mu,N}$, $\mathcal{H}^\oplus_{\mu',N'}$ *over the same measurable space* $(X, \mathcal{B})$ *are given.*
i)
If $[\mu] = [\mu']$ *and* $N = N'$ $\mu-$*a.e., if* U *is a fibre preserving measurable unitarity, then the operator* $V : \mathcal{H}_{\mu,N} \to \mathcal{H}_{\mu',N'}$ *defined by*

$$(V\psi)(x) := \sqrt{\frac{d\mu}{d\mu'}(x)}\; U(x)\; \psi(x) \tag{3.21}$$

is unitary and has the property $VF(B) = F'(B)V$ *for all* $B \in \mathcal{B}$.
ii)
If $V : \mathcal{H}_{\mu,N} \to \mathcal{H}_{\mu',N'}$ *is a unitary operator satisfying* $VF(B) = F'(B)V$ *for all* $B \in \mathcal{B}$ *then* $[\mu] = [\mu']$, $N = N'$ μ*-a.e. and* V *admits the presentation (3.21).*

Proof of theorem 3.21:
i)
As defined, V is certainly an isometry and since $[\mu] = [\mu']$ the function $d\mu'/d\mu$ is also positive μ'-a.e. and clearly $(d\mu'/d\mu)(d\mu/d\mu') = 1$ μ-a.e. Hence V has an inverse, is thus unitary and the intertwining property $VF(B) = F'(B)V$ follows from the fibre preserving nature of all $V, F(B), F'(B)$ and because $F(B), F'(B)$ are just multiplication by scalars.
ii)
Let $f \in L_2(X, d\mu)$, $f \neq 0$ $\mu-$a.e. and $< e_m(x), e_n(x) >_{\mathcal{H}_x} = \delta_{m,n}\theta(N(x) - n)$ where $\theta(y) = 1$ for $y \geq 0$ and $\theta(y) = 0$ for $y < 0$. Let $b_n(x) := f(x)e_n(x)$ then obviously $||b_n||_{\mathcal{H}_{\mu,N}} \leq ||f||_{L_2(X,d\mu)}$ where equality is reached certainly for $n = 1$ because $N(x) \geq 1$ $\mu-$a.e. Hence $b_n \in \mathcal{H}_{\mu,N}$. Define $b'_n := Vb_n$. Then by unitarity and the intertwining property (unitary equivalence of the spectral projections)

$$\begin{aligned} < b'_m, F'(B)b'_n >_{\mathcal{H}^\oplus_{\mu',N'}} &= < b_m, F(B)b_n >_{\mathcal{H}^\oplus_{\mu,N}} \\ &\Rightarrow \int_B d\mu'(x) < b'_m(x), b'_n(x) >_{\mathcal{H}'_x} = \int_B d\mu(x) < b_m(x), b_n(x) >_{\mathcal{H}_x} \end{aligned} \tag{3.22}$$

Setting $m = n = 1$ (3.22) turns into

$$\int_B d\mu'(x) ||b'_1(x)||^2_{\mathcal{H}'_x} = \int_B d\mu(x) |f(x)|^2 \tag{3.23}$$

Since B is arbitrary and $|f|^2$ positive $\mu-$a.e. while $||b'_1(x)||_{\mathcal{H}'_x}$ could vanish on sets of finite $\mu'-$measure we conclude that μ is absolutely continuous with respect to μ'. Interchanging the roles of (μ, N) and (μ', N') we see that actually $[\mu] = [\mu']$.

Set $\rho = d\mu/d\mu'$ and $m = n$ in (3.22) then

$$\int_B d\mu'(x) ||b'_m(x)||^2_{\mathcal{H}'_x} = \int_B d\mu'(x) \rho(x) |f(x)|^2 \theta(N(x) - m) \tag{3.24}$$

Since B is arbitrary it follows that $||b'_m(x)||_{\mathcal{H}'_x} = \sqrt{\rho(x)} |f(x)| \theta(N(x) - m)$ $\mu-$a.e. while for $m \neq n$ the same argument leads to $< b'_m(x), b'_n(x) >= 0$ $\mu-$a.e. Thus $< b'_m(x), b'_n(x) >= 0$ for $m \neq n$ up to a zero measure set $\mathcal{N}_{m,n}$ and $< b'_m(x), b'_m(x) >= 0$ up to a zero measure set $\mathcal{N}_{m,m}$ if $N(x) \geq m$. Let $\mathcal{N} := \cup_{m,n} \mathcal{N}_{m,n}$ (countable collection). Since μ is $\sigma-$additive we find $\mu(\mathcal{N}) = 0$ so that our conclusions hold on a common set X_0 of full $\mu-$measure on which in particular $\rho > 0$. It follows that $N'(x) \geq N(x)$ $\mu-$a.e. and interchanging (N, μ) and $(N.\mu')$ shows that $N = N'$ $\mu-$a.e.

On X_0 set $U(x) b_m(x) := \sqrt{\rho(x)}^{-1} b'_m(x)$ which defines a measurable isometry. Let $(V_1 \psi)(x) := \sqrt{\rho(x)} U(x) \psi(x)$ then by definition of b'_m and the intertwining property

$$(V_1 F(B) b_m)(x) = \sqrt{\rho(x)} U(x) \chi_B(x) b_m(x) = \chi_B(x) b'_m(x) = (F'(B) V b_m)(x) = (V F(B) b_m)(x) \tag{3.25}$$

Since the $F(B) b_m$ lie dense, $V = V_1$, so V admits the presentation (3.21).
□

The theorem reveals that direct integral Hilbert spaces on measurable spaces $(X, \mathcal{B})$ and their canonical p.v.m.'s are uniquely characterized, up to unitary equivalence, by the type $[\mu]$ of the underlying measure μ and the multiplicity function N.

The next theorem characterizes all bounded operators that commute with the canonical p.v.m. of a direct integral Hilbert space.

Theorem 3.3.
Let $\mathcal{H}^{\oplus}_{\mu,N}$ be a direct integral Hilbert space.
i)
Suppose that T is a measurable, fibre preserving, bounded – operator – valued function on $\mathcal{H}^{\oplus}_{\mu,N}$ such that $\mu - \sup ||T(x)||_{\mathcal{H}_x}|| < \infty$ (i.e. the operator norm in the fibres is uniformly bounded up to sets of measure zero). Then T defined by $(T\psi)(x) = T(x)\psi(x)$ is a bounded operator on $\mathcal{H}^{\oplus}_{\mu,N}$ which commutes with the canonical p.v.m.
ii)
If T is a bounded operator on $\mathcal{H}^{\oplus}_{\mu,N}$ which commutes with the canonical p.v.m. then T is a fibre preserving, $\mu-$a.e. uniformly bounded operator. Moreover, the operator norm coincides with the uniform fibre norm.

Proof of theorem 3.3:
i)
An elementary calculation shows that

$$||T||_{\mathcal{H}^{\oplus}_{\mu,N}} \leq \mu - \sup_{x \in X} ||T(x)||_{\mathcal{H}_x} \tag{3.26}$$

so T is bounded. That $[F(B), T] = 0$ for all measurable B is trivial.
ii)

Let $X_n = \{x \in X;\ N(x) = n\ \mu-\text{a.e.}\} = N^{-1}(n)$. These mutually disjoint sets are measurable due to measurability of N. If we set $\mathcal{H}^{\oplus}_{\mu,n} := \int_{X_n} d\mu(x)\ \mathcal{H}_x$ then clearly

$$\mathcal{H}^{\oplus}_{\mu,N} = \oplus_{n=1}^{M} \mathcal{H}^{\oplus}_{\mu,n} \tag{3.27}$$

where $M = \mu - \sup_{x\in X} N(x)$ is the maximal multiplicity.

Let $x \in X_m$ and $\psi \in \mathcal{H}^{\oplus}_{\mu,n}$ then by assumtion that $[F(B), T] = 0$

$$(T\psi)(x) = (TF(X_n)\psi)(x) = (F(X_n)T\psi)(x) = \chi_{X_n}(x)(T\psi)(x) = \delta_{mn}(T\psi)(x) \tag{3.28}$$

Thus T preserves all the $\mathcal{H}^{\oplus}_{\mu,n}$ and we may reduce the analysis to $x \in X_n$ so that $N(x) = n = const.$ and we may set $\mathcal{H}_x = \mathcal{H}_n = const.$ on X_n.

Let $\mathcal{B} \ni B \subset X_n$ then for $\psi \in \mathcal{H}^{\oplus}_{\mu,n}$ due to boundedness

$$\begin{aligned} &\int_B d\mu(x)\ ||(T\psi)(x)||^2_{\mathcal{H}_n} = ||F(B)T\psi||^2_{\mathcal{H}^{\oplus}_{\mu,N}} = ||TF(B)\psi||^2_{\mathcal{H}^{\oplus}_{\mu,N}} \\ \leq\ & ||T||^2_{\mathcal{H}^{\oplus}_{\mu,N}}\ ||F(B)\psi||^2_{\mathcal{H}^{\oplus}_{\mu,N}} = ||T||^2_{\mathcal{H}^{\oplus}_{\mu,N}} \int_B d\mu(x)\ ||\psi(x)||^2_{\mathcal{H}_n} \end{aligned} \tag{3.29}$$

Since B is arbitrary we conclude

$$||(T\psi)(x)||_{\mathcal{H}_n} \leq ||T||_{\mathcal{H}^{\oplus}_{\mu,N}}\ ||\psi(x)||_{\mathcal{H}_n} \tag{3.30}$$

$\mu-$a.e. Since ψ could be supported on arbitrary measurable sets we conclude that $(T\psi)(x) \in \mathcal{H}_x$ must be fibre preserving. We may therefore define $T(x)\psi(x) := (T\psi)(x)$. Then (3.30) automatically gives

$$||T(x)||_{\mathcal{H}_x} \leq ||T||_{\mathcal{H}^{\oplus}_{\mu,N}} \tag{3.31}$$

$\mu-$a.e. and $T(x)$ is uniformly bounded. Together with (3.26) we obtain

$$||T||_{\mathcal{H}^{\oplus}_{\mu,N}} = \mu - \sup_{x\in X} ||T(x)||_{\mathcal{H}_x} \tag{3.32}$$

□

We see that bounded operators commuting with the canonical p.v.m. are precisely the fibre preserving bounded operator valued functions on the direct integral. Such bounded operators are called decomposable. Since for fibre preserving bounded operators no domain questions arise, the operations of scalar multiplication, addition, multiplication and taking adjoints can be done fibre − wise and we see that bounded, self − adjoint, unitary, normal and projection operators in the commutant of the canonical p.v.m. are precisely the fibre preserving operators which are self − adjoint, unitary, normal and projection operators in every fibre $\mu-$a.e. Finally, if T is a bounded operator which commutes with every decomposable operator then it must be itself decomposble because all the $F(B)$ are decomposble. Therefore its fibre component must commute with every bounded operator on $\mathcal{H}_x$ and thus $T(x) = q(x)1_{\mathcal{H}_x}$ is multiplication operator by a scalars on each fibre.

3.3 Direct Integral Representation of Projection Valued Measures

Let $\mathcal{H}$ be a separable Hilbert space and E a p.v.m. on a measurable space $(X, \mathcal{B})$. Choose a unit vector $\Omega_1 \in \mathcal{H}$ and let $\mathcal{H}_{\Omega_1}$ be the closure of the vector space of vectors of the form $[\sum_{k=1}^{K} z_k E(B_k)]\Omega_1$ where $z_k \in \mathbb{C},\ K < \infty,\ B_k \in \mathcal{B}$. If $\mathcal{H}_{\Omega_1} \neq \mathcal{H}$ choose $\Omega_2 \in \mathcal{H}^{\perp}_{\Omega_1}$ and construct $\mathcal{H}_{\Omega_2}$. Clearly $\mathcal{H}_{\Omega_1} \perp \mathcal{H}_{\Omega_2}$. Suppose that mutually orthogonal $\mathcal{H}_{\Omega_1}, .., \mathcal{H}_{\Omega_n}$ have already been constructed but that $\mathcal{H}_{\Omega_1} \oplus .. \oplus \mathcal{H}_{\Omega_n} \neq \mathcal{H}$. Then choose Ω_{n+1} in the orthogonal complement and construct $\mathcal{H}_{\Omega_{n+1}}$ which is orthogonal to all the other spaces. The procedure must come to an end after at most a countable number M of steps because the Ω_n form a countable orthogonal system and $\mathcal{H}$ has a countable basis.

We consider the associated spectral measures $\mu_{\Omega_n}(B) =< \Omega_n, E(B)\Omega_n >_{\mathcal{H}}$ and the total measure

$$\mu_\Omega(B) := \sum_{n=1}^{M} c_n \mu_{\Omega_n}(B) \tag{3.33}$$

where $\Omega := \sum_{n=1}^{M} c_n^{1/2}\Omega_n$ and $c_n > 0,\ \sum_{n=1}^{M} c_n = 1$ are any positive constants. It is often convenient to choose $c_n = 2^{-n}/\sum_{n=1}^{M} 2^{-n}$.

Notice that $\mu_\Omega(B) =< \Omega, E(B)\Omega >$ and that all measures are probability measures. The measure μ_Ω has the following maximality feature:

Lemma 3.1.
For any $\Psi \in \mathcal{H}$ the associated spectral measure $\mu_\Psi(B) =< \Psi, E(B)\Psi >$ is absolutely continuous with respect to μ_Ω.

Proof of lemma 3.1:
A dense set of vectors in $\mathcal{H}$ is of the form $\Psi = \sum_n \Psi_n$ with $\Psi_n = \sum_{k=1}^{\infty} z_k^n E(B_k^n)\Omega_n$ and $z_k^n = 0$ for all but finitely many k. The Hilbert space $\mathcal{H}_{\Omega_n}$ is unitarily equivalent to $L_2(X, d\mu_{\Omega_n})$ via $\Psi_n \mapsto \sum_{k=1}^{\infty} z_k^n \chi_{B_k^n}$. It follows that

$$\mu_{\Psi_n}(B) = \int_B d\mu_{\Omega_n}(x)\ |\Psi_n(x)|^2 \tag{3.34}$$

hence μ_{Ψ_n} is absolutely continuous with respect to μ_{Ω_n}. Since every μ_{Ω_n} is absolutely continuous with respect to μ_Ω, the claim follows.
□
Thus, while the choice of Ω_n, c_n and thus Ω is not unique, the type of μ_Ω is unique.

Definition 3.4.
Let E be a p.v.m.. The type $[E]$ of E is given by $[\mu_\Omega]$ where Ω is any vector satisfying the maximality criterion of lemma 3.1 (which was shown to exist).

Notice that this would not hold if $\mathcal{H}$ is not separable. In the non – separable case it may take an uncountable collection of Ω_n in order to decompose $\mathcal{H}$ as above. Then $\mu = \sum_n c_n \mu_{\Omega_n}$ may still be formed but in order to be well – defined (not identical to the measurue which is infinite a.e.) we generically would need to set all but a countable number of the c_n equal to zero. But then for $c_n = 0$ we do not have that μ_{Ω_n} is absolutely continuous with respect to μ_Ω. Hence separability is essential in order that the type $[E]$ be well – defined.

