An algebraic extension of Dirac quantization: Examples

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Abstract
An extension of the Dirac procedure for the quantization of constrained systems is necessary to address certain issues that are left open in Dirac’s original proposal. These issues play an important role especially in the context of non-linear, diffeomorphism invariant theories such as general relativity. Recently, an extension of the required type was proposed by one of us using algebraic quantization methods. In this paper, the key conceptual and technical aspects of the algebraic program are illustrated through a number of finite dimensional examples. The choice of examples and some of the analysis is motivated by certain peculiar problems endemic to quantum gravity. However, prior knowledge of general relativity is not assumed in the main discussion. Indeed, the methods introduced and conclusions arrived at are applicable to any system with first class constraints. In particular, they resolve certain technical issues which are present also in the reduced phase space approach to quantization of these systems.

1 Introduction
A number of systems with first class constraints arise naturally in mathematical physics: interesting examples are provided by Yang-Mills theories, general relativity, string theory and topological field theories. The problem of non-perturbative quantization of such theories is of considerable interest from both physical and mathematical perspectives. In the case of QCD for example, one hopes that a non-perturbative quantization would provide a satisfactory explanation of the physical phenomenon of confinement. Similarly, a full quantization of topological field theories is expected to provide a wealth of information on the topology of low dimensional manifolds as well as a classification of knots.
There are two major avenues to the non-perturbative quantization of such systems. The first is the Dirac approach, in which, roughly speaking, one first ignores the constraints, quantizes the system and then selects the admissible physical states by demanding that they be annihilated by the quantum constraint operators. The second is the reduced phase space method where one first eliminates the constraints classically and then quantizes the resulting unconstrained system. In this paper, we shall focus on the Dirac method although some of the main points we raise and the conclusions we reach are relevant also to the reduced phase space method.

In an algebraic version of the Dirac quantization procedure [1]—essentially the one followed originally by Dirac— one first ignores the constraints and constructs a “kinematical” operator algebra \( \mathcal{A} \) starting from the phase space of the system. One then seeks a representation of \( \mathcal{A} \) by operators acting on a complex vector space \( \mathcal{V} \). Next, one represents the constraints as concrete operators on the chosen vector space. Imposition of constraints is then carried out by finding the kernel of the constraint operators. Since the operators are all linear, the kernel \( \mathcal{V}_{phy} \) has a natural vector space structure. This is the space of physical states and elements of \( \mathcal{A} \) which map \( \mathcal{V} \) to itself are the physical operators. In simple physical systems, one can carry out this program completely. For source-free Maxwell fields in Minkowski space, for example, the algebra \( \mathcal{A} \) is generated by \( \hat{A}(g) := \int d^3x \hat{A}_a(x) g^a(x) \) and \( \hat{E}(f) := \int d^3x \hat{E}^a(x)f_a(x) \), the smeared vector potentials and electric fields. For the vector space \( \mathcal{V} \), one can choose the space of functionals of vector potentials \( \Psi(A) \), represent \( \hat{A}(g) \) by a multiplication operator and \( \hat{E}(f) \) by a (directional) derivative (in the direction of \( f_a \)). One then imposes the Gauss constraint:

\[
\int d^3x \hat{E}^a \partial_a \Lambda \circ \Psi(A) = 0 \text{ for all suitably regular functions } \Lambda(x). 
\]

This equation can be readily solved. It tells us that \( \Psi(A) \) must be gauge invariant. Thus, as one might expect, the space \( \mathcal{V}_{phy} \) of physical states is precisely the space of gauge invariant functions of vector potentials.

This general procedure, however, is incomplete. The most significant limitation is that it leaves open the issue of finding the inner product on the space \( \mathcal{V}_{phy} \) of physical states; no prescription whatsoever is provided. In practice, one generally appeals to suitable symmetries and asks that the inner product be such that these symmetries are unitarily implemented in the quantum theory. In the above example of free Maxwell fields, the required symmetries are provided by the Poincaré group acting on the underlying Minkowski space-time. However, an appropriate symmetry group is not always available. In the case of general relativity, for example, there is no background space-time and hence no analog of the Poincaré group. One might imagine using the entire diffeomorphism group. However, just as the quantum constraint of Maxwell theory requires that all physical states be gauge invariant, those of general relativity require that they all be diffeomorphism invariant. The diffeomorphism group thus has a trivial action on \( \mathcal{V}_{phy} \); it is unitary with respect to any inner product! Thus, the fact that there is no prescription available to find the inner product is a severe limitation, especially in the context of diffeomorphism invariant theories.

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1 One might seek symmetries directly on the infinite dimensional phase space. However, it is known that appropriate symmetries fail to exist. For 4-dimensional general relativity, see [2, 3]. The results of [3] also hold in 3-dimensional relativity [4].
A second limitation arises already in the first step, in the construction of the algebra $\mathcal{A}$. In simple examples, such as the free Maxwell fields discussed above, the phase space is linear and the construction of $\mathcal{A}$ is straightforward. However, in general, the phase space is a genuine manifold, i.e., it does not admit a global chart. In the classical theory, then, it is not possible to specify a complete set of globally defined configuration and momentum variables unless they are overcomplete. We can associate operators with all these variables. However, then we have to face the overcompleteness squarely in the quantum theory. (This situation arises, for example, in lattice gauge theories, where the Wilson loop variables are overcomplete.) In the original Dirac program, this issue was not addressed.

These –and related– issues were considered by Isham in [5], where he developed a group-theoretic approach to quantization to resolve these difficulties. In this paper, we will focus on another approach, based on algebraic methods. These methods are more general in the sense that, if an appropriate “canonical group” on the classical phase space can be found to complete the Isham program for a given system, key steps of the algebraic program would be automatically completed. On the other hand, there also exist other methods to complete the program. Being more general, however, the algebraic program is correspondingly less specific: While the group theoretic methods are “tight” in the sense that once the appropriate group is found, very little new input is needed, as we will see in section 2, the algebraic program needs inputs at several stages.

In the algebraic approach, the problem of finding the inner product was addressed through the following prescription: roughly, it states that the inner product should be such that a complete set of real classical observables should be represented on $\mathcal{V}_{\text{phy}}$ by self-adjoint operators. It is now known [7] that such an inner product, if it exists, is unique (modulo a multiplicative, overall constant). The prescription seems rather trivial at first sight. However, it is both powerful and –in some respects– subtle. In the case of 3-dimensional general relativity, for example, although there are again no symmetries [4] (and, for a general spatial topology, no “deparametrization” is available), this principle does select the physical inner-product uniquely. The subtleties can be seen in the proof of uniqueness [4], as well as in the occasional occurrence of unforeseen superselected sectors, examples of which are discussed later in this paper. The second issue, that of overcompleteness, was addressed by providing a detailed prescription for the construction of the algebra $\mathcal{A}$; the new inputs required to pass from the classical to the quantum theory were isolated and a prescription was given to handle the possible overcompleteness. Note that these two issues arise also in the reduced phase space method: one again needs a guideline to select the inner product on the space of physical quantum states, and, since the reduced phase spaces are typically genuine manifolds without a natural cotangent bundle structure, one must deal with overcompleteness. Therefore, the algebraic program developed in [6] is relevant to the reduced phase space approach as well.

The purpose of this paper is to illustrate various aspects of the program through five examples. The examples are motivated primarily by the problem of quantum general relativity and each of them mimics one or more “peculiarities” of general relativity. However, for the main discussion, no prior knowledge of general relativity is required.