Consider any collection Ω_n such that Ω leads to maximal type $[E]$. Since all the measures μ_{Ω_n} and μ_Ω are actually finite measures, the Radon – Nikodym derivatives $\rho_n(x) := d\mu_{\Omega_n}(x)/d\mu_\Omega(x)$ exist and are non – negative $L_1(X, d\mu)$ functions. As such they are only defined $\mu-$a.e. but let us pick any representative. Let $S_n := \{x \in X;\ \rho_n(x) > 0\}$ be the support of these functions. These sets are measurable because the functions ρ_n are measurable (namely S_n is the support of μ_{Ω_n} which is $\mu_{\Omega_n}-$measurable and thus μ_Ω measurable). Given $x \in X$ we define $N_E(x) = n$ if there are precisely n integers $k_1(x) < .. < k_n(x)$ such that $x \in S_k,\ k \in \{k_1, .., k_n\}$. The function $N_E :\ X \to \mathbb{N}$ is measurable because $\mathbb{N}$ carries the discrete topology (all sets are open, in particular the one point sets $\{n\}$) and

$$X_n := N_E^{-1}(\{n\}) = X'_n - X'_{n+1} \text{ where } X'_n := \cup_{k_1<..<k_n} \cap_{l=1}^{n} S_{k_l} \tag{3.35}$$

is the set of points which are in at least n of the supports of the ρ_n (notice that $X'_{n+1} \subset X'_n$). Thus, X_n is the difference of a countable union of measurable sets, hence it is measurable for

every $n \in \mathbb{N}$, thus N_E is a measurable function.
Furthermore, the functions $k_l(x),\ l = 1,..,N(x)$ are measurable. To see this, consider the function $K:\ X \mapsto P(\mathbb{N});\ x \mapsto \{k_1(x),..,k_{N(x)}(x)\}$ where $P(S)$ denotes the power set (set of all subsets of) the set S. We have $K^{-1}(\{k_1,..,k_N\}) = S_{k_1} \cap .. \cap S_{k_N} - X'_{N+1} \subset X_N$ so M is clearly measurable because $P(\mathbb{N})$ carries the discrete topology. Next let $n:\ P(\mathbb{N}) \to \mathbb{N} \cup \{0\};\ \{k_1,..k_N\} \mapsto k_n$ if $n \le N$ with the convention that $k_1 < ..k_N$ and otherwise $\{k_1,..k_N\} \mapsto 0$. The function n is continuous because it maps between discrete topologies. Now $k_n(x) = (n \circ K)(x)$ is the composition of a measurable with a continuous function, hence it is measurable.

As an example choose $\mathcal{H} = \mathcal{H}_{\mu,N}$ and $E = F$ the canonical p.v.m. Let us show that $[F] = [\mu]$ and $N_F = N$. To see this, recall that the functions $e_{B,n}$ with $e_{B,n}(x) = f(x)\chi_B(x)e_n(x)$ where $f \in L_2(X,d\mu),\ f \ne 0\ \mu-$a.e. and $< e_m(x), e_n(x) >_{\mathcal{H}_x} = \delta_{m,n}\theta(N(x)-n)$ are dense in $\mathcal{H}^{\oplus}_{\mu,N}$. We may therefore choose $\Omega_n = fe_n$. We calculate

$$d\mu_{\Omega_n}(x)/d\mu(x) = |f(x)|^2||e_n(x)||^2_{\mathcal{H}_x} = |f(x)|^2\theta(N(x)-n) \tag{3.36}$$

Therefore, choosing not to normalize the $||\Omega_n|| \le 1$

$$d\mu_{\Omega}(x) \propto \sum_n 2^{-n} d\mu_{\Omega_n}(x) = |f(x)|^2 d\mu(x) \sum_{n=1}^{N(x)} 2^{-n} = [1 - 2^{-N(x)}]|f(x)|^2 d\mu(x) \tag{3.37}$$

Hence, $d\mu_\Omega$ and $|f|^2 d\mu$ are equivalent measures because $N(x) \ge 1\ \mu-$a.e. by convention (otherwise restrict X). This reveals $[F] = [\mu]$. It follows that $S_n = \{x \in X; \theta(N(x)-n) > 0\}$ and $N_F(x) = n$ if x lies precisely in n of the S_k, say $k_1 < .. < k_n$ which is precisely the case for $N(x) = k_n$. However, if $k_n > n$ then this is the case for all $k = 1,..,k_n$. Therefore $k_l = l,\ l = 1,..,n$ so that $N(x) = n$. Thus $N_F(x) = N(x)\ \mu-$a.e.

The worry is now that the function N_E depends not only on E but also on the choice of the Ω_n. This is excluded by the following theorem which proves more: N_E, as a measurable function, depends only on E and, moreover, any p.v.m. E is completely characterized by the type $[E]$ and the muliplicity function N_E up to unitary equivalence.

Theorem 3.4.
Let E be a p.v.m. on a Hilbert space $\mathcal{H}$ and $\mathcal{H}_{\mu,N}$ a direct integral Hilbert space together with its natural p.v.m. F. Of course, both E and μ are based on the same measurable space $(X,\mathcal{B})$.
i)
If $[E] = [\mu]$ and $N_E(x) = N(x)\ \mu-$a.e. then there is a unitary operator $V:\ \mathcal{H} \to \mathcal{H}_{\mu,N}$ such that $VE(B) = F(B)V$ for all measurable $B \in \mathcal{B}$.
ii)
a) N_E only depends on E and not on the concrete choice of the $\Omega_n,\ c_n$ that lead to N_E as above.
b) The spectral type $[E]$ and the multiplicity function N_E are unitary invariants of E.
iii)
The data $([E],N)$ determine E up to unitary equivalence.

Proof of theorem 3.4:
Without loss of generality we may assume that the measure μ underlying $\mathcal{H}_{\mu,N}$ is finite because by using an $f \in L_2(X,d\mu)$ with $f \ne 0\ \mu-$a.e. we can switch to the finite measure $d\mu' = |f|^2 d\mu$ which gives rise to $[\mu'] = [\mu]$ and $N = N'\ \mu-$a.e., hence by theorem 3.2 the corresponding direct integral Hilbert spaces and the canonical p.v.m. are unitarily equivalent.
i)
By assumption $[E] = [\mu]$ and $N_E(x) = N(x)\ \mu-$a.e. Given $x \in X$ let $M(x) = \{n_1(x) < .. < n_{N(x)}\}$ be the set of indices n such that $x \in S_{\Omega_n}$. Any vector $\Psi \in \mathcal{H}$ can be written in the form

$\Psi = \sum_{n=1}^M \Psi_n(E)\Omega_n$ for measurable Ψ_n and has the norm

$$
\begin{aligned}
||\Psi||^2_{\mathcal{H}} &= \sum_{n=1}^M \int_X d\mu_\Omega(x)\ \rho_n(x)|\Psi_n(x)|^2 \\
&= \int_X d\mu_\Omega(x)\ \sum_{n=1}^M \rho_n(x)|\Psi_n(x)|^2 \\
&= \sum_{m=1}^M \int_{X_m} d\mu_\Omega(x)\ \sum_{n=1}^M \rho_n(x)|\Psi_n(x)|^2 \\
&= \sum_{m=1}^\infty \int_{X_m} d\mu_\Omega(x)\ \sum_{n\in M(x)} \rho_n(x)|\Psi_n(x)|^2 \\
&= \sum_{m=1}^\infty \int_{X_m} d\mu_\Omega(x)\ \sum_{n=1}^m \rho_{k_n(x)}(x)|\Psi_{k_n(x)}(x)|^2
\end{aligned} \tag{3.38}
$$

In the second step we have used the fact that $L_2(X, d\mu; l_2^M) \cong l_2^M(L_2(X, d\mu))$, i.e. the Hilbert space of square integrable vector valued functions with values in the Hilbert space l_2^M of square summable sequences (with label set $n = 1, .., M \le \infty$) is isometrically isomorphic to the Hilbert space of square summable sequences of square integrable functions. This allowed us to interchange the sum and the integral (alternatively, use the Lebesgue dominated convergence theorem). In the third step we have decomposed X into the $X_m = N^{-1}(m)$, recall (3.35), and then could restrict the sum over n to the $k_1(x), .., k_m(x)$.

For $x \in X_m$ consider an orthonormal basis $e_n^{(m)},\ n = 1, .., m$ of the Hilbert space $\mathbb{C}^m$ equipped with the standard inner product. We extend this to vector valued functions $e_n(x)$ where

$$
e_n(x) = \sum_{m=1}^\infty \chi_{X_m}(x)\theta(N(x) - n)e_n^{(m)} \tag{3.39}
$$

and set $\mathcal{H}_x = \mathbb{C}^m$ if $x \in X_m$. Let

$$
\psi(x) := \sum_{n=1}^{N(x)} \sqrt{\rho_{k_n(x)}(x)}\Psi_{k_n(x)}(x)e_n(x) \tag{3.40}
$$

Then (3.38) shows that the map $V_1 :\ \mathcal{H} \to \mathcal{H}_{\mu_\Omega,N};\ \Psi \mapsto \psi$ is an isometry.

To show that it is unitary, we must show that its image is dense. Let $B \in \mathcal{B}$ and fix $n_0 \in \mathbb{N}$. Consider

$$
\Psi_n^{B,n_0}(x) := \chi_B(x)\theta(N(x) - n_0)\delta_{n,k_{n_0}(x)}/\sqrt{\rho_{k_{n_0}(x)}(x)} \tag{3.41}
$$

The function (3.41) is measurable: χ_B is obviously measurable, $x \mapsto \theta(N(x) - n_0)$ is the composition of the measurable map N and the continuous map $k \mapsto \theta(k - n_0)$ on $\mathbb{N}$ (discrete topology), $x \mapsto \delta_{n,k_{n_0}(x)}$ is the composition of the measurable map k_{n_0} (see above) and the continuous map $k \mapsto \delta_{n,k}$ on $\mathbb{N}$, $\rho_{k_{n_0}(x)}(x) = \sum_{m=1}^M \delta_{m,k_{n_0}(x)}\rho_m(x)$ and now we just need to use the fact that taking sums and products are continuous maps $\mathbb{R} \times \mathbb{R} \to \mathbb{R}$ (product topology) and taking square roots is a continuous map on $\mathbb{R}_+$ to see that (3.41) is measurable. It is easy to check that $V_1\Psi^{B,n_0} = F(B)e_{n_0}$. Since the functions $F(B)e_n$ are dense in $\mathcal{H}_{\mu_\Omega,N}$ it follows that V_1 is unitary. Moreover, it is trivial to see that $V_1E(B) = F(B)V_1$.

Now consider the given direct integral Hilbert space $\mathcal{H}_{\mu,N}$. By assumption we have $[\mu_\Omega] = [\mu]$. Hence, choosing $U(x) = \sqrt{d\mu_\Omega/d\mu}(x)\ 1_{\mathcal{H}_x}$ in theorem 3.2 i) as the measurable unitarity we conclude that there exists a unitary operator $V_2 :\ \mathcal{H}_{\mu_\Omega,N} \to \mathcal{H}_{\mu,N}$ satisfying $V_2F(B) = F'(B)V_2$

where we have also denoted by F the canonical p.v.m. on $\mathcal{H}_{\mu,N}$ therby slightly abusing the notation. Thus, $V = V_2 V_1 : \mathcal{H} \to \mathcal{H}_{\mu,N}$ is the searched for unitarity satisfying $VE(B) = F'(B)V$ for all $B \in \mathcal{B}$.
ii)
a) Consider two sets of vectors and constants $(\Omega_n,\ c_n)_{n=1}^M,\ (\Omega'_n,\ c'_n)_{n=1}^{M'}$ leading to two multiplicity functions N_E, N'_E but of course to equivalent measures $\mu_E,\ \mu'_E$ of type $[E] = [\mu_E] = [\mu'_E]$. Using theorem 3.4 i) we find unitary operators $V :\ \mathcal{H} \to \mathcal{H}_{\mu_E,N_E}$ and $V' :\ \mathcal{H} \to \mathcal{H}_{\mu'_E,N'_E}$ satisfying $VE(B) = F(B)V$ and $V'E(B) = F'(B)V'$ for all $B \in \mathcal{B}$ respectively. It follows that $\tilde{V} = V'V^{-1} :\ \mathcal{H}_{\mu_E,N_E} \to \mathcal{H}_{\mu_E,N_E}$ is a unitary operator satisfying $\tilde{V}F(B) = F'(B)\tilde{V}$. Hence, by theorem 3.2 ii) we find that $N_E(x) = N'_E(x)\ \mu_E-$a.e.
b)
Suppose we are given two p.v.m.'s E_j on Hilbert spaces $\mathcal{H}_j,\ j = 1,2$ which are unitarily equivalent, that is, there is a unitarity $V :\ \mathcal{H}_1 \to \mathcal{H}_2$ satisfying $VE_1(B) = E_2(B)V$ for all $B \in \mathcal{B}$. By theorem 3.4 i) we find unitary maps $V_j :\ \mathcal{H}_j \to \mathcal{H}_{\mu_{E_j},N_{E_j}}$ satisfying $V_j E_j(B) = F_j(B)V_j$. Thus the unitary operator $\tilde{V} := V_2 V V_1^{-1} :\ \mathcal{H}_{\mu_{E_1},N_{E_1}} \to \mathcal{H}_{\mu_{E_2},N_{E_2}}$ satisfies $\tilde{V}F_1(B) = F_2(B)\tilde{V}$. Thus, by theorem 3.2 ii) we have $[\mu_{E_1}] = [\mu_{E_2}]$ and $N_{E_1} = N_{E_2}\ \mu_{E_1}-$a.e.
iii)
Given $([E], N)$ choose representatives E_1, E_2 with $[E_j] = [E]$ and $N_{E_j} = N$ a.e. The corresponding unitarily equivalent models F_j on $\mathcal{H}_{\mu_{E_j},N_{E_j}}$ satisfy $[\mu_{E_1}] = [\mu_{E_2}],\ N_{E_1} = N_{E_2}$ a.e. by assumption, hence by theorem 3.2 i) the models are unitarily equivalent and so are E_1, E_2.
□

Remarks:
1.
Given a self − adjoint operator a represented on a Hilbert space $\mathcal{H}$ it is often easier to choose the Ω_n and to determine the Hilbert spaces $\mathcal{H}_{\Omega_n}$ as follows: $\mathcal{H}$ has a dense set of $C^\infty-$vectors Ω for a, that is, vectors which are in the domain of a^n for all $n = 0, 1, 2, ..$, see e.g. [22]. To see that the closure of the span of the $a^n\Omega$ coincides with the span of the $E(B)\Omega,\ B \in \mathcal{B}$ we notice that every measurable function on $\mathbb{R}$ can be approximated $\mu-$a.e. to arbitrary precision by smooth functions of rapid decrease which in turn have convergent Taylor expansions. The same is true for the linear span of the χ_B. Thus, given that mutually orthogonal $\mathcal{H}_{\Omega_n}$ with Ω_n $C^\infty-$vectors for a have already been constructed, we restrict a to the orthogonal complement of those spaces and simply choose a $C^\infty-$vector in that space.
2.
It is now evident why the function $N(x)$ is called multiplicity function: In each fibre $\mathcal{H}_x$ the operator a acts by multiplication by x as follows from the spectral theorem, we also formally derive this in section 3.5. Since $N(x) = \dim(\mathcal{H}_x)$ this means that the (generalized) eigenvalue x has multiplicity $N(x)$. Furthermore, on $\mathcal{H}_\mu^N := \int_{X_N}^\oplus d\mu(x)\mathcal{H}_x$ the operator a has constant multiplicity N and we have $\mathcal{H} \cong \oplus_{N=1}^M \mathcal{H}_\mu^N$. It follows that a is multiplicity free ($N \equiv 1$) if and only if there is a cyclic vector for a.

3.4 Direct Integral Representations and Spectral Types

We will need this section in order to properly deal with constraint quantization.

Given the measures $\mu_n := \mu_{\Omega_n}, \mu := \mu_\Omega = \sum_n c_n \mu_n$ denote by P_n, P respectively their pure point sets, that is, the set of points $p \in X$ such that $\mu_n(\{p\}) > 0$ and $\mu(\{p\}) > 0$ respectively. Obviously $P = \cup_n P_n$. Since the measures μ_n, μ are probability measures the sets P_n, P must have countable cardinality (this is not necessarily the case when $\mathcal{H}$ is not separable in which case the label set of the n may have uncountable cardinality). We define for $B \in \mathcal{B}$ the pure point measures

$$\mu_n^{pp}(B) := \mu_n(P_n \cap B), \quad \mu^{pp}(B) := \mu(P \cap B) \tag{3.42}$$

Then $\mu_n^c := \mu_n - \mu_n^{pp}$, $\mu^c := \mu - \mu^{pp}$ are positive measures with the property that their sets of pure points is empty because e.g. $\mu^c(B) = \mu(B - P)$. They are called continuous for that reason. Thus the measures allow for a unique decomposition, e.g. $\mu = \mu^{pp} + \mu^c$ into their pure point and continuous part respectively. In the case of interest, $X = \sigma(a)$ is a subset of $\mathbb{R}$ which carries the natural Borel $\sigma-$algebra $\mathcal{B}_{Borel}$. The measurable space $(\mathbb{R}, \mathcal{B}_{Borel})$ carries the natural $\sigma-$finite Lebesgue measure $d\mu_L(x) = dx$ and the Lebesgue decomposition theorem tells us that every measure μ on $(\mathbb{R}, \mathcal{B}_{Borel})$ can be uniquely decomposed into $\mu = \mu^{ac} + \mu^s$ where μ^{ac}, μ^s respectively is absolutely continuous and singular with respect to μ_L respectively (that is, $\mu_L(B) = 0$ implies $\mu^{ac}(B) = 0$ while there exists a measurable set S such that $\mu^s(S) = 0$ and $\mu_L(\mathbb{R} - S) = 0$). Since μ_L has no pure points we may apply the above observation to split μ^s further as $\mu^{pp} + \mu^{cs}$ where μ^{cs} is the continuous singular part of μ.

Coming back to our concrete direct integral construction $\mu = \sum_n c_n \mu_n$ with $c_n > 0$, $\sum_n c_n = 1$ we may decompose each of the μ_n and μ independently into the parts $* = pp, ac, cs$. We derive two simple results:

Lemma 3.2.
We always have $\mu^* = \sum_n c_n \mu_n^*$ for $* = pp, ac, cs$.

Proof of lemma 3.2:
By definition, using $P_n \subset P$

$$\mu^{pp}(B) = \mu(B \cap P) = \sum_n c_n \mu_n(B \cap P) = \sum_n c_n[\mu_n(B \cap P_n) + \mu_n(B \cap (P - P_n))] = \sum_n c_n \mu_n^{pp}(B) \tag{3.43}$$

because $B \cap (P - P_n)$ is a discrete set containing no pure points of μ_n. It follows that $\mu^c = \mu^{ac} + \mu^{cs} = \sum_n c_n[\mu_n^{ac} + \mu_n^{cs}] = \sum_n c_n \mu_n^c$. Next, let S_n, $n = 1,..,M$ be such that $\mu_n^{cs}(S_n) = 0$ and $\mu_L(\mathbb{R} - S_n) = 0$ and let S_0 be such that $\mu^{cs}(S_0) = 0$ and $\mu_L(\mathbb{R} - S_0) = 0$. Define $S = \cap_{n=0}^M S_n$. Then $\mu_L(\mathbb{R} - S) = \mu_L(\cup_{n=0}^M (\mathbb{R} - S_n)) \leq \sum_{n=0}^M \mu_L(\mathbb{R} - S_n) = 0$ by $\sigma-$additivity. This implies $\mu^{ac}(\mathbb{R} - S) = \mu_n^{ac}(\mathbb{R} - S) = 0$ for all n due to absolute continuity. Moreover, $\mu^{cs}(S) = \mu_n^{cs}(S) = 0$ for all $n = 1, 2, ..$ since $S \subset S_n$ for all $n = 0, 1, 2, ...$ Thus, if $B \subset \mathbb{R} - S$ then $\mu^c(B) = \mu^{cs}(B) = \sum_{n=1}^M c_n \mu_n^{cs}(B)$ and if $B \subset S$ then $\mu^{cs}(B) = \sum_{n=1}^\infty c_n \mu_n^{cs}(B) = 0$ anyway. Thus $\mu^{cs}(B) = \sum_{n=1}^\infty \mu_n^{cs}(B)$ for all B. It follows that $\mu^{ac}(B) = \sum_{n=1}^\infty \mu_n^{ac}(B)$ for all B as well. $\square$

Lemma 3.3.
Given two unitarily equivalent direct integral representations $\mathcal{H}_{\mu,N}$, $\mathcal{H}_{\mu',N'}$ of a so that necessarily $[\mu] = [\mu']$ and $N = N'$ $\mu-$a.e. we always have $[\mu^*] = [\mu'^*]$ for $* = pp, ac, cs$.

Proof of lemma 3.3:
Let P, P' be the pure points of μ, μ' respectively. Then $\mu(P' - P) = 0$ implies $\mu'(P' - P) = 0$ by absolute continuity, hence $P' \subset P$. Likewise, $\mu'(P - P') = 0$ implies $\mu(P - P') = 0$ by absolute continuity, hence $P \subset P'$. Thus $P = P'$ and so $[\mu^{pp}] = [\mu'^{pp}]$.

Let S, S' be such that $\mu_L(\mathbb{R} - S) = \mu_L(\mathbb{R} - S') = \mu^{cs}(S) = \mu'^{cs}(S') = 0$. Then also $\mu_L(\mathbb{R} - \tilde{S}) = \mu^{cs}(\tilde{S}) = \mu'^{cs}(\tilde{S}) = 0$ where $\tilde{S} = S \cap S'$.

Suppose $B \subset \mathbb{R} - (\tilde{S} \cup P)$. Then $\mu(B) = \mu^{cs}(B) = 0$ if and only if $\mu'(B) = \mu'^{cs}(B) = 0$ by absolute continuity. If $B \subset \tilde{S} \cup P$ then anyway $\mu^{cs}(B) = \mu'^{cs}(B) = 0$, hence $\mu^{cs}(B) = 0 \Leftrightarrow \mu'^{cs}(B) = 0$ for all $B \in \mathcal{B}$, that is, $[\mu^{cs}] = [\mu'^{cs}]$.

Suppose $B \subset \tilde{S} - P$. Then $\mu(B) = \mu^{ac}(B) = 0$ if and only if $\mu'(B) = \mu'^{ac}(B) = 0$ by absolute continuity. If $B \subset \mathbb{R} - (\tilde{S} - P) \subset (\mathbb{R} - \tilde{S}) \cup P$ then anyway $\mu^{ac}(B) = \mu'^{ac}(B) = 0$,

hence $\mu^{ac}(B)=0 \Leftrightarrow \mu'^{ac}(B)=0$ for all $B\in\mathcal{B}$, that is, $[\mu^{ac}]=[\mu'^{ac}]$.
□

Lemma 3.4.
Let $\mathcal{H}^*=\{\Psi\in\mathcal{H};\ \mu_\Psi=\mu_\Psi^*\}$ where $*\in\{pp,ac,cs\}$ and $\mu_\Psi(.)=<\Psi,E(.)\Psi>$ denotes the spectral measure of Ψ. Then $\mathcal{H}=\mathcal{H}^{pp}\oplus\mathcal{H}^{ac}\oplus\mathcal{H}^{cs}$. Moreover, each space $\mathcal{H}^*$ is invariant under the $E(B),\ B\in\mathcal{B}$.

Proof of lemma 3.4:
Let Ω_n be a cyclic system such that the $\mathcal{H}_n=\overline{\mathrm{span}\{E(B)\Omega_n;\ B\in\mathcal{B}\}}$ are mutually orthogonal and $\mathcal{H}=\oplus_n\mathcal{H}_n$. Let μ_n be the spectral measure of Ω_n and let the Ω_n be normalized such that $\mu=\sum_n\mu_n$ is a probability measure. Any $\Psi\in\mathcal{H}$ is of the form $\Psi=\sum_n\Psi_n(E)\Omega_n$ with measurable functions Ψ_n and thus

$$\mu_\Psi(B)=\sum_n\int_B d\mu_n\,|\Psi_n|^2=\int_B d\mu\,[\sum_n\rho_n|\Psi_n|^2] \tag{3.44}$$

i.e. $d\mu_\Psi=|\Psi|^2d\mu$ with $\rho_n=d\mu_n/d\mu$ and $|\Psi|^2:=\sum_n\rho_n|\Psi_n|^2$. Writing $\mu=\mu^{pp}+\mu^{ac}+\mu^{cs}$, let P be the pure points of μ and $\mu_L(\mathbb{R}-S)=\mu^{cs}(S)=0$. We may assume without loss of generality that $S\cap P=\emptyset$. We may write (3.44) as

$$\mu_\Psi(B)=\int_B d\mu^{pp}\,|\Psi|^2+\int_B d\mu^{ac}\,|\Psi|^2+\int_B d\mu^{cs}\,|\Psi|^2 \tag{3.45}$$

which gives rise to a map $V:\ \mathcal{H}=L_2(\mathbb{R},d\mu)\to L_2(\mathbb{R},d\mu^{pp})\oplus L_2(\mathbb{R},d\mu^{ac})\oplus L_2(\mathbb{R},d\mu^{cs})$ defined by $\Psi\mapsto(E(P)\Psi,E(S)\Psi,E(\mathbb{R}-(S\cup P))\Psi)$. Recall from the previous section that the type of the measure μ is uniquely determined and by lemma 3.3 the type of the measures μ^* is also uniquely determined, hence the sets P,S are also determined uniquely $\mu-$a.e. The map V is an isometry by (3.45) and it is invertible because $E(P)+E(S)+E(\mathbb{R}-(P\cup S))=1_\mathcal{H}$, hence it is unitary.

We must show that $\mathcal{H}^*=L_2(\mathbb{R},d\mu^*)$ for $*=pp,ac,cs$ or, in other words, that $\mathcal{H}^{pp}=E(P)\mathcal{H},\ \mathcal{H}^{ac}=E(S)\mathcal{H},\ \mathcal{H}^{cs}=E(\mathbb{R}-(S\cup P))\mathcal{H}$. Since $d\mu_{E(B)\Psi}=\chi_Bd\mu_\Psi=\chi_B|\Psi|^2d\mu$ it is clear that $d\mu_{E(B^*)\Psi}=|\Psi|^2d\mu^*$ where $B^*=P,S,[\mathbb{R}-(S\cup P)]$ for $*=pp,ac,cs$. Hence $E(B^*)\mathcal{H}\subset\mathcal{H}^*$. Conversely, since $d\mu_\Psi=|\Psi|^2d\mu$, it follows that μ_Ψ is absolutely continuous with respect to μ. Thus, by the method of proof of lemma 3.3 it follows that μ_Ψ^* is absolutely continuous with respect to μ^*. Hence, if $\Psi\in\mathcal{H}^*$, i.e. $\mu_\Psi=\mu_\Psi^*$ then $d\mu_\Psi=|\Psi|^2d\mu^*$ so $\Psi\in E(B^*)\mathcal{H}$.

That $E(B)$ preserves $\mathcal{H}^*$ is evident since $E(B)\mathcal{H}^*=E(B\cap B^*)\mathcal{H}\subset\mathcal{H}^*$.
□
Lemma 3.4 shows that any Hilbert space $\mathcal{H}$ is reducible with respect to a given p.v.m. E. The invariant subspaces $\mathcal{H}^*$ are defined only with respect to E and do not depend on the choice of a system of cyclic vectors Ω_n.

Corollary 3.1.
Let E' be a p.v.m. commuting with the p.v.m. E, that is, $[E(B),E'(B')]=0$ for all $B,B'\in\mathcal{B}$. Then the spaces $\mathcal{H}^*$ defined with respect to E are preserved by E'.

This follows trivially from $E'(B)\mathcal{H}^*=E'(B)E(B^*)\mathcal{H}=E(B^*)E'(B)\mathcal{H}\subset\mathcal{H}^*$.

The total decomposition $\mu=\mu^{pp}+\mu^{ac}+\mu^{cs}$ gives rise to a corresponding breakup of the spectrum $\sigma(a)$.

Definition 3.5.
One defines the pure point spectrum $\sigma^{pp}(a)$ *as the set of eigenvalues of* a*. This set may not be closed, however,* $\sigma^*(a) := \sigma(a_{|\mathcal{H}^*})$ *is closed.* $\sigma^c(a) := \sigma^{ac}(a) \cup \sigma^{cs}(a)$ *is called the continuous spectrum.*

The three sets may not be disjoint and only $\overline{\sigma^{pp}(a)} \cup \sigma^{ac}(a) \cup \sigma^{cs}(a) = \sigma(a)$. Roughly speaking, $\mathcal{H}^{pp}$, $\mathcal{H}^{ac}$, $\mathcal{H}^{cs}$ correspond to bound, scattering and states without physical interpretation respectively and a good deal of work in the spectral analysis of a given self – adjoint operator is focussed on proving that $\sigma^{cs}(a) = \emptyset$. A sufficient criterion is that there is a dense set D of vectors ψ such that for each $x \in \mathbb{R}$ the function $z \mapsto <\psi, R(z)\psi>$ is bounded as $z \to x$ where the bound is uniform, for given ψ, as x takes values in any open interval. Here $R(z) = (a - z)^{-1}$ is the resolvent of a. The decomposition of the spectrum made above should not be confused with the disjoint decomposition into the discrete spectrum $\sigma^d(a)$ and the essential spectrum $\sigma^e(a)$ which are defined as the subset of $\sigma(a)$ consisting of the points x such that $E((x - \epsilon, x + \epsilon))$ is a projection onto a finite or infinite subspace of $\mathcal{H}$ for any $\epsilon > 0$. It is not difficult to show that $\sigma^d(a)$ consists of the isolated eigenvalues of finite multiplicity and that $\sigma^e(a)$ contains $\sigma^c(a)$, the limit points of $\sigma^{pp}(a)$ and the eigenvalues of infinite multiplicity. In particular it contains embedded eigenvalues, i.e. those which are also part of the continuous spectrum.

3.5 Direct Integral Representations and Constraint Quantization

By the theory just reviewed in section 3.3, given a self – adjoint operator a with p.v.m. E on a Hilbert space $\mathcal{H}$ we find a unitarily equivalent representation on a direct integral Hilbert space $\mathcal{H}_{\mu,N}$ such that $VE(B) = F(B)V$ for all Borel sets $B \in \mathcal{B}$ in $X = \mathbb{R}$ and the type $[\mu]$ and the multiplicity function N are uniquely determined $\mu-$a.e. up to unitary equivalence ($V : \mathcal{H} \to \mathcal{H}_{\mu,N}$ is the corresponding unitary map). We have by the spectral theorem for $\psi \in D(a)$

$$<\psi, VaV^{-1}\psi'>_{\mathcal{H}_{\mu,N}} = \int_{\mathbb{R}} x\, d<\psi, F(x)\psi'>_{\mathcal{H}_{\mu,N}} = \int_{\mathbb{R}} x\, d\mu(x)\ <\psi(x), \psi'(x)>_{\mathcal{H}_x} \tag{3.46}$$

hence VaV^{-1} is represented as mutiplication by x on $\mathcal{H}_x$.