In section 2, we summarize the algebraic program of [6] on which the rest of the
paper is based, with special attention to the new ingredients. In section 3, we consider an unconstrained system to illustrate how the prescription for finding the inner product can enable one to quantize systems with “hybrid” canonical variables, in which the configuration variable, for example, may be complex but its conjugate momentum, real. (Such variables arise in 4-dimensional general relativity and simplify the structure of Einstein’s equations considerably). In sections 4-6, we discuss four constrained systems. In each case, we carry out the quantization program in detail to illustrate its various subtle aspects. The example discussed in section 5 is especially interesting as it illustrates how the program can be used to resolve ambiguities that may have important physical consequences. In all these cases, we are motivated primarily by issues in mathematical physics. Therefore, issues of detailed physical interpretation and those associated with the measurement theory will be left untouched.

The program of [6] was distilled and refined from a number of examples. Because of this and because we have tried to make our discussion here self-contained, there is some inevitable overlap between [6] and the material covered in this paper. The previous discussion was, however, incomplete in certain respects and also contained a minor error. We have taken this opportunity to rectify the situation.

2 Quantization Program

In this section we will outline the extension of the Dirac quantization procedure for constrained systems—which constitutes the basis for the rest of the paper—and discuss in some detail its key features. The extension is based on the algebraic approach to quantum mechanics [8, 9].

2.1 The main steps

Consider a classical system for which the phase space \( \Gamma \) is a real symplectic manifold (which will be finite dimensional in all examples discussed in the paper). We are particularly interested in systems which are subject to first class constraints. To quantize such a system, we proceed in the following steps:

1. Select a subspace \( \mathcal{S} \) of the vector space of all smooth, complex-valued functions on \( \Gamma \) subject to the following conditions:

   (a) \( \mathcal{S} \) should be large enough so that any sufficiently regular function on the phase space can be obtained as (possibly a suitable limit of) a sum of products of elements \( F^{(i)} \) in \( \mathcal{S} \). Technically, \( \mathcal{S} \) is (locally) complete if and only if the gradients of the functions \( F \) in \( \mathcal{S} \) span the cotangent space of \( \Gamma \) at each point. The unit function “1” should also be included in \( \mathcal{S} \).

   (b) \( \mathcal{S} \) should be closed under Poisson brackets, i.e. for all functions \( F,G \) in \( \mathcal{S} \), their Poisson bracket \( \{F,G\} \) should also be an element of \( \mathcal{S} \).

   (c) Finally, \( \mathcal{S} \) should be closed under complex conjugation, i.e. for all \( F \) in \( \mathcal{S} \), the complex conjugate \( \bar{F} \) should be a function in \( \mathcal{S} \).
Each function in $S$ is to be regarded as an *elementary classical variable* which is to have an *unambiguous quantum analog* \cite{9}. The first requirement on $S$ ensures that the space of the resulting elementary quantum operators is “large enough,” the second enables us to define commutators between these operators unambiguously while the third will lead us to the $\star$-relations between these operators. It is often the case that in order to satisfy the completeness requirement, one is forced (say by the non-trivial topology of the phase space) to include more functions in the set $S$ than the dimension of the phase space. In this case, there are algebraic relations between them.

2. Associate with each element $F$ in $S$ an abstract operator $\hat{F}$. Construct the free algebra generated by these *elementary quantum operators*. Impose on it the canonical commutation relations, $[\hat{F}, \hat{G}] = i\hbar \{\hat{F}, \hat{G}\}$, and, if necessary, also the (anticommutation) relations which capture the algebraic identities satisfied by the elementary classical variables. (The details are discussed in section 2.2.) Denote the resulting algebra by $A$.

3. On this algebra, introduce an involution operation\footnote{An involution operation on $A$ is a map $\star$ from $A$ to itself satisfying the following three conditions for all $A$ and $B$ in $A$: i) $(A + \lambda B)^\star = A^\star + \lambda B^\star$, where $\lambda$ is any complex number and $\bar{\lambda}$ its complex conjugate; ii) $(AB)^\star = B^\star A^\star$; and, iii) $(A^\star)^\star = A$.} denoted by $\star$, by requiring that if two elementary classical variables $F$ and $G$ are related by $\bar{F} = G$ (where $\bar{F}$ denotes the complex conjugate of $F$), then $\hat{F} \star = G$ in $A$. Denote the resulting $\star$-algebra by $A^{(\star)}$. As can be seen from its definition, the $\star$-relation on $A^{(\star)}$ reflects the reality relation between the elementary variables.

4. Construct a linear representation of the abstract algebra $A$ via linear operators on some complex vector space $V$. (Because of the structure of $A$ the canonical commutation relations and the anticommutation relations (if any) should, in particular, be satisfied on $V$.) Note that for now the $\star$-relations on $A^{(\star)}$ are to be ignored.

5. Obtain explicit operators $\hat{\mathcal{C}}$ on $V$, representing the quantum constraints. In general, a choice of factor ordering (and, in the case of systems with an infinite number of degrees of freedom, also of regularization) has to be made at this stage. Physical states lie in the kernel $V_{phy}$ of these operators. That is, $|\psi\rangle$ is a physical state only if it is a solution to the quantum constraint equation:

$$
\hat{\mathcal{C}} |\psi\rangle = 0.
$$

(2.1)

6. Extract the physical subalgebra, $A_{phy}$, of operators that leave $V_{phy}$ invariant. Not all operators in $A$ are of this type. An operator $\hat{A}$ in $A$ will leave $V_{phy}$ invariant if and only if $\hat{A}$ commutes weakly with the constraints, i.e.

$$
[\hat{A}, \hat{\mathcal{C}}_{I}] = \sum_{J} f_{I}^{J} \hat{\mathcal{C}}_{J}.
$$

(2.2)
Operators that satisfy (2.2) are the quantum observables or physical operators. From the ⋆-relation on \(A^{(\ast)}\), we induce an involution (denoted again by ⋆) on the physical algebra \(A_{\text{phy}}\). (See the remark in section 2.4.) Denote the resulting ⋆-algebra of physical operators by \(A_{\text{phy}}^{(\ast)}\).

7. Introduce on \(V_{\text{phy}}\) a Hermitian inner product so that the ⋆-relations on \(A_{\text{phy}}^{(\ast)}\) are represented as Hermitian adjoint relations on the resulting Hilbert space. In other words, if \(\hat{F}^{\ast} = \hat{G}\) in the abstract algebra \(A_{\text{phy}}^{(\ast)}\), then the inner product on physical states should be chosen such that the corresponding explicit operators in the representation satisfy \(\hat{F}^\dagger = \hat{G}\), where \(\dagger\) is the Hermitian adjoint with respect to the physical inner product.

Note that the steps listed above are meant to be broad guidelines which help streamline the procedure. They are not meant to be rigid rules. We will now discuss in some detail those features of the program which involve some subtleties.

### 2.2 Algebraic relations

As we mentioned above, in the case when the phase space \(\Gamma\) is a genuine manifold, the completeness requirement on the space \(S\) of elementary classical observables leads one to an overcompleteness; there are algebraic relations between elements of \(S\). These have to be incorporated in the quantum theory in an appropriate fashion. Let us illustrate this point by a simple example. Consider a particle confined to a circle. Then, the configuration space is \(S^1\), the simplest non-trivial manifold, and the phase space \(T^\ast(S^1)\) is topologically \(S^1 \times \mathbb{R}\). Since \(S^1\) does not admit a global chart, we let \(S\) be the four-dimensional vector space generated by, say, the set of functions \((1, \cos \theta, \sin \theta, p_\theta)\), where \(\theta\) is the standard angular parameter on \(S^1\), and \(p_\theta\), its canonically conjugate momentum. Thus, although the phase space is two dimensional, \(S\) contains three nontrivial generators. Hence, in this case (in addition to the canonical commutation relations) there is one algebraic relation to incorporate in the quantum theory: we should require that \((\cos \theta)^2 + (\sin \theta)^2 = 1\). If we simply ignore this relation, we would be quantizing a theory which is quite different from the one we started out with. More generally, if the phase space \(\Gamma\) is \(m\)-dimensional and there are \(n\) non-trivial generators of \(S\), one expects \(n - m\) algebraic relations between the elementary variables, which would “cut the physical algebra down to the right size”.