The kernel of a is therefore the Hilbert space $\mathcal{H}_{x=0}$ and if a is a constraint operator, we identify $\mathcal{H}_{phys} := \mathcal{H}_{x=0}$ with the physical Hilbert space. However, this prescription is too naive for the following reasons:

- Suppose that $\mu = \mu^c$ has no pure points. Then the set $\{x = 0\}$ has $\mu-$measure zero and there is no harm, as far as the unitary equivalence with the direct integral representation is concerned, in choosing $N(x = 0)$ arbitrarily, in particular setting $N(x = 0) = 0$ is allowed. In other words, in the case of only continuous spectrum the prescription is ambiguous.

- Suppose that $x = 0$ is an embedded eigenvalue, in other words, $\mu = \mu^{pp} + \mu^c$ with $\mu^{pp}(\{0\}) > 0$ and $\mu^c((-\epsilon, \epsilon)) > 0$ for all $\epsilon > 0$. By the Radon – Nikodym theorem $\mu_n(B) = \int_B \rho_n d\mu$ for non – negative $\rho_n \in L_1(\mathbb{R}, d\mu)$. Since we have defined $N(x)$ as the number of n such that $\rho_n(x) > 0$ we are interested in the value of $\rho_n(0)$. Since $x = 0$ is an eigenvalue there is at least one n, say $n = n_0$ such that $\mu_{n_0}(\{0\}) > 0$. Consequently $\mu(\{0\}) \geq c_{n_0}\mu_{n_0}(\{0\}) > 0$. It follows that $\mu_n(\{0\}) = \rho_n(0)\mu(\{0\})$. Thus, if $\mu_n^{pp} = 0$ then we conclude $\rho_n(0) = 0$ even if $\mu_n((-\epsilon, \epsilon)) = \mu_n^c((-\epsilon, \epsilon)) > 0$ for all $\epsilon > 0$. Thus we see that the presence of a single zero eigenvector would delete all generalized zero eigenvectors as one can see by comparing the situation with the one that resulted from deleting from $\mu = \sum_n c_n\mu_n$ all terms corresponding to those n such that $0 \in P_n$.

To see that it is physically wrong to suppress the continuous spectrum in case of embedded zero eigenvalues, consider the operator $C = p_1 \otimes p_2$ on $L_2(\mathbb{R}, dx_1) \otimes L_2(S^1, dx_2)$ where zero is both an eigenvalue (corresponding to the eigenfunction $e_m(x_2) := e^{imx_2},\ m \in \mathbb{Z}$ of p_2 with $m = 0$) and a generalized eigenvalue (corresponding to the generalized eigenfunction $f_k(x_1) = e^{ikx_1},\ k \in \mathbb{R}$ of p_1 with k=0). Classically $C = 0$ corresponds to a particle moving on a cylinder which is constrained to move parallel to the direction of its axis or perpendicular to it. Thus one expects that the physical Hilbert space is spanned (in the appropriate sense) by vectors of the form $f_0 \otimes \psi_2 + \psi_1 \otimes e_0$ with $\psi_j \in \mathcal{H}_j$ arbitrary which is isomorphic to $\mathcal{H}_1 \oplus \mathcal{H}_2$. However, the naive prescription would lead to the following result: Switching to the momentum representation with respect to p_1 we choose as our cyclic system of vectors the $\Omega_{0,m} := H_0 \otimes e_m,\ m \in \mathbb{Z} - \{0\}$ and $\Omega_{n,0} := H_n \otimes e_0,\ n \in \mathbb{N}$ where H_n is the orthonormal basis of $\mathcal{H}_1 = L_2(\mathbb{R}, dk)$ consisting of Hermite functions. The spectral measures are computed as

$$\begin{aligned}
\mu_{0,m}(B) &= <\Omega_{0,m}, \chi_B(C)\Omega_{0,m}>= \int_{\mathbb{R}} dk \chi_B(mk)|H_0(k)|^2 = \mu_{0,-m}(B) \\
\mu_{n,0}(B) &= <\Omega_{n,0}, \chi_B(C)\Omega_{n,0}>= \int_{\mathbb{R}} dk \chi_B(0)|H_0(k)|^2 = \chi_B(0)
\end{aligned} \tag{3.47}$$

We see that $\mu_{0,m} = \mu^{ac}_{0,m}$ and $\mu_{n,0} = \mu^{pp}_{n,0}$ The total measure can be chosen to be

$$\mu(B) = \frac{1}{3}[\sum_{m=1}^{\infty} 2^{-m}[\mu_{0,m}(B) + \mu_{0,-m}(B)] + \frac{1}{2}\sum_{n=0}^{\infty} 2^{-n}\mu_{0,n}(B)] = \frac{1}{3}[2\sum_{m=1}^{\infty} 2^{-m}\mu_{0,m}(B) + \chi_B(0)] \tag{3.48}$$

The Radon – Nikodym derivatives are

$$\begin{aligned}
\mu_{0,m}(B) &= \int_B \rho_{0,m}(x)d\mu(x) = \frac{1}{3}[2\sum_{k=1}^{\infty} 2^{-k}\int_B \rho_{0,m}(x)d\mu_{0,k}(x) + \rho_{0,m}(0)\chi_B(0)] \\
\mu_{n,0}(B) &= \int_B \rho_{n,0}(x)d\mu(x) = \frac{1}{3}[2\sum_{k=1}^{\infty} 2^{-k}\int_B \rho_{n,0}(x)d\mu_{0,k}(x) + \rho_{n,0}(0)\chi_B(0)]
\end{aligned} \tag{3.49}$$

Now choosing $B = (-\epsilon, \epsilon)$ and letting $\epsilon \to 0$ we deduce $\rho_{0,m}(0) = 0$ and $\rho_{n,0}(0) = 3 > 0$. Thus it would follow from our naive prescription that $\mathcal{H}_{phys} = \mathcal{H}_{x=0}$ is spanned by the $\Omega_{n,0}$ and thus we would miss out completely the contribution from the continuous spectrum: Quantum mechanically the particle would only be allowed to move along the axis of the cylinder while classically it may also wrap around the cylinder. This is clearly physically wrong.

Thus, the naive prescription is ambiguous in the case that zero is only in the continuous spectrum, wrong in the case that zero is an embedded eigenvalue and unambiguous only if zero is an isolated eigenvalue in which case however the whole machinery of the direct integral is not needed at all because then $\mathcal{H}_{x=0} \subset \mathcal{H}$ and the physical inner product coincides with the kinematical one.

To improve this we prescribe the following procedure:

PRESCRIPTION:

The obvious solution to the second problem is to use the orthogonal decomposition of $\mathcal{H}$ into the pieces $\mathcal{H}^{pp}$, $\mathcal{H}^{ac}$, $\mathcal{H}^{cs}$ derived in section 3.4 before applying the direct integral decomposition. As we have shown, this preliminary decomposition only depends on the type $[E]$ of E and reduces both the p.v.m. E of the self – adjoint operator a of interest as well as the p.v.m.'s E' of self – adjoint operators b which commute with a. (Notice that self – adjoint operators a, b are said to commute if and only if all their spectral projections commute. This avoids domain questions of unbounded operators.) We may therefore apply all the results of the previous section to the pieces individually.

In practice, we then have to compute the individual Radon – Nikodym derivatives

$$\rho_n^* := d\mu_n^*/d\mu^*, \;\; \mu^* = \sum_n c_n^* \mu_n^* \tag{3.50}$$

While $\rho_n^{pp}(x)$ is unambiguously defined, $\rho_n^{ac}(x), \rho_n^{cs} \geq 0$ are only defined $\mu^{ac}, \mu^{cs}-$a.e. respectively. In order to fix this ambiguity we need additional physical input. Namely, first of all we add the the requirement that a complete subalgebra[11] of bounded Dirac (weak or strong) observables be represented irreducibly as self adjoint operators on the physical Hilbert space[12].

Let us see what this implies given the structure already available: By theorem 3.4 ii), different choices of Ω_n^* and c_n^* in $\mu^* = \sum_n c_n^* \mu_n^*$ lead to unitarily equivalent direct integral representations $\mathcal{H}_{\mu^*,N^*}$ where the type $[\mu^*]$ and the μ^*-class of the function N^* are unique. By theorem 3.2 i) there exists a unitary operator mediating between these two realizations of the form $V^* : \mathcal{H}_{\mu^*,N^*} \to \mathcal{H}_{\mu^{*\prime},N^{*\prime}}$; $(V\psi)(x) = \sigma_*(x)U(x)\psi(x)$ where $U(x) : \mathcal{H}_x^{\oplus *} \to \mathcal{H}_x^{\oplus *\prime}$ is a measurable, fibre preserving unitarity and $\sigma_*^2(x) = [d\mu^*/d\mu^{*\prime}](x)$. Moreover, given a bounded, self – adjoint strong Dirac observable, A we see from theorem 3.3 ii) that it gives rise to a measurable, bounded, self – adjoint and fibre preserving operator of the form $(a\psi)(x) = a(x)\psi(x)$ in any direct integral representation. It follows that $(VaV^{-1})(x) = U(x)a(x)U^{-1}(x)$, in other words, different direct integral representations give rise to unitarily equivalent representations of strong Dirac observables in $\mu-$a.e. fibre. It follows that once we have chosen the $\rho_n^*(0)$ for one choice of Ω_n^*, c_n^* we may fix them for all others by requiring that the representations of the strong Dirac observables be exactly unitarily equivalent in the fibre $x = 0$. This means that in particular the number $N^*(0)$ of those n for which $\rho_n^*(0) > 0$ is fixed for all those choices of Ω_n^*, c_n^*. Notice that the positive constants $K_* := \sigma_*(0)$ by which the norms of $||\psi(0)||_{\mathcal{H}_0^{\oplus *}}$, $\sigma_*(0)||U(0)\psi(0)||_{\mathcal{H}_0^{\oplus *\prime}}$ of the induced physical inner products differ are irrelevant for strong Dirac observables because they drop out in the normalization of states. However, they play a role for weak Dirac observables which may mix the sectors $\mathcal{H}^*$.

Thus we may restrict attention to one choice Ω_n^*, c_n^* and are left with the choice of the representatives $\rho_n^*(0)$ for those fixed data (and the three undetermined numbers K_*, $* = \{pp, ac, cs\}$ which we should have added anyway because it is anway ad hoc to equip the physical Hilbert space with the inner product of $\mathcal{H}_0^{\oplus *}$ rather than any positive scalar multiple thereof). Fortunately, as we will see in the next section, either choice of $\rho_n^*(0)$ induces a self – adjoint representation of bounded strong Dirac observables. Moreover, since weak Dirac observables can be characterized by the fact that they preserve at least the fibre $x = 0$, they are therefore equivalent to strong Dirac observables as far as the fibre $x = 0$ is concerned and hence the self – adjointness criterion also does not fix the remaining ambiguity, although they may fix the constants K_*. However, non – trivial restrictions arise from the fact that we want a reresentation of the *algebra* of observables. This will in general prohibit to alter the $\rho_n^*(0)$ arbitrarily.

If this still does not fix the ambiguity, we must look for other criteria, such as whether the resulting physical Hilbert space admits a sufficient number of semiclassical states[13]. Fortunately, as suggested by the examples, the a priori knowledge of good physical semiclassical states or the algebra of Dirac observables seems not to be necessary but rather one can take the following practical approach: We choose a minimal set of Ω_n (which is always possible and measure theoretically unique, see below) and for such a minimal set we choose an everywhere non – negative representative, from the equivalence class of the measurable functions which equal ρ_n^{ac} $\mu^{ac}-$a.e. (and similar for ρ_n^{cs}), which is continuous at $\lambda = 0$ from the right, if such a representative exists.

[11]The corresponding classical functions should separate the points of the reduced phase space and form a closed Poisson subalgebra.

[12]We may allow quantum corrections to the classical Poisson algebra of these observables.

[13]In some sense this granted by Fell's theorem [7] once we have a representation on the physical Hilbert space of the C^* algebra of our preferred algebra of bounded Dirac observables.

If it does, then $\rho_n^c(0) := \lim_{x\to 0+} \rho_n^c(x)$ is well defined. If such a representative does not exist, a case which was not encountered so far in the examples we studied, then we must really resort to the physical criteria or, if even that does not fix the ambiguity, we must adopt an ad hoc prescription such as arbitrarily setting $\rho_n^c(0) = 0$ in this case. Further restrictions may come from the irreducibility criterion[14].

We stress that the fundamental, physical prescription is always the irreducible self – adjoint representation of a complete subalgebra of Dirac observables and a good semiclassical behaviour. Ideally one would want to show that the freedom in the more practical continuity prescription is equivalent to the freedom left in the physical prescription. In the examples encountered that happened to be the case but in general there seems to be little known about the relation between these two prescriptions. It is conceivable that in general the physical representations induced from a kinematical one are simply not uniquely determined. We will come back to this issue in section 3.7 where we compare with the amount of ambiguities in other approaches.
This ends our prescription.

As follows from the proof of the spectral theorem which uses the Riesz Markov theorem, all the measures μ_n^*, μ^* are regular, finite Borel measures on $\mathbb{R}$ and therefore we may apply Lusin's theorem [21] which says that $\rho_n^{ac},\ \rho_n^{cs}$ can be approximated, up to sets of arbitrarily small μ^{ac}, μ^{cs} measure, by a continuous function. Hence the continuity part in our prescription makes sense. In practice the continuous singular part is mostly absent and then it will be sufficient to choose a representative, defined a.e. with respect to Lebesgue measure, which is maximally continuous and non – negative. Also in practice the representatives that one computes are naturally non – negative everywhere.

The reason for why we choose the number of Ω_n to be minimal is in order to remove the following, trivial ambiguity: Suppose for instance that $\mathcal{H}$ even has a cyclic vector Ω_0. Let $I_n,\ n = 1,..,m$ be a system of mutually disjoint intervals whose union is $\mathbb{R}$ and set $\Omega_n := E(I_n)\Omega_0/||E(I_n)\Omega_0)||$. Then the Ω_n provide an orthonormal cyclic system as well whose total measure is equivalent to the spectral measure of Ω_0. We have $\mu_n(B) =< \Omega_0, E(B\cap I_n)\Omega_0 >$ hence $\rho_n = \chi_{I_n}$ for $n = 1,..,m$ while $\rho_0 = 1$. We see that we can make the Radon – Nikodym derivatives arbitrarily discontinuous at any values by an unfortunate, that is, redundant choice of Ω_n and to avoid that it is obviously necessary to minimize the number of necessary Ω_n. This number is given by the maximal multiplicity $M = \mu - \max(N)$ of the function N. That this is always possible is the content of the subsequent lemma:

Lemma 3.5.
The cyclic system Ω_n can be chosen in such a way that with $\Omega = \sum_{n=1}^M 2^{-n/2}\Omega_n/\sqrt{\sum_{n=1}^M 2^{-n}}$ we have $[\mu_\Omega] = [\mu_{\Omega_1}] \ge [\mu_{\Omega_2}] \ge ...$ where the notation $[\mu] \ge [\nu]$ means that ν' is absolutely continuous with respect to μ' for any $\mu' \in [\mu],\ \nu' \in [\nu]$. Moreover, the above types are uniquely determined.