How do we incorporate the algebraic constraints in the quantum theory in a more general setting? Consider first the simplest case. Suppose \(F_1, \ldots, F_n\) are elementary variables, all the Poisson brackets between which vanish. Then, if they are subject to a relation \(f(F_1, \ldots, F_n) = 0\) on the classical phase space, we require that

\[
f(\hat{F}_1, \ldots, \hat{F}_n) = 0
\]

on \(A\). This condition generalizes the circle example considered above. Next, let us consider relations between elementary variables whose Poisson brackets do not necessarily vanish. Now, the idea is that if the three functions \(F, G, H \equiv F \cdot G\) on \(\Gamma\) are all in the
space $S$ (and thus are to have unambiguous quantum analogs), then we should require that in $\mathcal{A}$:

$$\hat{F} \cdot \hat{G} + \hat{G} \cdot \hat{F} - 2\hat{H} = 0.$$  \hspace{1cm} (2.4)

More generally, suppose there is a set of $m$ elementary functions, $(F_1, \ldots, F_m)$, which are such that the product $H = F_1 \cdot F_2 \cdots F_m$ is also an elementary variable. Then, the prescription is to impose

$$\hat{F}_1 \cdot \hat{F}_2 \cdots \hat{F}_m - \hat{H} = 0,$$  \hspace{1cm} (2.5)

on the algebra constructed from $S$, where as usual $(1 \cdots m)$ denotes $1/m!$ times the sum of all the permutations. Technically, the imposition of these relations simply amounts to taking the quotient of the free algebra by the ideal generated by the left sides of (2.3) and (2.5).

Note that even though we are imposing “anti-commutation relations”, there is nothing fermionic about the system. Note also that the purpose of (2.3) and (2.5) is not to resolve factor ordering ambiguity since all $\hat{F}_i$ in (2.3) commute and since $\hat{H}$ in (2.3) is, by assumption, an elementary operator. Rather, (2.3) and (2.5) are imposed to remove unwanted sectors in the final quantum description. In the circle example considered above, in particular, the prescription rules out quantizations in which the sum $(\cos \theta)^2 + (\sin \theta)^2$ of operators fails to equal the identity. More generally, the algebraic identities arise due to a “failure of global coordinatization” of the phase space. We cannot classically solve the algebraic identity and eliminate one of the elementary functions globally on the phase space. The identity is then incorporated in quantum theory through the anti-commutation relations.

Given a classical identity $F \cdot G = H$, one might imagine incorporating it in the quantum theory only “up to terms of the order $\hbar$.” Indeed, in place of the ACR (2.4), we could impose a nonsymmetric condition of the form

$$\hat{F} \cdot \hat{G} + \hat{G} \cdot \hat{F} + \delta \hbar \{\hat{F}, \hat{G}\} - 2\hat{H} = 0.$$  \hspace{1cm} (2.6)

Since in the limit $\hbar \to 0$ the extra term on the left side vanishes, independent of the (real) value of $\delta$ we obtain the correct classical limit. Our prescription (2.4) just sets $\delta$ to zero. This choice is motivated by two considerations. First is simplicity. For definiteness, we need to give a specific guideline to construct the $\star$-algebra of quantum operators and setting $\delta$ to zero is the simplest choice. Secondly, in the standard Schrödinger-type quantization of systems whose configuration space is a manifold (see, e.g., [4], or [6, appendix C]), $\delta$ does turn out to be zero. Since this is a very large class of examples, it is reasonable to adopt our prescription as a rule of thumb to begin with. If in certain systems, there are specific physical and/or mathematical reasons not to make this choice, we can treat them as exceptional cases and resort to the more general prescription of (2.6).

\footnote{In all the examples considered in this paper as well as in [3, 10], overcompleteness arises due to algebraic relations between elementary variables of the type discussed here. In general, however, the relations may be more complicated and we do not have a general prescription to handle such cases.}
2.3 Selection of the inner product

The idea behind our strategy is simply to require that real classical observables should become self-adjoint (or, rather, symmetric) quantum observables. In a certain sense, the idea is rather elementary. After all, in elementary quantum mechanics, the (real) physical observables always become Hermitian operators on the Hilbert space of quantum states. However, the notion of using this as a general principle to select the inner product appears to be new. As we emphasized in section 1, the Dirac quantization program itself does not provide a strategy to select the inner product on physical states. As a general rule, underlying symmetries —such as the Poincaré invariance— are invoked to arrive at the inner product. However, in many physical systems, such as general relativity or the the finite dimensional systems considered in this paper, there are no obvious symmetries that can be invoked. The strategy of using the reality conditions can then be quite powerful.

It is important to note the precise manner in which the reality conditions are to be imposed. For simplicity of discussion let us, for a moment, consider an unconstrained system. Then, one begins with a vector space representation of the algebra $A$ of operators and invokes the reality conditions to select the inner product on the vector space such that the $*$-relations between abstract operators in $A$ become Hermitian-adjoint conditions on the concrete operators in the given representation. A theorem due to Rendall [7] ensures that, if the inner product exists, then it is unique up to an overall multiplicative constant on each irreducible representation of $A$. Note, however, that the procedure is tied to the initial choice of the vector space representation. Therefore, one can still have inequivalent quantizations. In linear field theories in Minkowski space, for example, there are infinitely many inequivalent representations of the CCRs in all of which the field operators are self-adjoint. From the perspective of the reality conditions, the inequivalence arises essentially because of the freedom in the initial vector space representation.

Note that there is no a priori guarantee that the vector space would admit an inner product satisfying the required quantum reality conditions. If it does not, one must change the vector space representation judiciously and start all over again. Thus, the success of the procedure does depend on the initial choice. A simple example in which no inner-product implementing the reality conditions exists in an "obvious" vector space representation, but can be found uniquely in a slightly modified one, is discussed in [6, p. 155]).

Perhaps the most interesting examples of the success of this strategy are provided by toy models that arise from general relativity: mini-superspaces (see, e.g., [11, 12, 13]) and 2+1-dimensional gravity (see, e.g., [6, §17]). Let us focus on 2+1 gravity because it shares all the conceptual difficulties with the 3+1-dimensional theory. In this case, it was generally believed that it would be impossible to find the physical inner product without "deparametrizing" the theory first (i.e., separating an internal time variable from the true, dynamical degrees of freedom). In the general case when the Cauchy slices are of a genus greater than one, the problem of deparametrization is still open. However, the strategy of using the reality conditions does work and selects the inner product unambiguously (in the connection representation, see e.g. [6, §17]). Thus, the
strategy enables one to separate the problem of time from the problems of finding the complete mathematical structure, including the Hilbert space structure on the space of physical states. In full, 3+1-dimensional quantum gravity, it may well be that time can be introduced only as an approximate notion. It is therefore important to have alternate strategies available to construct the complete mathematical framework.

In this paper, we will consider only finite dimensional examples and will need to introduce the inner product just on physical states, i.e., solutions to constraints. Indeed, even if one introduced an inner product on the space $V$, solutions to constraints will typically not be normalizable with respect to this inner product. In certain cases – especially for systems with an infinite number of degrees of freedom – it is nonetheless useful to have an inner product available on $V$ for technical reasons: this structure can restrict the factor ordering choices, enable one to regulate products of operator-valued distributions that may feature in the expressions of constraints and naturally suggest the appropriate function spaces in which the solutions to constraints should lie [14]. In such cases, then, one can use the reality conditions on $V$ to introduce a fiducial, kinematic inner product.

2.4 Physical $\star$-algebra

Let us explore the space of physical operators. An operator $\hat{A}$ in $\mathcal{A}$ will leave the space of solutions to the quantum constraint equation (2.1) invariant if and only if $[\hat{A}, \hat{C}_I] = \sum_J f^I_J \hat{C}_J$. The collection of all such operators –which includes the constraints themselves– forms a sub-algebra of $\mathcal{A}$. Denote it by $\mathcal{A}_{phy}'$. Since constraints annihilate all physical states, the algebra $\mathcal{A}_{phy}$ of physical observables can be obtained “by setting the constraint operators to zero” in $\mathcal{A}_{phy}'$. More precisely, one constructs the ideal $\mathcal{I}_C$ of $\mathcal{A}_{phy}'$ generated by the constraints and takes the quotient of $\mathcal{A}_{phy}'$ by this ideal: $\mathcal{A}_{phy} := \mathcal{A}_{phy}' / \mathcal{I}_C$. Since there may be some ambiguity in the correspondence between the classical and quantum observables, it is at this stage that some factor ordering choices for the physical operators may have to be made, before one quotients by $\mathcal{I}_C$.

Now, if $\hat{A}$ in $\mathcal{A}$ belongs to $\mathcal{A}_{phy}'$, its $\star$-adjoint in $\mathcal{A}$, $\hat{A}^\star$, may not belong to $\mathcal{A}_{phy}'$. Hence, in general the $\star$-relation on $\mathcal{A}$ does not induce an involution on $\mathcal{A}_{phy}$. In this case, no prescription is available to select the physical inner product in the simple program outlined in section 2.1. If, on the other hand, $\hat{A}^\star \in \mathcal{A}_{phy} \forall \hat{A} \in \mathcal{A}_{phy}$, then we do obtain an involution on $\mathcal{A}_{phy}$ (denoted again by $\star$) and hence a physical $\star$-algebra $\mathcal{A}_{phy}^{(\star)}$, which can now be used to select the inner product. For what kind of physical systems is the above condition guaranteed to be satisfied? Consider, for example, the case when the constraint operators satisfy: $\hat{C}_I^\star = \hat{C}_I, \forall I$ (i.e. the classical constraint functions are all real). Now, if a physical operator $\hat{A}$ commutes strongly with the constraints, i.e. if $[\hat{A}, \hat{C}_I] = 0$, then $\hat{A}^\star$ is also a physical operator, even though $\hat{A}^\star \neq \hat{A}$. We will see that this situation occurs in a number of model systems. In these cases, the quantization program can be completed successfully. Note however, that it is not essential that the operators commute strongly with the constraints for the $\star$-relations to be well-defined on the physical algebra. For example, if a set of generators of $\mathcal{A}_{phy}$ are their own $\star$-adjoints (i.e. if they correspond to real functions on the phase space), the $\star$-relations on $\mathcal{A}$ induce an unambiguous $\star$-relation on $\mathcal{A}_{phy}$.
Finally, note that to capture the full physics of the model under investigation, the algebra $\mathcal{A}_{\text{phy}}$ has to be complete in an appropriate sense: the set of classical functions corresponding to the generators of $\mathcal{A}_{\text{phy}}$ should be complete on the reduced phase space. In terms of the constraint surface itself, this amounts to the requirement that the set of Hamiltonian vector fields of the classical observables corresponding to the generators of $\mathcal{A}_{\text{phy}}'$ span the tangent space to the constraint surface. In practice, it is often the case that, if the completeness condition is not met globally, the theory has superselection rules; the “obvious” vector space representations are not irreducible.

2.5 Remarks

We will conclude with a few remarks.

Completeness of $\mathcal{V}_{\text{phy}}$:

Is there a criterion which will determine whether the space of solutions to the quantum constraint equation is physically “large enough”? Since –after one has found an inner product– $\mathcal{V}_{\text{phy}}$ is complete as a Hilbert space (and any vector space with a norm can be completed) this notion of completeness cannot help resolve the above question. However, we do have a physical notion of completeness of $\mathcal{A}_{\text{phy}}$, and thus we can require that $\mathcal{V}_{\text{phy}}$ be large enough to carry a faithful representation of the algebra of observables.

Solutions and physical states:

Physical states are normalizable solutions to the quantum constraint equation. However, not all solutions to the quantum constraints are normalizable with respect to the physical inner product. Thus, there is a distinction between physical states and solutions. Of course, physical states form a (generically proper) subspace of the kernel of the constraint operator. While one must keep this distinction in the back of one’s mind, we will no longer emphasize it.

Inputs to the program:

As we have emphasized, the steps outlined in section 2.1 do not constitute a crank that can be turned to convert a constrained classical theory to a quantum theory. Rather, the steps constitute broad guidelines that clarify and streamline the choices that are available in the transition. These choices arise through three main inputs: i) the choice of the space $\mathcal{S}$ of elementary classical variables; ii) the choice of the vector space representation of the algebra $\mathcal{A}$; and, iii) the choice of factor ordering in the expression of constraints. While these choices are restricted by a number of consistency conditions, there is nonetheless considerable freedom left at the end. In making these choices, therefore, one must use physical input. Generally, the final quantum theory one obtains does depend on the choices in quite a sensitive manner. This is not surprising: since the goal of quantization is to obtain the more complete quantum description starting from the “coarse-grained” classical theory, it necessarily requires a certain amount of new information which is hard to specify universally at the outset.

A particularly natural avenue to making these choices is provided by the group theoretic approach developed by Isham [4]. If the appropriate “canonical group” is identified,
it automatically provides the elementary variables, the operator expressions of the constraints, and the inner product on physical states. (For interesting examples, see, e.g., [4, 15].) Thus, this approach succinctly reduces the problem of finding the inputs needed in the algebraic program to that of finding an appropriate group action on the phase space. Another avenue is provided by geometric quantization: If a polarization which is appropriately compatible with the constraints can be found, one is led to physical states and a complete set of physical observables (see, e.g., [16]). One must still find, however, the inner product on the physical states via, e.g., the reality conditions.

3 Harmonic oscillator in the \((q, z)\) variables

We now present the simplest application of the quantization program. The aim is only to illustrate the role of the reality conditions. Therefore, in this section, we will ignore constraints.

As we discussed in the introduction, several features of our extension of the Dirac quantization scheme have been motivated by peculiarities of general relativity. One of these is the fact that the Hamiltonian formulation simplifies if one uses a “hybrid” pair of canonical variables (see e.g. [17, 6]), where one variable is real and the other is complex. In quantum theory it is then simplest to work in a representation in which the states are holomorphic functionals of the complex variable, treat the real variable as momentum and represent it by a functional derivative [17, 6]. A question that arises immediately is whether the procedure is consistent: can the momentum conjugate to a complex variable be itself Hermitian?

To address this issue in a simple context, in this section we will consider the harmonic oscillator in terms of hybrid variables. More precisely, we will quantize the oscillator using hybrid elementary variables and find that the implementation of the Hermiticity conditions leads to a quantum theory which is unitarily equivalent to the usual one. Thus there is no \textit{a priori} obstruction to using such variables.