Proof of lemma 3.5:
Let Ω_1 be any vector such that its spectral measure has maximal type, see lemma 3.1. Suppose now that we have found already mutually orthogonal $\Omega_1,..,\Omega_n$ such that the $\mathcal{H}_k := \overline{\text{span}\{E(B)\Omega_k;\ B\in\mathcal{B}\}}$ are mutually orthogonal and such that $[\mu_{\Omega_1}] \ge .. \ge [\mu_{\Omega_n}]$. Put $\mathcal{H}^{(n)} := \oplus_{k=1}^n \mathcal{H}_k$. We have $\mathcal{H}^{(k)} \subset \mathcal{H}^{(k+1)}$ for $k = 1,..,n-1$ and $\mathcal{H}^{(k+1)\perp} \subset \mathcal{H}^{(k)\perp}$ for $k = 0,..,n-1$ where we have set $\mathcal{H}^{(0)\perp} := \mathcal{H}$. Let $[E_k^\perp]$ be the maximal type of the spectral measures $\mu_\psi,\ \psi \in \mathcal{H}^{(k)\perp}$, that is $[\mu_\psi] \le E_k^\perp$ for all $\psi \in \mathcal{H}^{(k)\perp}$. Since $\mathcal{H}^{(k+1)\perp} \subset \mathcal{H}^{(k)\perp}$ we also have $[\mu_\psi] \le [E_k^\perp]$ for all $\psi \in \mathcal{H}^{(k+1)\perp}$. It follows that $[E_{k+1}^\perp] \le [E_k^\perp]$ for $k = 0,..,n-1$ where of course $[E_0^\perp] = [E]$.

[14]The set of bounded operators on a Hilbert space is always represented irreducibly. However, here the question is whether the subset of bounded operators induced from the kinematical Hilbert space is represented irreducibly.

We now make the additional induction assumption that $[\mu_{\Omega_k}]=[E_{k-1}^\perp]$ for $k=1,..,n$ which is obviously satisfied for $k=1$. Choose some $\Omega_{n+1}\in\mathcal{H}^{(n)\perp}$ of maximal type, i.e. $[\mu_{\Omega_{n+1}}]=[E_n^\perp]$. Then obviously $[E_n^\perp]=[\mu_{\Omega_{n+1}}]\le[\mu_{\Omega_n}]=[E_{n-1}^\perp]$ as claimed.

To see that the measure classes $[\mu_{\Omega_n}]$ are uniquely determined, consider the supports $S_n := \{x\in X;\ \rho_n(x):=d\mu_{\Omega_n}(x)/d\mu_{\Omega_1}(x)>0\}$. It follows that up to $\mu_{\Omega_1}-$measure zero sets we have $S_{n+1}\subset S_n$. Then $X_n:=S_n-S_{n+1}$ coincides with the set $N^{-1}(n)=\{x\in X;\rho_k(x)>0$ for precisely n of the $k\}$. Since N is uniquely determined up to sets of $\mu-$measure zero, so are the X_n and thus the $S_n:=\cup_{k=1}^n X_k$. Thus $[\mu_{\Omega_n}]$ is uniquely determined.
□

Let us see how our prescription affects the direct integral and dimension function N. We write for $\Psi\in\mathcal{H}$

$$\begin{aligned}||\Psi||^2 &= \sum_{n=1}^M\int_X d\mu_n\,|\Psi_n(x)|^2=\sum_{*=pp,ac,cs}\sum_{n=1}^M\int_X d\mu_n^*\,|\Psi_n(x)|^2\\ &= \sum_{*=pp,ac,cs}\sum_{n=1}^M\int_X d\mu^*\,\rho_n^*(x)|\Psi_n(x)|^2\\ &= \sum_{*=pp,ac,cs}\int_X d\mu^*\,[\sum_{n=1}^M|\sqrt{\rho_n^*(x)}\Psi_n(x)|^2]\end{aligned} \tag{3.51}$$

In other words, all of section 3.3 applies, the only difference being that now we have a unitary map between $\mathcal{H}^*$ and $\mathcal{H}_{\mu^*,N^*}$ where $N^*(x)$ are defined μ^*-a.e. as the number of n such that $\rho_n^*(x)>0$. If we compare (3.51) with the unitarity equivalence between $\mathcal{H}$ and $\mathcal{H}_{\mu,N}$ given as in section 3.3 by

$$||\Psi||^2=\int_X d\mu\,[\sum_{n=1}^M|\sqrt{\rho_n(x)}\Psi_n(x)|^2]=\sum_{*=pp,ac,cs}\int_X d\mu^*\,[\sum_{n=1}^M|\sqrt{\rho_n(x)}\Psi_n(x)|^2] \tag{3.52}$$

then we conclude that $\rho_n^*=\rho_n\ \mu^*-$a.e. Thus ρ_n^{pp} can differ from ρ_n everywhere except at the pure points $p\in P$ of μ while $\rho_n^{ac},\ \rho_n^{cs}$ may differ from ρ_n in particular at the pure points of μ. It is precisely this fact which allows us to repair the second problem mentioned above. Without loss of generality and in order to be specific we may choose $\rho_n^{pp}(x)=0$ for $x\notin P$ while $\rho_n^{pp}(x)=\rho_n(x)$ is fixed for $x\in P$. Thus $\rho_n^{pp}(x)=\sum_{p\in P}\delta_{x,p}\rho_n(p)$. For $\rho_n^{ac},\ \rho_n^{cs}$ we use our prescription spelled out above. Notice that it is possible and of practical advantage to split the set pf Ω_n into the respective sets of $\Omega_n^*\in\mathcal{H}^*,\ n=1,2,..,M^*$ and to define $\mu^*=\sum_n c_n^*\mu_n^*$ and $\Psi=\sum_{n,*}\Psi_n^*(a)\Omega_n^*$. We will assume to have done that in what follows.

The physical Hilbert space is then evidently the direct sum $\mathcal{H}_{phys}:=\mathcal{H}^{pp}_{x=0}\oplus\mathcal{H}^{ac}_{x=0}\oplus\mathcal{H}^{cs}_{x=0}$. Notice that the physical Hilbert space can be represented as an ℓ_2 space consisting of sequences of complex numbers $z_n^*,\ n=1,..,M^*$ subject to $\sum_{n,*}K_*|z_n^*|^2\rho_n^*(0)<\infty$. It is clear that different choices of $\Omega_n^*,\ c_n^*$ result in unitarily equivalent Hilbert spaces since by our prescription the numbers $N^*(0)$ of those n with $\rho_n^*(0)>0$ is fixed.

Whether the superselection structure concerning the spectral types with respect to the strong Dirac observables remains intact if we also allow weak Dirac observables cannot be answered in general and will probably depend on the concrete constraint operator under investigation. See e.g. [24] where this actually happens in a different context.

Let us verify that our prescription leads to the correct answer in the example discussed above: We have

$$\mu_{0,m}(B)=\int dk\chi_B(mk)|H_0(k)|^2=\frac{1}{|m|}\int_B dx|H_0(x/m)|^2 \tag{3.53}$$

hence $d\mu_{0,m}(x)/dx = |H_0(x/m)|^2/|m|$ and $d\mu^c(x)/dx = 2/3 \sum_{k=0}^\infty 2^{-k} d\mu_{0,k}(x)/dx$ so that

$$\rho^c_{m,0}(x) = \frac{3|H_0(x/m)|^2/|m|}{2\sum_{k=0}^\infty 2^{-k}/|k||H_0(x/k)|^2} \tag{3.54}$$

This function is already continuous, even smooth and actually everywhere positive, in particular

$$\rho^c_{m,0}(0) = \frac{3}{2|m|\sum_{k=0}^\infty 2^{-k}/k} > 0 \tag{3.55}$$

for all $m \neq 0$. Thus $N^c(x) = N^{pp}(x) = |\aleph|$ have countable cardinality independent of x.

Introducing orthonormal bases $e_{m,0};\ m \in \mathbb{Z} - \{0\}$ in the associated l_2 space and likewise $e_{0,n};\ n = 0, 1, 2, ..$ we have that under the unitary map $V:\ \mathcal{H} \to \mathcal{H}_{\mu^{pp},N^{pp}} \oplus \mathcal{H}_{\mu^c,N^c}$

$$(V\Psi)(0) = \sum_{m\neq 0} \Psi_{m,0}(0)\sqrt{\rho_{m,0}(0)}e_{m,0} \oplus \sum_n \Psi_{0,n}(0)\sqrt{\rho_{0,n}(0)}e_{0,n} \tag{3.56}$$

In particular for $\Psi = \Omega_{m,0},\ \Psi_{k,0} = \delta_{k,m},\ \Psi_{0,k} = 0$ and $\Psi = \Omega_{0,n},\ \Psi_{0,k} = \delta_{k,n},\ \Psi_{k,0} = 0$ we find

$$(V\Omega_{m,0})(0) = \sqrt{\rho_{m,0}(0)}e_{m,0} \text{ and } (V\Omega_{0,n})(0) = \sqrt{\rho_{0,n}(0)}e_{0,n} \tag{3.57}$$

which shows that the heuristic expectation is correct, namely that the span of the $\Omega_{m,0}$ which is isomorphic to the orthogonal complement of the vector 1 in the Hilbert space $L_2(S^1, dx_2)$ is isometric isomorphic to the span of the $e_{m,0}$ while the span of the $\Omega_{0,n}$ which is isomorphic to the Hilbert space $L_2(\mathbb{R}, dx_1)$ is isometric isomorphic to the span of the $e_{0,n}$. Moreover, these two physical Hilbert spaces are realized as direct sums. Notice that we could attribute the vector $\Omega_{0,0}$ also to $L_2(S^1, dx_2)$ but then we would have to subtract it from $L_2(\mathbb{R}, dx_1)$. This effect is related to the fact that the point $p_1 = p_2 = 0$ also classically plays a special role: Namely the reduced phase space with respect to the constraint $C = p_1p_2$ is as follows: The constraint surface is not a manifold but a variety of varying dimension consisting of the five disjoint pieces $S_1^\pm = \{(x_1, x_2, \pm p_1 > 0, p_2 = 0)\},\ S_2^\pm = \{(x_1, x_2, \pm p_2 > 0, p_1 = 0)\},\ S_0 = \{(x_1, x_2, p_1 = 0, p_2 = 0)\}$. The constraint generates gauge motions on each of these pieces except for S_0 and leads to the reduced phase space consting of the disjoint pieces $P_1^\pm = \{(x_1, \pm p_1 > 0)\},\ P_2^\pm = \{(x_2, \pm p_2 > 0)\},\ P_0 = \{(x_1, x_2)\}$. Notice that P_0 has a degenerate symplectic structure and thus should be discarded. But even then we see that the reduced phase space is not the union of two cotangent bundles over $\mathbb{R}$ but rather of four cotangent bundles over $\mathbb{R}_+$. This non − trivial topology is reflected in the above direct sum which is not the direct sum of the two Hilbert spaces corresponding to the union of two topologically trivial contangent bundles. We will not dwell further on this point, the discussion is just to reveal that the unusual form of $\mathcal{H}_{phys}$ is not surprising.

3.6 Explicit Action of Dirac Observables on the Physical Hilbert Space

As we have explained we may focus attention on either of the sectors $\mathcal{H}^*$ seperately. We will drop the $*$ for the purposes of this section.

Let E be the p.v.m. of a self − adjoint constraint operator a and let E' be the p.v.m. of a strong Dirac observable b. Let $V:\ \mathcal{H} \to \mathcal{H}_{\mu,N}$ be an associated direct integral representation based on a cyclic system of vectors Ω_n. Let f be a measurable function and $\Psi' \in D(f(b))$. From section 3.3 we know that $Vf(b)V^{-1}$ is fibre preserving and determines $\mu-$a.e. uniquely an operator $[f(b)](x)$ on $\mathcal{H}_x$. This applies in particular to the spectral projections $E'(\lambda) := E'((-\infty, \lambda])$.

By the spectral theorem

$$
\begin{aligned}
<\psi, V f(b) V^{-1}\psi' >_{\mathcal{H}_{\mu,N}} &= \int_{\mathbb{R}} f(\lambda)\; d <\psi, V E'(\lambda) V^{-1}\psi' >_{\mathcal{H}_{\mu,N}} \\
&= \int_{\mathbb{R}} f(\lambda) \int_{\mathbb{R}} d\mu(x)\; d <\psi(x), [E'(\lambda)](x)\psi' >_{\mathcal{H}_x} \\
&= \int_{\mathbb{R}} d\mu(x) \int_{\mathbb{R}} f(\lambda)\; d <\psi(x), [E'(\lambda)](x)\psi' >_{\mathcal{H}_x}
\end{aligned} \tag{3.58}
$$

whence $\mu-$a.e.

$$
[f(b)](x) = \int_{\mathbb{R}} f(\lambda)\; d_\lambda [E'(\lambda)](x) \tag{3.59}
$$

Thus we only need to know $[E'(\lambda)](x)$. There are measurable functions $x \mapsto G^\lambda_{nm}(x)$ such that

$$
E'(\lambda)\Omega_m = \sum_n G^\lambda_{mn}(a)\; \Omega_n \tag{3.60}
$$

Therefore for all $\Psi, \Psi' \in \mathcal{H}$

$$
\begin{aligned}
<\Psi, E'(\lambda)\Psi' >_{\mathcal{H}} &= = \sum_n \int d\mu_n(x)\; \overline{\Psi_n(x)} \sum_m G^\lambda_{mn}(x)\Psi'_m(x) \\
&= \int d\mu(x) \sum_{n\in M(x)} \rho_n(x)\overline{\Psi_n(x)} \sum_m G^\lambda_{mn}(x)\Psi'_m(x)
\end{aligned} \tag{3.61}
$$

On the other hand

$$
(V\Psi)(x) = \psi(x) = \sum_{n\in M(x)} \sqrt{\rho_n(x)}\Psi_n(x) e_n(x) \tag{3.62}
$$

with $e_n(x),\ n \in M(x)$ an orthonormal basis of $\mathcal{H}_x$ and $M(x) = \{n :\ \rho_n(x) > 0\}$ as described in section 3.3. Thus defining

$$
[E'(\lambda)](x) e_m(x) =: \sum_{n\in M(x)} ([E'(\lambda)](x))_{mn} e_n(x) \tag{3.63}
$$

we have

$$
\begin{aligned}
<\Psi, E'(\lambda)\Psi' >_{\mathcal{H}} &= \int d\mu(x)\; <\psi(x), [E'(\lambda)](x)\psi'(x) >_{\mathcal{H}_x} \\
&= \int d\mu(x) \sum_{m,n\in M(x)} \overline{\Psi_n(x)}([E'(\lambda)](x))_{mn}\Psi'_m(x)\sqrt{\rho_n(x)\rho_m(x)}
\end{aligned} \tag{3.64}
$$

We conclude that $\mu-$a.e.

$$
([E'(\lambda)](x))_{mn} = \chi_{M(x)}(m)\; \chi_{M(x)}(n) \sqrt{\frac{\rho_n(x)}{\rho_m(x)}}\; G^\lambda_{mn}(x) \tag{3.65}
$$

In order to fix (3.65) one must choose a representative $G^\lambda_{mn}(x)$ such that (3.65) is self – adjoint which is always possible $\mu-$a.e. by the results of section 3.3. For the pure point sector these numbers are uniquely determined while for the continuous sectors we will use our prescription to fix the freedom in (3.65) at $x = 0$. For instance we may reduce the freedom by insisting that $\lambda \to [E'(\lambda)](0)$ has to be a system of spectral projections on $\mathcal{H}_x$. See below for the general case.