Consider the phase space of a harmonic oscillator of unit mass and spring constant. \(\Gamma\) is coordinatized by the real canonically conjugate functions \((q, p)\). In analogy with general relativity in the connection variables, let us introduce the complex variable \(z = q - ip\). Note that the phase space is real; \((q, z)\) do not constitute a chart on \(\Gamma\). However, we choose as \(S\) the vector space spanned by the (complex) functions \((1, q, z)\). This set is complete, and closed under Poisson brackets. \(S\) is also closed under complex conjugation, since \(\bar{q} = q\) is real and \(\bar{z} = 2q - z\). These hybrid reality conditions are analogous to those for the new variables in linearized general relativity. The canonical commutation relations between the corresponding operators are

\[
[\hat{q}, \hat{z}] = \hat{1},
\]  

and the \(\star\)-relations are:

\[
\hat{q}^\star = \hat{q}, \quad \hat{z}^\star = 2\hat{q} - \hat{z}.
\]  

(These are completely analogous to those one encounters if one linearizes general relativity in the hybrid canonical variables [18, 6, section 11.5].) We next have to find a representation of this algebra. The hybrid variables suggest a new approach. We can represent the above operators on the space of \textit{holomorphic} functions of one complex
variable. Let $\mathcal{V}$ be the space of holomorphic functions $\psi = \psi(z)$, and represent the operators by:

$$\hat{z} \circ \psi(z) = z \cdot \psi(z) \quad \text{and} \quad \hat{q} \circ \psi(z) = \frac{d}{dz} \psi(z).$$

(3.3)

For linearized gravity, and indeed for general relativity itself, the analogous holomorphic (or self-dual) connection representation is particularly convenient since it greatly simplifies the form of the constraints.

A natural ansatz for the inner product on these holomorphic states is

$$\langle \psi | \chi \rangle = \int \frac{dz \wedge d\bar{z}}{2\pi i} e^{\mu(z, \bar{z})} \bar{\psi} \chi,$$

(3.4)

where $\mu = \bar{\mu}$ is a function to be determined. We now have to impose the Hermiticity conditions (3.2) on these operators. This is the crucial step: it is quite counterintuitive to have a real momentum (represented by a holomorphic derivation) “canonically conjugate” to a complex variable, and hence the consistency of the formalism is not immediately obvious.

However, the calculation is straightforward. The Hermiticity condition on $\hat{q}$ yields a differential equation for $\mu$ which constrains $\mu$ to be of the form $\mu = \mu(z + \bar{z})$. Next, using the holomorphicity of the wavefunctions, the Hermiticity condition on $\hat{z}$ yields another differential equation for $\mu$ which is solved by:

$$\mu(z, \bar{z}) = -\frac{(z + \bar{z})^2}{4}.$$

(3.5)

Hence, the Hermiticity conditions do determine the measure uniquely. Note that even though the measure does not “fall-off” as expected (for example in the $\text{Im}(z)$ direction), there exist normalizable states: these are of the form $\psi(z) = e^{\frac{z^2}{4}} f(z)$, where $f(z)$ are polynomials in $z$. The inner product (3.4,3.5) now yields:

$$\langle \psi | \psi \rangle = \int \frac{dz \wedge d\bar{z}}{2\pi i} e^{-\frac{z^2}{4}} |f(z)|^2.$$

(3.6)

How is this quantization related to the Bargmann quantum theory? Apart from a factor of 2 in the exponent which arises because the $z$ we have defined is $\sqrt{2}$ times the usual Bargmann variable, the inner product (3.4,3.6) corresponds to the standard Gaussian measure on the Bargmann states, establishing a unitary map between the two Hilbert spaces. Next, we can use this unitary map to compare the actions of the operators $(\hat{q}, \hat{z})$ in the two representations. The result is that the two quantum theories are unitarily equivalent.

Thus, we have completed the quantization of the 1-dimensional oscillator in the hybrid $(q, z)$ variables. The Hermiticity conditions on the elementary operators can be implemented, and they fix the inner product. This indicates that there is a priori no obstruction to the use of a hybrid set of variables of the type used in general relativity.

\[4\text{Alternately, one could represent } \hat{q} \text{ by } \hat{q} \circ \psi(z) = \frac{1}{\sqrt{2}}(\sqrt{2} \frac{d}{dz} + \frac{z}{\sqrt{2}})\psi(z). \text{ Then, the commutation relations are still satisfied, but the measure } \mu(z, \bar{z}) \text{ is the usual Bargmann measure } e^{-\frac{z^2}{4}}. \text{ The unitary equivalence is then manifest. (Recall that } z/\sqrt{2} \text{ is the usual Bargmann variable.)}\]
Remark:
As we noted after Eq.(3.2), the variables \((z, q)\) we used above and the resulting reality conditions are completely analogous to those encountered in the linearized version of general relativity. In the exact theory, however, one of the reality conditions is non-polynomial. To mimic this situation, Kuchař [19] has proposed the following model. Let the phase space be 2-dimensional, labelled by the real canonically conjugate variables \((Q, P)\), with \(Q > 0\), and let the Hamiltonian be \(h = QP^2 + 1/Q\). Then, if we set \(Z = 1/Q - iP\), and treat \(Q, Z\) as the hybrid canonical variables, the Hamiltonian simplifies to \(h = 2Z - QZ^2\); as in general relativity, it becomes a low order polynomial in the new variables. However, now one of the reality conditions is non-polynomial: \(\bar{Z} = -Z + 2/Q\). It was thought that its complicated nature would be an unsurmountable obstacle in carrying out the quantization program and concern was expressed that the situation may be similar in full general relativity [19].

It turns out however, that, by appropriately choosing a vector space representation of the algebra \(\mathcal{A}\) and an ansatz for the inner product, the quantization program can be completed in the Kuchař model too. The final description is as follows. We can choose \((1, Q, QZ)\) as the elementary variables. The \(*\)-relations are: \(Q^* = Q\) and \((QZ)^* = 2 - (QZ)\). Let us choose for the vector space \(\mathcal{V}\) the space of holomorphic functions \(\Psi(z)\) of one complex variable \(z = x + iy\), and set:

\[
\hat{Q} \circ \Psi(z) = \left(\frac{d}{dz} + \frac{z}{2}\right) \Psi(z) \quad \text{and} \quad (3.7)
\]

\[
\hat{QZ} \circ \Psi(z) = \left(\frac{z}{2} \frac{d}{dz} + \frac{z^2}{2} + \frac{3}{2}\right) \Psi(z), \quad (3.8)
\]

It is easy to check that the CCR are satisfied; we have a vector space representation of \(\mathcal{A}\). The inner product which implements the \(*\)-relations is:

\[
\langle \Psi | \Phi \rangle = \int dy \ e^{-\frac{1}{2}y^2} \left(\overline{\Psi(z)} \Phi(z)\right) \bigg|_{x=0}, \quad (3.9)
\]

where we have used the fact that holomorphic functions are completely determined by their restriction to the \(x = 0\) line. The Hamiltonian which generates the quantum dynamics is given by:

\[
\hat{h} \circ \Psi(z) = -\left(\frac{z^2}{2} \frac{d}{dz} + \frac{z^3}{2} + z\right) \Psi(z). \quad (3.10)
\]

It is straightforward to check that all three operators defined above are Hermitian and their commutators are \(i\) times the Poisson brackets of their classical analogs. Thus, the non-polynomiality of the reality conditions is not necessarily an obstacle to the completion of the program.

4 Coupled Oscillators
In the previous section we quantized an unconstrained system and used the (nontrivial) Hermiticity conditions on the elementary variables to determine the inner product on
quantum states. In this section we will consider two constrained systems, and illustrate how one can use the Hermiticity conditions on physical observables to obtain an inner product on physical states. Each of these systems will be built out of two harmonic oscillators with the same frequency, which will be set to 1 for simplicity.

In the more interesting of the two models, the oscillators are coupled to each other via a first class constraint on the difference between their energies. This model is of interest especially because it mimics certain features of general relativity in the geometrodynamical variables: i) the constraint is quadratic in momenta; ii) the kinetic piece of the constraint is of indefinite signature; and, iii) the potential term is also of indefinite sign. Due to these similarities, some of the qualitative results are of interest to quantum gravity, particularly quantum cosmology. In fact, this specific model corresponds precisely to the Friedman-Robertson-Walker universe (with $S^3$ spatial topology), conformally coupled to a massless scalar field (see section 4.3).

However, we will begin with a simpler but related model in which the two oscillators are coupled to each other via a first class constraint on the sum of their energies. This model has been used in the past as a testing ground for various ideas (e.g. the issue of time [20, 21]). Since it is simpler than the “energy difference” model, it will allow us to implement some of the new features of the quantization program in a familiar setting. We will then use the same approach for the energy difference model.

In the first two subsections, we will construct the Dirac quantum theories for the two models. (The reduced space quantum theories have been constructed in [10].) In the last subsection, we discuss several features of the energy difference model, including its relation to the minisuperspace mentioned above.

### 4.1 Constrained total energy

The 4-dimensional phase space of the system is described by position and momentum coordinates $(x_I, p_I, I = 1, 2)$. The first class constraint we wish to impose is

$$C \equiv \frac{1}{2}(p_1^2 + x_1^2 + p_2^2 + x_2^2) - E \approx 0,$$  

(4.1)

where $E \geq 0$ in order for the classical system to be well defined. Choose as the set $S$ of elementary classical variables the standard “creation” and “annihilation” functions on $\Gamma$

$$z_I = \frac{1}{\sqrt{2}}(x_I - ip_I) \quad \text{and} \quad \bar{z}_I = \frac{1}{\sqrt{2}}(x_I + ip_I),$$  

(4.2)

as well as the constant function. Since these elementary variables are algebraically independent, there are no ACRs in the quantum algebra $A$. In these variables, the constraint function is

$$C = (z_1\bar{z}_1 + z_2\bar{z}_2) - E.$$  

(4.3)

The quantum $\star$-algebra $A(\star)$ is straightforward to construct. To make the notation transparent we will denote the elementary quantum operators $\hat{z}_I$ by $\hat{c}_I$ and $\hat{\bar{z}}_I$ by $\hat{a}_I$. $A(\star)$ is then generated by the set of elementary quantum operators $(1, \hat{a}_1, \hat{c}_1, \hat{a}_2, \hat{c}_2)$ which satisfy the canonical commutation relations:

$$[\hat{a}_I, \hat{a}_J] = 0 = [\hat{c}_I, \hat{c}_J] \quad \text{and} \quad [\hat{a}_I, \hat{c}_J] = \delta_{IJ}, \quad I, J = 1, 2;$$  

(4.4)
and are subject to the ∗-relation
\[ \hat{a}_I^\dagger = \hat{c}_I, \quad \forall I. \] (4.5)

In terms of these operators, the quantum constraint we wish to impose is
\[ \hat{C} | \psi \rangle_{\text{phy}} := (\hat{c}_1 \hat{a}_1 + \hat{c}_2 \hat{a}_2 + 1 - E) | \psi \rangle_{\text{phy}} = 0, \] (4.6)
where we have symmetrized the operator product to resolve the ordering ambiguity in the constraint. (See the remark at the end of this section.)

The next step in the quantization program is to represent the algebra \( \mathcal{A} \) by means of concrete operators on a vector space \( \mathcal{V} \). (Recall that the ∗-relations are ignored at this stage.) Let us choose the vector space representation of \( \mathcal{A} \) as follows. Since any complete set of commuting operators consists of only two of the elementary operators, let us choose for \( \mathcal{V} \) the complex vector space spanned by states of the form \( | j, m \rangle \), where \( j \) and \( m \) are any complex numbers, and let us represent the elementary quantum operators as follows:
\[
\hat{a}_1 | j, m \rangle = \alpha_1 (j + m)| j - \frac{1}{2}, m - \frac{1}{2} \rangle, \\
\hat{c}_1 | j, m \rangle = \gamma_1 (j + m + 1)| j + \frac{1}{2}, m + \frac{1}{2} \rangle, \\
\hat{a}_2 | j, m \rangle = \alpha_2 (j - m)| j - \frac{1}{2}, m + \frac{1}{2} \rangle \\
\text{and} \quad \hat{c}_2 | j, m \rangle = \gamma_2 (j - m + 1)| j + \frac{1}{2}, m - \frac{1}{2} \rangle; \] (4.7)
where the coefficients, \( \alpha_I(k) \) and \( \gamma_I(k) \), functions only of their argument \( k \), are chosen to satisfy
\[ \alpha_1(k)\gamma_1(k) = k \quad \text{and} \quad \alpha_2(k)\gamma_2(k) = k. \] (4.8)

It is straightforward to check that the commutation relations (4.4) are satisfied by any representation (4.7) in which (4.3) is satisfied. Thus, so far we have a (rather large) family of vector space representations and none of them is preferred. Eq. (4.7) implies that the number operators \( \hat{N}_I = \hat{c}_I \hat{a}_I \) are represented simply by \( \hat{N}_1 | j, m \rangle = (j + m)| j, m \rangle \) and \( \hat{N}_2 | j, m \rangle = (j - m)| j, m \rangle \). Each \( | j, m \rangle \) is an eigenket of the total number operator \( \hat{N} = \hat{c}_1 \hat{a}_1 + \hat{c}_2 \hat{a}_2 \) with eigenvalue \( 2j \), as well as the difference between the number operators \( \hat{N}_1 - \hat{N}_2 \) with eigenvalue \( 2m \). (Thus, had we represented states as Bargmann type holomorphic wave functions, we would have \( \psi(z_1, z_2) := \langle z_1, z_2 | j, m \rangle \equiv z_1^{j+m}z_2^{-m}. \) The notation \( | j, m \rangle \) to represent the kets may seem strange at first. However, these angular momentum like states arise naturally because, as we will see below, the Poisson bracket algebra of physical observables is the Lie algebra of \( SO(3) \). The \( | j, m \rangle \) representation will therefore be more convenient than the number representation.

Since \( \hat{C} \) is diagonal in this representation, with eigenvalues \( 2j + 1 - E \), the quantum constraint is easy to solve. A basis for the space \( \mathcal{V}_{\text{phy}} \) of solutions to the quantum constraint equation is given simply by the kets \( \{ | j = L, m \rangle \} \), where \( L \) is now a fixed number, \( L = \frac{E - 1}{2} \). Note that this is a “small” subspace of \( \mathcal{V} \); \( j \) was an arbitrary complex number to begin with, but is now a fixed real number. However, \( m \) is still allowed to be an arbitrary complex number. Physical operators are the elements of \( \mathcal{A} \) that map \( \mathcal{V}_{\text{phy}} \) to itself; their action should preserve the total energy of the two oscillators. Clearly, operators that simultaneously raise the energy of one and lower the energy of the other

15
oscillator by a unit, and an operator that measures the energy difference, are physical operators. Hence, let us consider the algebra generated by the set of operators \( \{ \hat{L}_z, \hat{L}_\pm \} \), where \( \hat{L}_z := \frac{1}{2}(\hat{N}_1 - \hat{N}_2) \), \( \hat{L}_+ := \hat{c}_1 \hat{a}_2 \) and \( \hat{L}_- := \hat{c}_2 \hat{a}_1 \) are physical operators. The commutator algebra is given by

\[
[\hat{L}_+, \hat{L}_-] = 2\hat{L}_z \quad \text{and} \quad [\hat{L}_z, \hat{L}_\pm] = \pm \hat{L}_\pm; \quad (4.9)
\]

it is isomorphic to the Lie algebra of \( SO(3) \). The Hilbert space of physical states will thus provide a unitary representation of \( SO(3) \).