In practice one is directly interested in the Dirac observables b themselves and thus one will try to choose the Ω_n to be in their common domain and as $C^\infty-$vectors of the constraint operator a. One can then directly determine the measurable functions $G_{mn}(a)$ via $b\Omega_m = \sum_n G_{mn}(a)\Omega_n$. The resulting expression for $(b(x))_{mn}$ then is analogous to (3.65). Notice that for bounded, strong, self adjoint Dirac observables the induced operator on the physical Hilbert space is bounded and self – adjoint no matter how the $\rho_n(0)$ were chosen because the $(b(x))_{mn}$ are non vanishing only if both $m, n \in M(x)$. This follows because by self – adjointness of b we have $\mu-$a.e. $\rho_m \overline{G_{nm}} = \rho_n G_{mn}$ and so we may choose a Hermitean representative b_{mn}. Moreover, since all possible direct integral representations of a given Hilbert space induced by different choices of Ω_n, c_n are unitarily equivalent as we showed in section 3.5 inducing a measurable fibre preserving unitarity, we may always arrange that different such choices lead to unitarily equivalent induced representations on the physical Hilbert space. Interestingly, if we find strong, unitary Dirac Observables u then we may simplify the spectral analysis because then the two vectors Ω_1 and $\Omega_2 := U\Omega_1$ have the same spectral measures.

The discussion of weak Dirac observables is more complicated because they are not necessarily fibre preserving. We will only sketch some ideas and reserve a complete discussion for future publications. By definition, if we write $\Psi = \sum_{*,n} \Psi_n^*(\widehat{\mathbf{M}})\Omega_n^*$ for measurable functions Ψ_n^* then the direct integral representation of Ψ is given by $(V\Psi)(x) = \psi(x) = \sum_{*,n} \sqrt{\rho_n^*(x)}\Psi_n^*(x)e_n^*$ where $V:\ \mathcal{H} \to \mathcal{H}_{\mu,N}$ is the unitary operator which realizes $\mathcal{H}$ as a direct integral. Weak bounded s.a. Dirac observables are of the form $(V\hat{D}\Psi)(x) = \int d\nu^D(x')d(x',x)\psi(x')$ for some measure ν^D and some kernel $d(x',x):\ \mathcal{H}_{x'}^\oplus \mapsto \mathcal{H}_x^\oplus$. The classical condition for a weak Dirac observable $\{D,\{D,\mathbf{M}\}\}_{\mathbf{M}=0} = 0$ translates into the condition that $A := V[\hat{D},[\hat{D},\widehat{\mathbf{M}}]]V^{-1}$ should annihilate the fibre $\mathcal{H}_0^\oplus$. In other words, if $a(x',x):\ \mathcal{H}_{x'}^\oplus \mapsto \mathcal{H}_x^\oplus$ is the kernel of A, that is, $(A\psi)(x) = \int d\nu^A(x')a(x',x)\psi(x')$ then $a(0,x) = 0$ for $\mu-$a.a. x. In terms of the measure ν^D and the kernel d we have explicitly $\nu^A = \nu^D$ and $a(x',x) = \int d\nu^D(x'')d(x'',x)d(x',x'')[x + x'' - 2x']$. This condition is implied by $d(0,x) = 0$ for ν^D-a.a. x which would mean that the fibre $\mathcal{H}_0^\oplus$ is preserved but not necessarily the individual sectors $\mathcal{H}_0^{\oplus *}$. This is in fact the only sensible choice if $\mathcal{H}_0^\oplus$ is to carry an induced representation of the weak Dirac observables. We conclude that $(V\hat{D}\Psi)(0) = \nu^D(\{0\})d(0,0)(V\psi)(0)$ where $\nu^D(\{0\}) \neq 0$.

In future publications we will elaborate more on representations of weak Dirac observables and investigate the question under which circumstances the superselection structure with respect to strong Dirac observables is destroyed by the weak ones. Notice, however, that also self – adjointness of weak, bounded self – adjoint Dirac observables cannot fix the ambiguity in the choice of the $\rho_n(0)$ since they must preserve the fibre $x = 0$ as we just showed and are then automatically self – adjoint there for the same reason as the strong Dirac observables.

We now will exhibit that the requirement of a self – adjoint representation of the *algebra* of strong Dirac observables will impose severe constraints on the sets $M(x) = \{n \in \mathbb{N}; \rho_n(x) > 0\}$. Let $D^j,\ j = 1,2,3$ be strong Dirac observables on $\mathcal{H}$ with $D^1D^2 = D^3$ and $D^j\Omega_m = \sum_n D^j_{mn}(a)\Omega_n$. It follows for the measurable functions that $\sum_k D^2_{mk}D^1_{kn} = D^3_{mn}$. The corresponding operators in the fibres are then given by $d^j(x)e_m = \sum_n d^j_{mn}(x)e_n$ where $d^j_{mn}(x) = \sqrt{\rho_n/\rho_m}(x)\chi_{M(x)}(m)\chi_{M(x)}(n)D^j_{mn}(x)$. Now a short calculation reveals

$$d^1(x)d^2(x) = \sqrt{\frac{\rho_n(x)}{\rho_m(x)}}\chi_{M(x)}(m)\chi_{M(x)}(n) \sum_{k \in M(x)} D^2_{mk}(x)D^1_{kn}(x) \tag{3.66}$$

which coincides $\mu-$a.e. with

$$d^3(x) = \sqrt{\frac{\rho_n(x)}{\rho_m(x)}}\chi_{M(x)}(m)\chi_{M(x)}(n)D^3_{mn}(x) = \sqrt{\frac{\rho_n(x)}{\rho_m(x)}}\chi_{M(x)}(m)\chi_{M(x)}(n)\sum_k D^2_{mk}(x)D^1_{kn}(x) \tag{3.67}$$

The point is now that (3.66) and (3.67) differ by the fact that in (3.66) the sum over k is restricted to the set $M(x)$ while in (3.67) it is not. Requiring that these two expressions coincide, at least at $x = 0$, numerically rather than a.e. should impose restrictions on the choice of the representatives of $\rho_n(0), D^j_{mn}(0)$ and all other Dirac observables. Intuitively, this requirement will amount to choosing representatives $\rho_n(0)$ which are positive for a maximal number of n so that we are not missing necessary terms while irreducibility will require to have a maximal number of the $\rho_n(0)$ vanishing so that at least heuristically these two requirements have the tendency to restrict the freedom.

3.7 Comparison Between Refined Algebraic Quantization (RAQ) and the Direct Integral Decomposition (DID)

The main purpose of the Master Constraint Programme is to deal with situations where RAQ [23] fails: Namely in the case of an infinite dimensional set of constraints with no or little control on the resulting group they generate or, even worse, when there is no group at all (the constraints close with non – trivial structure functions on phase space rather than structure constants). In such situations there are presently only formal BRST procedures available [25] which apply at most in the case of a finite number of degrees if freedom and which have not yet been shown to produce a non negative physical inner product. On the other hand, the Master Constraint Programme offers a rigorous alternative *whose mathematics always works.*

In the present section we would like to compare the direct integral decomposition (DID) method with the RAQ programme in a situation to which RAQ applies: This is the case of a *single* constraint or the Master Constraint considered as a *single* constraint.

In its most general form, RAQ consists of the following steps [23]:

1. *Choose* a dense and invariant domain Φ for a. Φ^* is defined as the algebraic dual of Φ, i.e. the set of all linear functionals on Φ equipped with the weak * topology of pointwise convergence.

2. An element $F \in \Phi^*$ is said to be a physical "state" provided that $F[a^\dagger f] = 0$ for all $f \in \Phi$. Denote the vector space of these generalized solutions by Φ^*_{phys}.

3. Turn (a subspace of) Φ^*_{phys} into a pre – Hilbert space by supplementing it with an anti – linear "Rigging Map"

$$\eta : \; \Phi \to \Phi^*_{phys}; \; f \mapsto \eta(f); \;\; <\eta(f), \eta(f')>_{phys} := (\eta(f'))[f] \tag{3.68}$$

   and then complete it with respect to the sesqui – linear form $< .,. >_{phys}$ to obtain a physical Hilbert space $\mathcal{H}_{phys}$ (possibly after dividing out a null space). In order that η be a rigging map, (A) (3.68) must be a positive semi – definite sesqui – linear form and, moreover, (B) for any strong Dirac observable defined on Φ we should have $b'\eta(f) = \eta(bf)$ where b' is the dual of b defined on Φ^* via $(b'F)[f] := F(b^\dagger f)$ and $b^\dagger$ is the adjoint of b on $\mathcal{H}$. One says that b commutes with the rigging map. It is easy to see that condition (B) implies that symmetric operators on $\mathcal{H}$ are promoted to symmetric operators on $\mathcal{H}_{phys}$.

A heuristic procedure for constructing η from a is to set $(\eta(f))[f'] :=< f, \delta(a)f' >$ where the $\delta-$distribution is formally defined via the spectral theorem as $\delta(a) = \int \; \delta(\lambda)dE(\lambda)$. It is clear that this formally solves the requirements on η to qualify as a rigging map, however, the meaning of the $\delta-$distribution must be made more precise and depends on the spectral properties of a. In fact, the direct integral representation of $\mathcal{H}$ now enables us to precisely do that as follows: Recall the decomposition $\mathcal{H}=\sum_{*=pp,ac,cs}\mathcal{H}^*$. The "operator" $\delta(a)$ is reduced by this decomposition and we define $\delta^*(a)$ as the restriction of $\delta(a)$ on $\mathcal{H}^*$. Use a direct integral representation $\mathcal{H}_{\mu^*,N^*}$ of $\mathcal{H}^*$. Then, if V^* denotes the corresponding unitary operator

$$<\Psi,\delta(a)\Psi'>_{\mathcal{H}^*}:=\int d\mu^*(x)\;\delta^*(x)<\psi(x),\psi'(x)>_{\mathcal{H}^*_x} \tag{3.69}$$

for all $\Psi,\Psi'\in\Phi$. It follows that if $\delta^*(x)$ is such that $\int d\mu^*(x)\delta^*(x)g(x)=g(0)$ for all measurable g then

$$<\eta^*(\Psi),\eta^*(\Psi')>^*_{phys}=<\psi'(0),\psi(0)>_{\mathcal{H}^*_0} \tag{3.70}$$

so RAQ reproduces the results of the direct integral decomposition provided that $\{\psi(0);\;\Psi\in\Phi\}$ is dense in $\mathcal{H}^*_0$ and that there exist a rule for choosing representatives $x\mapsto\psi(x)$ for all $\Psi\in\Phi$ such that the numbers $<\psi(x),\psi'(x)>_{\mathcal{H}^*_x}$ are finite, at least at $x=0$. Notice that this issue about the representatives only arises in the construction of the physical inner product: For the elements $F\in\Phi^*$ the numbers $F[f]$ are of course well defined for any $f\in\Phi$, however, the complication lies in the Rigging Map $\eta:\;\Phi\to\Phi^*_{phys}$ without which there is no physical inner product and which may actually not produce elements of Φ^* unless one has a rule for choosing appropriate representatives. In other words, if one has an element $F\in\Phi^*$ which solves the constraints, then it may not be possible to display it in the form $F=\eta(f)$ for some $f\in\Phi$ unless one has resolved the issue about the representatives.

Several remarks are in order:

i) *Group Averaging*
Group averaging is a heuristic method to define the rigging map or, in other words, the $\delta-$"operator " $\delta(a)$. For a single self – adjoint constraint C it consists of the formula

$$\eta(f):=\int_{-\infty}^{\infty}\frac{dt}{2\pi}\;<e^{it\hat{C}}f,.> \tag{3.71}$$

where the inner product indicated is the one on the unreduced Hilbert space. We now show that (3.71) is wrong in general.

1. *Purely Continuous Spectrum*
Consider the operator $C=p^2$. We have, using the momentum space representation

$$<\eta(f),\eta(f')>=\int_{\mathbb{R}}dp[\int_{\mathbb{R}}\frac{dt}{2\pi}e^{itp^2}]\overline{f'(p)}f(p)=\lim_{p\to 0}\frac{\overline{f'(p)}f(p)}{|p|} \tag{3.72}$$

which is ill defined even for f,f' in the dense subspace of functions of rapid decrease. The reason of failure is that in this case (3.71) does not take into account the appropriate spectral measure μ: We may choose $\Omega_1=\sqrt{\exp(-p^2/2)/\sqrt{2\pi}},\;\Omega_2=p\Omega_1$. A straightforward calculation reveals that $\rho_1(x)=2/(1+x),\;\rho_2(x)=2x/(1+x)$ and $d\mu(x)=\frac{dx}{2\sqrt{2\pi x}}e^{-x/2}(1+x)$ where with $f=f_1(p^2)\Omega_1+f_2(p^2)\Omega_2$ we have

$$<f,f'>=\int_{\mathbb{R}^+}d\mu(x)\;[\rho_1(x)\overline{f_1(x)}f_1'(x)+\rho_2(x)\overline{f_2(x)}f_2'(x)] \tag{3.73}$$

Since $\rho_1(0)=2>0,\;\rho_2(0)=0$ our prescription yields the correct result that the physical Hilbert space is one dimensional, isomorphic to $\mathbb{C}$, and can be thought of as the span of the vector Ω_1.

2. *Purely Discrete Spectrum*
   In the previous example one could rescue the proposal (3.71) by selecting a "reference vector" f_0 and to formally define a new rigging map $\eta'(f) := \eta(f)/\eta(f_0)[f_0]$. This would take care of the singularity at $p = 0$. We now show that even with this modification (3.71) is completely wrong in the case of an entirely discrete spectrum. Take this time the harmonic oscillator $H = (p^2 + q^2)/2$ with spectrum $x_n = \hbar(n + 1/2),\ n \in \mathbb{N}_0$. Applying (3.71) now yields on the eigenstates e_n of the harmonic oscillator

$$< \eta(e_n), \eta(e_m) >_{Phys} := \int_{\mathbb{R}} \frac{dt}{2\pi} < e_m, e^{itC} e_n > = \delta_{m,n}\delta(\hbar(m + 1/2), 0) = 0 \qquad (3.74)$$

   The physical Hilbert space would be empty because zero is not in the spectrum. Obviously we must normal order C to remove the zero point energy, i.e. we quantize the quantum corrected classical expression $C' := (p^2 + q^2)/2 - \hbar/2$ which is semiclassically equivalent to C. But then the physical inner product diverges on the physical state e_0. Here one could repair the situation by integrating over the "period" $t \in [-\pi/\hbar, \pi/\hbar]$ but one sees already at this point that as compared to the case of the continuous spectrum the integration range cannot be chosen universally but depends on the spectrum of C. In particular, integrating over a finite period does not lead to the correct result in the case of a continuous spectrum.

   However, one can think of even more generic situations. Consider the case of an operator with entirely discrete spectrum for which at least two eigenvalues are rationally independent. An example from LQG would be the area operator with a spectrum whose simplest eigenvalues are of the form $x = \ell_p^2 \sum_p \sqrt{j_p(j_p + 1)}$ where the sum runs over a finite set of points, the j_p are half integral spin quantum numbers and ℓ_p^2 is the Planck area. Consider the family of operators $C_a = \mathrm{Ar}(H) - a\ell_p^2$ where $\mathrm{Ar}(H)$ is the area operator of an isolated horizon [26] and a is a real number. This kind of operators appear in the quantum entropy calculations in LQG. The entropy is given by

$$S = \ln(\mathrm{Tr}(P(a_0)), \quad P(a_0) := \sum_{a \in [a_0 - 1, a_0 + 1]} P_a \qquad (3.75)$$

   where P_a is the projector onto the kernel of C_a. Now even if a is in the spectrum of $\mathrm{Ar}(H)$ it is *impossible* to define P_a via (3.71) no matter how one chooses the period since C_a has an infinite number of incommensurable eigenvalues. The way out here would be to replace $\mathbb{R}$ by the Bohr compactification of the real line and dt by the corresponding Haar measure. More in elementary terms one would define

$$< f, P_a f' > := \lim_{T \to \infty} \int_{-T}^{T} dt < f, e^{itC_a} f' > \qquad (3.76)$$

   However, this ergodic mean again does not lead to the correct result in the case of the continuous spectrum.