These representations are of course well known. However, we will arrive at them systematically following the various steps in the quantization program. This procedure will also help prepare the reader for our next example where the representation theory of the observable algebra is not so well known.

Using (4.7), we can evaluate the action of the physical operators on the physical states. Doing so, we get

\[
\hat{L}_z |L,m\rangle = m |L,m\rangle, \\
\hat{L}_+ |L,m\rangle = \lambda_+(m+1) |L,m+1\rangle \\
\hat{L}_- |L,m\rangle = \lambda_-(m) |L,m-1\rangle, \quad (4.10)
\]

where \( \lambda_\pm \) —functions of their arguments only— are just products of the coefficients \( \alpha_I, \gamma_I \) in (4.7). Since \( \alpha_I, \gamma_I \) are (non-unique) solutions of (4.8), the coefficients \( \lambda_\pm \) satisfy

\[
\lambda_+(m)\lambda_-(m) = (L + \frac{1}{2})^2 - (m - \frac{1}{2})^2. \quad (4.11)
\]

Since only the \( \lambda_\pm \) are relevant to the observable algebra, we can view (4.11) directly as a condition on \( \lambda_\pm \). With this condition, the canonical commutation relations of the observable algebra are also identically satisfied. Recall that we had considerable freedom in our choice of the representation (4.7) of the operator algebra \( \mathcal{A} \) since the coefficients \( \alpha_I \) and \( \gamma_I \) were arbitrary to a large extent. This freedom descends to the physical operator algebra: due to the existence of a multitude of solutions to (4.11), the representation (4.10) of the physical algebra is also not unique.

Recall that the program requires us to construct a complete algebra of observables. Let us pause to analyze this issue. The classical analogs of \( \{ \hat{L}_z, \hat{L}_\pm \} \) are the functions \( L_z := \frac{1}{2}(z_1 \bar{z}_1 - z_2 \bar{z}_2) \), \( L_+ := z_1 \bar{z}_2 \), \( L_- := \bar{z}_1 z_2 \) on phase space. One can easily check that the set \( \{ L_+, L_- \} \) is by itself complete, the set suffices to coordinatize the reduced phase space. It is in order to ensure that the algebra of observables is closed under Poisson brackets that one has to include \( L_z \) in the set of generators of \( \mathcal{A}_{phy} \), and thus make the set overcomplete. There is an algebraic relation satisfied by this overcomplete set which, it turns out, fixes a value of the Casimir invariant of \( \mathcal{A}_{phy} \). Using the definitions of \( \hat{L}_\pm \) and the commutation relations (4.4), one

\[\text{We have denoted these observables by } (L_z, L_\pm) \text{ rather than } (J_z, J_\pm) \text{ only to distinguish them from a related but different set of functions —that serve as observables in the next example— which will be denoted by } (J_z, J_\pm). \text{ No relation with orbital (as opposed to total) angular momentum is intended.}\]
finds that the algebraic relation is
\[ \hat{L}^2 := \hat{L}_z^2 + \frac{1}{2}[\hat{L}_+, \hat{L}_-] = L(L + 1). \]
(Recall that the value \( L = \frac{E - 1}{2} \) is determined by the classical constraint.) Equivalently, the relation can be expressed as
\[ \hat{L}_+ \hat{L}_- = (L + \frac{1}{2})^2 - (\hat{L}_z - \frac{1}{2})^2, \] (4.13)
in which form it is manifest that this condition on the operators is automatically satisfied because of (4.11). Thus the completeness requirement has been incorporated in our representation.

The next step in the program is to obtain an inner product on the space of physical states by requiring that the *-relations on the physical operators become Hermitian adjointness relations on the resulting Hilbert space. From the expressions for the physical operators in terms of the elementary quantum operators \( \hat{a}_I, \hat{c}_I \) and the *-relation (4.5), one obtains the *-relation induced on \( A_{\text{phy}} \):
\[ \hat{L}^*_+ = \hat{L}_- \quad \text{and} \quad \hat{L}^*_z = \hat{L}_z. \] (4.14)

First, consider only the operator \( \hat{L}_z \). Since it is to be Hermitian on the physical Hilbert space, its eigenvalues must be real, and its eigenkets with distinct eigenvalues must be orthogonal to each other. Hence \( m \) is real. (Note that \( L \) is already real on all solutions to the constraint.) Next, recall that the Hermiticity conditions are to be implemented separately on each irreducible representation of the algebra. The representation (4.10), however, is reducible: the physical operators either leave the value of \( m \) unchanged, or change it by an integer. Thus, the fractional part of \( m \) —denoted by \( \epsilon = \text{frac}(m) \)—is invariant under the action of \( \hat{L}_z, \hat{L}_\pm \). Now, consider \( \mathcal{V}^\epsilon_{\text{phy}} \), the vector space of states with the same fixed value of \( \epsilon \). Each subspace \( \mathcal{V}^\epsilon_{\text{phy}} \) carries an irreducible representation of the \( \text{SO}(3) \) Lie algebra (4.9). Let \( m = n + \epsilon \), \( n = \cdots -2, -1, 0, 1, 2 \cdots \). Each \( \mathcal{V}^\epsilon_{\text{phy}} \) has a countable basis, the elements of which are labelled by \( n \)—the integer part of \( m \)—and it is on these irreducible representations that we now wish to implement the remaining Hermiticity conditions. Prior to this implementation, we have a 1-parameter family of ambiguities in the quantization of the system, labelled by the parameter \( \epsilon \in [0, 1) \).

For definiteness, consider a representation with a fixed value of \( \epsilon \). The Hermiticity of \( \hat{L}_z \) implies that on \( \mathcal{V}^\epsilon_{\text{phy}} \) there exists an inner product in which the above basis is orthogonal; without any loss of generality, we can choose it to be orthonormal. Thus the inner product can be chosen to be:
\[ \langle \hat{L}, m' = n' + \epsilon | \hat{L}, m = n + \epsilon \rangle = \delta_{n', n}, \] (4.15)
where both states on the left have the same fractional part of \( m \). Note that it is only because we implement the Hermiticity conditions on an irreducible sector— with a countable basis—that we can postulate a Kronecker-\( \delta \) normalization on \( \mathcal{V}^\epsilon_{\text{phy}} \). Had we tried to introduce an inner product on the entire \( \mathcal{V}_{\text{phy}} \), we would have been led to a Dirac-\( \delta \) normalization. Finally, as in the familiar quantization of the \( \text{SO}(3) \) algebra, it is straightforward to show that the Hermiticity conditions (4.14) fix the coefficients \( \lambda_{\pm}(m) \). One finds that there exist non-trivial representations only when \( \epsilon = \text{frac}(L) \), and then only when \( L \) itself is half integer or integer (and thus for integer \( E \) only). The representation of the generators of \( A_{\text{phy}} \) is
\[ \hat{L}_z | L, m \rangle = m | L, m \rangle, \]
\[ \hat{L}_+ |L,m\rangle = \sqrt{(L-m)(L+m+1)} |L,m+1\rangle \]
\[ \hat{L}_- |L,m\rangle = \sqrt{(L+m)(L-m+1)} |L,m-1\rangle, \] (4.16)

where as before \( L = \frac{(E-1)}{2} \). It is easy to check that in the inner product (4.15), the Hermiticity conditions \( \hat{L}_+^\dagger = \hat{L}_- \) and \( \hat{L}_-^\dagger = \hat{L}_+ \) are satisfied, implementing the \( \star \)-relations.