3. *Mixed spectrum*
   Finally consider again the case of a mixed spctrum, e.g. the operator $C = C_1 \otimes C_2$ on a Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ where C_1 has purely continuous spectrum such as in 1. and C_2 has purely discrete spectrum such as in 2. Now integrating over $\mathbb{R}$ in (3.71) projects onto a physical Hilbert space which is isomorphic to the orthogonal complement of the ground state of C_2 in $\mathcal{H}_2$. Integrating over a finite period does not lead to any sensible result because the period of the eigenvalue $p^2 n\hbar$ of C is p dependent. Finally, ergodic averaging gives a physical Hilbert space isomorphic to

$\mathcal{H}_1$. Hence in none of the cases does one recover the correct result which would be roughly isomorphic to the direct sum of $\mathcal{H}_1$ and $\mathcal{H}_2$ as we saw in section 3.5.

We conclude that already in these simple examples group averaging only leads to the correct physical result if one already knows the spectrum. Even then it fails in the case of a mixed spectrum. Thus one must, similar as we observed in section 3.5, first split the Hilbert space into its pure point and continuous part respectively. Again, this requires detailed knowledge of the spectrum so that rigorous methods more closely tied to the spectral analysis of the operator such as the direct integral method suggest themselves.

ii) *Superselection Sectors, Non – Amenable Groups and Group Averaging Constants*
In [8] we find an example where group averaging has been carried out with respect to an infinite dimensional Lie group, the group of diffeomorphisms. With respect to the corresponding strong Dirac observables a certain superselection structure was discovered (these have a different origin than the separation between the types of spectrum discussed here). On each of those sectors the group averaging measures had to be carried out independently for the following reasons:
1. The diffeomorphism group is not amenable, there is no finite Haar measure on the diffeomorphism group. The only known Haar measures are counting measures.
2. In order to apply group averaging anyway one must renormalize the averaging procedure by formally dividing by the "volume" of the effective gauge group on each sector. The effective gauge group on a sector is the subgroup of the diffeomorphism group each of whose elements has non – trivial action on all vectors of the given sector.
This sector dependent volume is formally infinite and therefore the renormalized average is only well defined up to a positive constant which could be different for each sector. This therefore leads to a huge class of diffeomorphism invariant inner products depending on the choice of relative normalization constants between the group averaging measures of the respective sectors. It seems to be generic that group averaging leads to ambiguities, so – called group averaging constants, for every system with superselection sectors and non – amenable gauge groups. For the example in [8] it is conceivable that these constants can be fixed by adding the weak Dirac observables to the analysis which is precisely what happened in the lower dimensional model of [24].

In contrast, the Master Constraint Programme in connection with DID, where applicable, does not lead to these ambiguities as we have seen, intuitively because the gauge group generated by the Master constraint is Abelean and hence amenable. We will see this explicitly in the examples of [28]. In fact, the general analysis carried out in this paper did not depend at all on possible superselection sectors with respect to the strong Dirac observables.

iii) *Separability*
Notice that the Master Constraint Programme is not immediately applicable to the example of [8] because the Hilbert space given there is not separable. However, that Hilbert space is an uncountably infinite direct sum of separable Hilbert spaces which are invariant under the spatial diffeomorphism group and which are labelled by diffeomorphism invariant continuous data (moduli) (that have to do with vertices of valence higher than four). Thus we may apply DID to each of these sectors separately, at least in principle, although this would be rather involved, see [10, 30]. Hence DID also applies to non – separable Hilbert spaces which are (possibly uncountably infinite) direct sums of $\widehat{\mathbf{M}}$ −invariant separable Hilbert spaces.

iv) *Continuity of the Dimension Function*
In [23] the RAQ programme was also compared with the direct integral method (called

"spectral analysis inner product" there) but the multiplicity function $N(x)$ was assumed to be constant in a neighbourhood of $x = 0$. This is a somewhat reasonable assumption for the case of a single constraint. However, as we will see in the examples, not only do we not need this assumption but, moreover, the assumption is unphysical for the Master Constraint because in most examples the function N is stronly discontinuous at $x = 0$ as one should expect: This happens when, roughly speaking, the classical constraint manifolds $\mathbf{M} - x = 0$ have different dimension for different x. A typical example would be that $\mathbf{M} = x > 0$ is a (high dimensional) sphere but $\mathbf{M} = 0$ is a point. In quantum theory this is technically implemented by the fact that while e.g. the functions ρ_n^{ac} can be chosen to be continuous for all n, usually an infinite number of them are non-zero for $x \neq 0$ but vanish at $x = 0$. Thus, while the $\rho_n^{ac}(x)$ are actually continuous, the function $N(x)$ is not.

v) *Direct Integrals and Rigged Hilbert Spaces*
In [23] it was already noticed that the choice of Φ is critical for the size of the resulting $\mathcal{H}^*_{phys}$ (the superselection structure corresponding to pure point and continuous spectrum was also noticed there). From that perspective it is surprising that the direct integral decomposition does not depend on the additional structure Φ. In fact, modulo the prescription for how to choose the $\rho_n^c(x)$ for the continuous part of the spectrum, the physical Hilbert space does not need the structure of Φ. Notice that the choice of the $\rho_n^*(x)$ is in one to one correspondence with the choice of representatives for the direct integral decomposition of a given cyclic system of vectors Ω_n, that is, with representatives $\omega_n(x) = \sqrt{\rho_n(x)} e_n$.

However, it might be useful, at least for reasons of completeness, to relate the elements of $\mathcal{H}$ and of $\mathcal{H}_{Phys}$ and to display the relation between RAQ and the direct integral decomposition (DID). In [14] we find one method for how to do that, see also the summary in the appendix of [10]. It uses the machinery of Rigged Hilbert Spaces and we recall here the essential steps of the construction, see [14, 10] for more details. We drop the label $*$ for simplicity, focussing on one sector only for the remainder of this section.

A Rigged Hilbert Space consists of a so – called Gel'fand triple $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$ consisting of a topological vector space Φ which is dense in $\mathcal{H}$ (in the topology of $\mathcal{H}$) and the topological (rather than algebraic) dual of Φ (continuous linear functionals). These spaces arise from a chain of separable Hilbert spaces $\Phi_N,\ N = 1, 2, ..$ equipped with inner products $< ., . >_N$ subject to the condition $||.||_N \leq ||.||_{N+1}$ and $\Phi_{N+1} \subset \Phi_N$. One now defines $\Phi := \cap_N \Phi_N$, equips it with the metric $d(F, F') := \sum_N 2^{-N} ||F - F'||_N (1 + ||F - F'||_N)^{-1}$ and completes. This makes Φ a Fréchet space, i.e. a complete, metrizable locally convex topological space[15]. Such a structure is called a countably Hilbert space. One also defines $\Phi_{-N} := \Phi'_N,\ n = 1, 2, ..$ where Φ'_N is the topological dual of Φ_N. (By the Riesz lemma, Hilbert spaces are reflexive and hence we may identify Φ'_N with Φ_N.) From $\Phi_{N+1} \subset \Phi_N$ we conclude that any $l \in \Phi'_N$ is also an element of Φ'_{N+1}, hence $\Phi'_{-N} \subset \Phi'_{-(N+1)}$. One now defines $\Phi' := \cup_N \Phi'_N$. A nuclear space is a countably Hilbert space such that for all M there exists $N \geq M$ and such that the natural embedding $T_{NM} : \Phi_N \to \Phi_M$ is trace class (nuclear) , i.e. if $B_k^{(N)}$ is an orthonormal basis of Φ_N then $T_{NM} F = \sum_k \lambda_k < B_k^{(N)}, F >_N B_k^{(M)}$ where $\sum_k \lambda_k < \infty,\ \lambda_k \geq 0$. Finally one needs an inner product $< ., . >_0$ and defines $\Phi_0 := \mathcal{H}$ as the completion of Φ in that inner product. One can show that one obtains a chain of Hilbert spaces $\Phi_{N+1} \subset \Phi_N,\ N \in \mathbb{Z}$. A Rigged Hilbert space is such a chain of Hilbert spaces such that convergence in the topology of Φ implies convergence in the topology of $\mathcal{H}$.

[15] A topological space is called locally convex if its topology is defined by a family of seminorms separating the points. A seminorm is a norm just that the requirement $||F|| = 0 \Rightarrow F = 0$ is dropped. A locally convex topological space is metrizable if and ond if its family of seminorms is countable.

To see that this structure is naturally available in the context of the Master Constraint Programme, notice that every self-adjoint operator $\widehat{\mathbf{M}}$ on a Hilbert space has a dense set $\mathcal{D}$ of $C^\infty-$vectors of the form $\Omega_g = \int_{\mathbb{R}} dt\, g(t) \exp(it\widehat{\mathbf{M}})\Omega$ where $g \in C_0^\infty(\mathbb{R})$ is a smooth function of compact support and $\Omega \in \mathcal{H}$ and one computes $\widehat{\mathbf{M}}^n \Omega_g = (-1)^n \Omega_{g^{(n)}}$. We now define for $F, F' \in \mathcal{D}$

$$< F, F' >_N := \sum_{k=0}^{N} < F, \widehat{\mathbf{M}}^k F' >_{\mathcal{H}} \tag{3.77}$$

which defines positive semi definite inner products *because $\widehat{\mathbf{M}}$ is positive semi definite.* We define $\Phi_N,\ N = 0, 1, 2..$ as the Cauchy completion of $\mathcal{D}$ in the norm defined by (3.77) and see that the conditions on a countably Hilbert space are satisfied. Moreover, using a direct integral decomposition of $\mathcal{H}$ and a cyclic system of vectors Ω_n we find that

$$||F||_N^2 = \int_{\mathbb{R}_+} d\mu(x)\ \frac{x^N - 1}{x - 1}\ \sum_n \rho_n(x) |F_n(x)|^2 \tag{3.78}$$

where $F = \sum_n F_n(\widehat{\mathbf{M}})\Omega_n$ which shows that the norms of F grow rapidly with N provided that $\widehat{\mathbf{M}}$ is an unbounded operator. This typiically implies that Φ will be a nuclear space because, suppose that $B_k^{(0)}$ is an orthonormal basis of $\mathcal{H}$ constructed from functions in $\mathcal{D}$ by the Gram – Schmidt algorithm. This means we may choose

$$\sum_n \rho_n(x) \overline{b_{kn}^{(0)}(x)} b_{k'n}^{(0)}(x) = \delta_{kk'} \sigma_k(x) \tag{3.79}$$

$\mu-$a.e for some measurable function σ_k where $B_k^{(0)} = \sum_n b_{kn}^{(0)}(E)\Omega_n$. This means that $B_k^{(N)} := \sqrt{\mu_{Nk}}^{-1} B_k^{(0)}$ is an orthonormal basis of Φ_N where

$$\mu_{kN} := \int d\mu(x) \sigma_k(x) \frac{x^N - 1}{x - 1} \tag{3.80}$$

If these moments of μ grow sufficiently fast then by the completeness relation for $F \in \Phi_N$

$$T_{NM} F = \sum_k < B_k^{(N)}, F >_N B_k^{(N)} = \sum_k \sqrt{\frac{\mu_{kM}}{\mu_{kN}}} < B_k^{(N)}, F >_N B_k^{(M)} \tag{3.81}$$

and we identify $\lambda_k = \sqrt{\frac{\mu_{kM}}{\mu_{kN}}}$ which will satisfy the trace class condition depending on the growth of the moments. Notice that also the compatibility condition between the topologies of Φ and $\mathcal{H}$ is automatically stisfied here because convergence in the topology of Φ implies convergence with respect to all the $||.||_N$ in particular $||.||_0 = ||.||_{\mathcal{H}}$.

In any case, if a Rigged Hilbert Space Structure is available, one has the following result:

Theorem 3.5.
Let $\Phi \hookrightarrow \mathcal{H} \hookrightarrow \Phi'$ be a separable Rigged Hilbert Space. Let $\mathcal{H} \equiv \mathcal{H}_{\mu,N}$ be a direct integral representation of $\mathcal{H}$ subordinate to a self – adjoint operator $\widehat{\mathbf{M}}$.
i)
Then there exists a nuclear operator $T_x :\ \Phi \to \mathcal{H}_x^\oplus$ such that $T_x F = f(x)$ $\mu-$a.e. where $(f(x))_{x\in\mathbb{R}^+}$ is the direct integral representation of $F \in \Phi$. Moreover, the norms $||T_x f||_{\mathcal{H}_x}$ of the the vector valued function $x \mapsto T_x F$ are uniquely defined through the operator T_x

(and not only $\mu-$a.e.).
ii)
The maps

$$\eta_x:\ \Phi\to\Phi';\ F\mapsto\eta_x(F),\ \ \eta_x(F)[F']:=<T_xF,T_xF'>_{\mathcal{H}_x^\oplus} \tag{3.82}$$

are Rigging Maps and η_0 defines the physical Hilbert space. Moreover, the subset of Φ' defined by the images under the η_x defines a complete set of generalized eigenvectors, that is, $\eta_x(F)[\widehat{\mathbf{M}}\,F']=x\eta_x(F)[F']$ for all $F,F'\in\Phi$ and $\cup_x\eta_x(\Phi)\subset\Phi'$ separates the points of Φ.

Actually in order to prove the theorem it is sufficient that Φ is a Fréchet space and that there exists a map $T=T_2T_1$ where $T_1:\ \Phi\to\mathcal{H}_1$ is a continuous embedding of Φ into some Hilbert space $\mathcal{H}_1$ and T_2 is a nuclear operator. To prove the theorem one proceeds as follows: Given a direct integral representation of $\mathcal{H}$ and an orthonormal basis B_k of $\mathcal{H}$ with direct integral representation $(b_k(x))_{x\in\mathbb{R}}$ one *chooses* for each x a representative $b_k(x)$ once and for all. This means that on top of choosing values for the $\rho_n(x)$ which define the $\mathcal{H}_x^\oplus$ we must also choose values for the measurable functions $b_{kn}(x)$ where $B_k=\sum_n b_{kn}(E)\Omega_n$. The nuclear structure enables one to show that there exists an N, independent of x, $\lambda_k\geq 0$ with $\sum_k\lambda_k<\infty$ and an orthonormal basis $B_k^{(N)}$ of Φ_N such that the operator

$$T_xF:=\sum_k\lambda_k<B_k^{(N)},F>_N b_k(x)=\sum_n\sqrt{\rho_n(x)}[\sum_k\lambda_k<B^{(N)},F>_N b_{kn}(x)]e_n \tag{3.83}$$

is nuclear (where $e_n,\ \rho_n(x)>0$ is an orthonormal basis of $\mathcal{H}_x^\oplus$) and coincides with $f(x)$ $\mu-$a.e. More precisely, the norm of (3.83) converges $\mu-$a.e. to a finite number and T_xF is then defined *everywhere* by setting it to zero at those x for which the norm of (3.83) does not converge.

What has been gained?
Notice that the theorem supposes that one has already chosen the Hilbert spaces $\mathcal{H}_x^\oplus$, the ambiguity in the $\rho_n(x)$ has been fixed by making a definite choice. Furthermore, one must make a choice of the bases $B_k,B_k^{(N)}$ and one must choose representatives $b_k(x)$. One will make the cyclic system consisting of the Ω_n part of the basis B_k so that $b_{kn}(x)=\delta_{mn}$ for $B_k=\Omega_n$ but clearly there are more B_k than Ω_n. This is more than one has to choose in order to define the $\mathcal{H}_x^\oplus$. The only advantage of this theorem is that once one has made these choices to define the T_x, one can assign definite numbers to the inner products $<T_xF,T_xF'>_{\mathcal{H}_x}$ or in other words one can reduce the ambiguity in choosing the representative $f(x)$ universally (i.e. independently of $F\in\Phi$).

Hence we see that RAQ, even in its precise form given in theorem 3.5, is more ambiguous than DID. This seems surprising in view of the fact that using the Rigged Hilbert space based on the nuclear space of test functions of rapid decrease on $\mathbb{R}$ and a direct integral representation of $L_2(\mathbb{R},dx)$ subordinate to the momentum operator the T_xF are just the Fourier coefficients of the Fourier integral defining F in the sense of L_2 functions and that these coefficients are naturally smooth and of rapid decrease again. However, notice that secretly one has made also choices here, nobody can prevent one to make those Fourier coefficients arbitrarily discontinuous on a countable subset of $\mathbb{R}$. Moreover, in the case of the Fourier transform one has actually a cyclic vector for the momentum operator(s) and therefore the ρ_n are naturally identical to the constant function equal to one. In general little seems to be known in the mathematical literature about the connection between the "natural" continuity of the T_xF and the choice of Φ.

In summary we see that DID not only extends RAQ to the case of structure functions, it can also be used in order to reduce the ambiguity even for the rigorous version of RAQ since one is not in the need to choose the additional structures Φ, T_x. These additional structures are of no interest whatsoever to the direct integral decomposition because $\mathcal{H}_0^\oplus$ is determined by independent means, subject to the physical prescription of enforcing an irrducible, self – adjoint representation of a complete subalgebra of all Dirac observables with a good semiclassical limit which fixes the values of the $\rho_n(0)$ as much as it possibly can[16]. The physical Hilbert space is then isomorphic to the ℓ_2 space of sequences (z_n) for which $\sum_n \rho_n(0)|z_n|^2$ converges. We do not need to worry about the question whether the z_n can be thought of as the values $\Psi_n(0)$ of the measurable functions Ψ_n defined by $\Psi = \sum_n \Psi_n(a)\Omega_n$ and whether there is a natural representative $x \mapsto \Psi_n(x)$ in the corresponding equivalence class. Finally, there is no need to deal with the formal "operator" $\delta(a)$.

4 Algorithmic Description of the Direct Integral Decomposition

Given a self – adjoint operator $\widehat{\mathbf{M}}$ on a separable Hilbert space $\mathcal{H}$, the Direct Integral Decomposition (DID) method to solve the constraint $\widehat{\mathbf{M}} = 0$ consists of the following steps:

Step I. *Spectral Measures*

For any Lebesgue measurable set B and any $\Psi \in \mathcal{H}$ determine the spectral measures $\mu_\Psi(B) :=< \Psi, E(B)\Psi >$ where E is the p.v.m. underlying the operator $\widehat{\mathbf{M}}$, that is, $E(B) = \chi_B(\widehat{\mathbf{M}})$ where χ_B is the characteristic function of the set B. It is actually sufficient to construct these for the sets $B_x := (-\infty, x]$ and we set $\mu_n(x) := \mu_n(B_x)$. To construct the $\mu_\Psi(x)$ explicitly from a given operator $\widehat{\mathbf{M}}$ is very hard in general, however, if one can construct the bounded resolvent $R(z) := (\widehat{\mathbf{M}} - z\mathbf{1})^{-1}$ for $\Im(z) \neq 0$ which one can often determine by Green function techniques then one can use Stone's formula

$$\frac{1}{2}(E([a,b]) + E((a,b)) = s - \lim_{\epsilon \to 0} \int_a^b dt[R(t+i\epsilon) - R(t-i\epsilon)] \tag{4.1}$$

In fortunate cases the operator $\widehat{\mathbf{M}}$ is of the form $F(\{\hat{a}_\alpha\})$ where the $\hat{a}_\alpha$ form a mutually commuting set of other self – adjoint operators for which one knows explicitly a representation as multiplication operators on a space of square integrable functions in some variables y_α. Then $\mathcal{H}$ can be represented as some L_2 space on the space of y_α and $\widehat{\mathbf{M}}$ acts by multiplication by $F(\{y_\alpha\})$. The same applies when some of the $\hat{a}_\alpha$ have discrete spectrum in which case the L_2 space is replaced by an l_2 space and y_α by the corresponding eigenvalue.

Step II. *Separation of Discrete and Continuous Spectrum*

We say that μ_Ψ is of pure point or continuous type respectively if μ_Ψ has support on a discrete set of points or is not supported on one point sets respectively. Let $\mathcal{H}^{pp}$, $\mathcal{H}^c$ be the completion of the linear span of vectors such that μ_Ψ is of the respective type. Then it is always true that $\mathcal{H} = \mathcal{H}^{pp} \oplus \mathcal{H}^c$.

Step III. *Cyclic System*

For each sector $\mathcal{H}^*$, $* = \{pp, c\}$ determine a minimal sysyem of mutually orthogonal $C^\infty-$vectors, that is, normalized vectors Ω_n^*, $n = 1, .., M^* \leq \infty$ such that

A. all powers of $\widehat{\mathbf{M}}$ are defined on Ω_n^*,

[16] The additional structure Φ, T_x might be helpful, however, in order to fix the values of the measurable functions $G_{mn}(x)$ for all x, not only for $x = 0$, although this is not particularly interesting from the point of view of the physical Hilbert space.

B. $< \Omega^*_m, \widehat{\mathbf{M}}^N \Omega^*_n >= 0$ for all $N = 0, 1, 2, ..$ and all $m \neq n$,
C. the finite linear span of the $\widehat{\mathbf{M}}^N \Omega^*_n$ is dense in $\mathcal{H}^*$,
D. M^* cannot be reduced without violating condition C.
In practice one starts from a known orthonormal basis B_k for $\mathcal{H}$ and tries to identify elements Ω^*_n of that basis such that any B_k is a finite linear combination of the $\widehat{\mathbf{M}}^N \Omega^*_n$. Different choices of Ω^*_n satisfying A. – D. lead to unitarily equivalent direct integral decompositions $\mathcal{H}^*_{\mu^*,N^*} = \int d\mu^*(x)\, \mathcal{H}^{*\oplus}_x$ of $\mathcal{H}^*$ and in fact the measure class of μ^* and the dimension $N^*(x)$ of $\mathcal{H}^{*\oplus}_x$ is unique μ^*-a.e. (independent of the Ω^*_n). The minimal set of Ω^*_n is such that the supports S^*_n of the functions ρ^*_n defined below are ordered such that $S^*_{n+1} \subset S^*_n$.

Step IV. *Total Measure and Radon Nikodym Derivatives*
Let $\mu^*_n(B) :=< \Omega^*_n, E(B)\Omega^*_n >$ and define $\mu^*(x) := \sum_n c^*_n \mu^*_n(x)$ where where $c^*_n > 0$, $\sum_n c^*_n = 1$. Its measure class is actually unique (indendent of the choice of Ω^*_n, c^*_n). Let, if the limit exists

$$\rho^*_n(x) := \lim_{y \to 0+} \frac{\mu^*_n(x+y) - \mu^*_n(x-y)}{\mu^*(x+y) - \mu^*(x-y)} \tag{4.2}$$

For $* = pp$ the numbers (4.2) always exist, they are always non – negative and the number $N^{pp}(x)$ of those n for which $\rho^{pp}_n(x)$ does not vanish is independent of the Ω^{pp}_n. For $* = c$ they are granted to exist only μ^c-a.e., are naturally non – negative (but might be infinite) and the number $N^c(x)$ is only unique μ^c-a.e. (i.e. independent of the Ω^*_n, c^*_n). For a given system Ω^*_n, c^*_n fix these constants once and for all by choosing a representative subject to the requirement that the resulting physical Hilbert space is an irreducible self – adjoint representation of a complete subalgebra of all Dirac observables and admits a sufficient number of semiclassical states. For any other choice of Ω^*_n, c^*_n these constants are then fixed by the requirement that the induced representation of the strong Dirac observables is unitarily equivalent to the given one, see below. In practice, it is often sufficient to choose a representative, if it exists, which is continuous from the right at $x = 0$ and to set $\rho^c_n(0) := \lim_{x \to 0+} \rho^c_n(x)$. If it does not exist, set $\rho^c_n(0) = 0$ if also not fixed by the aforementioned physical criteria.

Step V. *Physical Hilbert Space*
Let e^*_n, $n = 1, 2, .., M^*$ be an orthonormal basis in some abstract Hilbert space. The Hilbert space $\mathcal{H}^{\oplus}_x$ is the space of vectors of the form $\sum_{*=\{pp,c\}} K_* \sum_{n=1}^{M^*} \sqrt{\rho^*_n(x)} z^*_n e^*_n$ with $z^*_n \in \mathbb{C}$ for which the norm squared $K_{pp} \sum_n \rho^{pp}(x)|z^{pp}_n|^2 + K_c \sum_n \rho^c(x)|z^c_n|^2$ converges. The positive constants K_* can possibly be determined if there are weak Dirac observables which mix the continuous and discrete part of the Hilbert space in which case they must be chosen so that the algebra of weak Dirac observables are also represented self – adjointly. The physical Hilbert space coincides with $\mathcal{H}^{\oplus}_{x=0}$.

Step VI. *Representation of Dirac Observables*
We will restrict the discussion to strong Dirac observables. See section 3.6 for the more interesting case of weak Dirac observables. A strong bounded Dirac observable D commutes with $\widehat{\mathbf{M}}$ and then preserves the fibres $\mathcal{H}^{*\oplus}_x$. In terms of a cyclic C^∞ system Ω^*_n we find measurable functions G^*_{mn} such that $D\Omega^*_m = \sum_n G^*_{mn}(\widehat{\mathbf{M}})\Omega^*_n$. Then

$$D(x)e^*_m = \sum_n D^*_{mn}(x)e^*_n, \quad D^*_{mn}(x) = \chi_{M^*(x)}(m)\chi_{M^*(x)}(n)\sqrt{\frac{\rho^*_n(x)}{\rho^*_m(x)}}G^*_{mn}(x) \tag{4.3}$$

where $M^*(x) = \{n \in \mathbb{N};\ \rho^*_n(x) > 0\}$ and a representative for $G^*_{mn}(x)$ was chosen. For symmetric choice of $\rho^*_n(x)G^*_{mn}(x)$ expression (4.3) is automatically self − adjoint and bounded on $\mathcal{H}_{phys}$ if D is on $\mathcal{H}$ no matter how the $\rho^*_n(0)$ are chosen. Moreover, for different choices of Ω^*_n, c^*_n we can always choose the corresponding different $\rho^*_n(0), G^*_{mn}(0)$ such that the induced representations of the strong Dirac observables on the physical Hilbert space are unitarily equivalent, see above. This makes in particular the dimension $N^*(0)$ of $\mathcal{H}^{*\oplus}_0$ independent of the $\Omega^*_n,\ c^*_n$. Thus we need to choose the $\rho^*_n(0), G^*_{mn}(0)$ only once and then only the weak Dirac observables can fix the ambiguity in the K_*. The $\rho^*_n(0)$ should be constrained by the requirement that the physical Hilbert space contains a sufficient number of semiclassical states and the requirement that the physical Hilbert space should be an irreducible representation for the induced action of a complete subalgebra of bounded self − adjoint Dirac observables which are defined on the unconstraned Hilbert space $\mathcal{H}$, see above.

5 Conclusions

In our companion papers [27, 28, 29, 30] we will apply the Master Constraint Programme and in particular the Direct Integral Decomposition (DID) to models of varying degree of complexity, starting with finite dimensional systems with a finite number of Abelean first class constraints linear in the momenta and ending with infinite dimensional systems (interacting field theories) with an infinite number of first class constraints not even polynomial in the momenta which close with structure functions only rather than with structure constants. This latter worst case scenario is precisely the case of 3+1 dimensional General relativity plus matter and therefore we believe that the Master Constraint Programme has been scrutinized in sufficiently complicated situations.

We hope to be able to convince the reader that the Master Constraint Programme can be very successfully applied to this wide range of constrained theories including those where other methods fail. While due care must be taken when squaring constraints, the Master Constraint Programme is sufficiently flexible in order to deal with the associated factor ordering problems and the worsened ultraviolet behaviour in these examples.

The Master Constraint Programme was invented in [17] in order to overcome the present obstacles in implementing the dynamics in LQG outlined in the introduction and in more detail in [10]. That it also provides the physical inner product of theory and even offers some handle on the Dirac observables comes at quite a surprise. So far the only systematic procedure in order to arrive at the physical inner product of a constrained theory was the group averaging method of RAQ [11] reviewed in section 3.7 and RAQ ideas were used very successfully in LQG in order to derive the Hilbert space of spatially diffeomorphism invariant states [8]. However, the RAQ method usually fails when the constraint algebra is not a finite dimensional Lie algebra.

It is here where the Master Constraint Programme can take over and enables us to make progress, since the (infinite) dimensional constraint algebra, whether it closes with structure functions or structure constants, is replaced by a one − dimensional Abelean Lie algebra. The only restriction is that the Hilbert space be separable, or that it can be decomposed into a possibly uncountably infinite direct sum of $\widehat{\mathbf{M}}$ −invariant separable Hilber spaces. For this case the RAQ method and the Master Constraint Programme essentially coincide with the difference that the Master Constraint Programme does not require the additional input of a nuclear topology on a dense subspace of the kinematical Hilbert space, the Master Constraint Programme just uses the spectral theory of the $\widehat{\mathbf{M}}$ and other physically motivated structures outlined in section 3.5 which involve less ambiguities than in the RAQ programme as shown in section 3.7. On the other hand the Master Constraint Operator itself generically provides a natural nuclear topology [14] as explained in [10] and also in section 3.7 so that in this case both procedures are really rather close.

The success of the programme of course rests on the question whether we can really quantize 3+1 General Relativity (plus matter) with this method. While we will show in [17] that there are no more mathematical obstacles on the way in order to complete the programme, it is not yet clear whether the resulting physical Hilbert space contains a sector which captures the semiclassical regime of both General Relativity and Quantum Field Theory on curved spacetimes. In order to show this, it will be necessary to develop approximation methods to construct the physical Hilbert space, such as path integral methods using coherent states, thus defining a new type of spin foam models as outlined in [10]. Approximation methods are mandatory because General Relativity is a fantastically difficult interacting quantum field theory with no hope to be solvable exactly. In order to complete this step we must develop spatially diffeomorphism invariant coherent states because the Master constraint is defined only on the spatially diffeomorphism invariant Hilbert space. After having constructed the physical Hilbert space by DID methods, at least approximately, one must eventually construct physical semiclassical states. All of these steps are parts of a hard but, we believe, not hopeless research project which is now in progress. At least the mathematical obstacles concerning the solution of the Hamiltonian constraints are now out of the way and we can in principle carry out the mathematical quantization programme to the very end.

The results of this series of papers, in our mind, demonstrate that the mathematics of the Master Constraint Programme succeeds in a large class of typical examples to capture the correct physics so that one can be hopeful to be able to do the same in full 3+1 quantum gravity.

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