This representation (4.16,4.15) of the observable algebra is unique up to unitary equivalence, since the Hermiticity conditions can only be implemented on the subspace labelled by \( \epsilon = \text{frac}(E) \). Not surprisingly (since the reduced phase space is compact), the representation is finite-dimensional, of dimension \( 2L+1 \). A basis is provided by states with \( m = -L, -L+1, \cdots L-1, L \). In the final analysis, the representation we have obtained is not surprising, given that \( \mathcal{A}_{\text{phy}} \) is just the Lie algebra of \( SO(3) \). However, we took this long route to to show that the quantization program, when implemented step by step, does lead one to the expected result.

Note that the coefficients \( \alpha_I, \gamma_I \) in (4.7) are left undetermined, and we have not obtained an inner product on the original representation space. However, (4.15) provides us with an inner product on \( \mathcal{V}_{\text{phy}} \). Let us summarize the steps by which the reality conditions have led us to the final result. Prior to imposing the reality conditions, there was considerable freedom in the choice of representation of the physical algebra: there exist representations of the observable algebra on solutions to the constraint labelled by complex-valued \( m \), the coefficients \( \lambda_\pm \) are not unique, and for each choice of \( \lambda_\pm \), there is a one parameter family of irreducible representations, labelled by \( \epsilon \). However, not all these representations are compatible with the reality conditions. The Hermiticity condition on one of the physical operators, \( \hat{L}_+^\dagger = \hat{L}_- \), allows only representations on states labelled by real \( m \), with the inner product (4.15). The further reality condition, \( \hat{L}_+^\dagger = \hat{L}_- \), then implies that there exist representations only for integer values of \( E \), and then the representation is unique.

The representations we have constructed above are only for integer \( E \). Is it possible to construct representations for arbitrary (positive) \( E \)? For the factor-ordering of the constraint that we have chosen, there is no quantum theory for non-integral \( E \). From the point of view of geometric quantization, this is not surprising since the reduced phase space is a compact manifold, \( S^2 \), and it admits a Kähler structure only for integer values of the radius [22, 23]. From ordinary quantum mechanics, we are familiar with the fact that the commutation relations (4.3) have only the integer and half-integer spin representations. Note however that there is a factor-ordering ambiguity in the choice of constraint operator. If we allow \( z_I \bar{z}_I \) to be represented by an undetermined convex linear combination of \( \hat{c}_I \hat{a}_I \) and \( \hat{a}_I \hat{c}_I \), then the resulting quantum constraint equation is

\[ \hat{C} | \psi \rangle_{\text{phy}} \equiv (\hat{c}_1 \hat{a}_1 + \hat{c}_2 \hat{a}_2 + 1 + \kappa - E) | \psi \rangle_{\text{phy}} = 0, \] (4.17)

where \( \kappa \in [-1, 1] \) represents the factor-ordering ambiguity. Now, even though \( L = \frac{E-\kappa-1}{2} \) is still integer or half-integer, \( E \) is no longer forced to be integer. Thus, there are (two) choices of ordering of the quantum constraint operator which allow us to find a non-trivial physical quantum theory, even when \( E \) is not an integer.
4.2 Constrained energy difference

The unconstrained phase space $\Gamma$ for this model is again $\mathbb{R}^4$, coordinatized by real variables $(x_I, p_I)$ or complex variables $(z_I, \bar{z}_I)$, $I = 1, 2$. The first class constraint we now wish to impose is however different. We will require that the difference between energies be a constant, $\delta$:

$$C := \frac{1}{2} (z_1 \bar{z}_1 - z_2 \bar{z}_2) - \delta \approx 0. \quad (4.18)$$

We will use the elementary operators (4.4-4.5) and representation (4.7) defined in the previous section. In terms of these operators, the quantum constraint we wish to impose is

$$\hat{C} | \psi \rangle_{phys} := \left[ \frac{1}{2} (\hat{c}_1 \hat{c}_2 - \hat{c}_2 \hat{c}_1) - \delta \right] | \psi \rangle_{phys} = 0, \quad (4.19)$$

where, since the constraint is the difference between the energies of the two oscillators, as long as we use the same ordering for each term $z_I \bar{z}_I$, there is no ambiguity in the constraint operator.

Since $\hat{C}$ is diagonal in this representation, with eigenvalues $m - \delta$, the quantum constraint is easy to solve. A basis for the physical subspace $V_{phys}$ is given simply by the kets $\{ | j, m = \delta \rangle \}$, where $j$ is an arbitrary complex number. Note that the situation here is reversed from the previous example: there, the constraint forced $j = L$ to be real and left $m$ arbitrary.

Next let us consider physical operators: these are elements of $\mathcal{A}$ that map $V_{phys}$ to itself and should thus maintain the difference in energies of the two oscillators. Clearly, operators that raise and lower the energy of each oscillator by a unit, and an operator that measures the total energy, are physical operators. Hence, consider the algebra generated by the set $\{ \hat{J}_+, \hat{J}_-, \hat{J}_z \}$; where $\hat{J}_+ := \hat{c}_1 \hat{c}_2$ raises the energy of each oscillator by a unit, $\hat{J}_- := \hat{a}_1 \hat{a}_2$ lowers the energy of each oscillator by a unit, and $\hat{J}_z := \frac{1}{2} (\hat{N} + 1)$ is half the total energy. The commutation relations between these operators are

$$[\hat{J}_+, \hat{J}_-] = -2 \hat{J}_z \quad \text{and} \quad [\hat{J}_z, \hat{J}_\pm] = \pm \hat{J}_\pm, \quad (4.20)$$

from which it is clear that they generate the Lie algebra of $SO(2, 1)$. (Note the difference from (4.3) in the sign of the first commutator.) $\hat{J}_+$ and $\hat{J}_-$ are the (angular momentum) raising and lowering operators, respectively. Note also that it is in order to ensure the closure of the commutation relations in (4.20) that we have chosen the definition $\hat{J}_z := \frac{1}{2} (\hat{N} + 1)$, as opposed to $\hat{J}_z = \frac{1}{2} \hat{N}$.

Using (4.7,4.8), we can evaluate the action of the physical operators on the physical states to obtain

$$\hat{J}_z | j, \delta \rangle = (j + \frac{1}{2}) | j, \delta \rangle,$$

$$\hat{J}_+ | j, \delta \rangle = \kappa_+ (j + 1) | j + 1, \delta \rangle$$

and

$$\hat{J}_- | j, \delta \rangle = \kappa_- (j) | j - 1, \delta \rangle, \quad (4.21)$$

where $\kappa_{\pm}$ — functions of their arguments only — are, as in the previous model, just products of the coefficients $\alpha_I, \gamma_I$ in (4.7). Analogous to (4.11), the coefficients $\kappa_{\pm}$ satisfy

$$\kappa_+(j) \kappa_- (j) = j^2 - \delta^2. \quad (4.22)$$
Since only the $\kappa_{\pm}$ are relevant to the observable algebra, we can view (4.22) as a condition on $\kappa_{\pm}$. With this condition, the CCRs (4.20) are also identically satisfied.

Let us consider, as before, the completeness of the set of observables. The classical analogs of $\{\hat{J}_z, \hat{J}_{\pm}\}$ are the functions

$$J_z = \frac{1}{2}(z_1 \bar{z}_1 + z_2 \bar{z}_2), \quad J_+ = z_1 z_2, \quad J_- = \bar{z}_1 \bar{z}_2$$

(4.23)
on phase space. (Note that there is an ambiguity in the correspondence between the operator $\hat{J}_z$ and the classical function $J_z$. This ambiguity is resolved by requiring the Poisson bracket algebra between the classical functions to be the Lie algebra of $SO(2,1)$.)

As in the previous model, one can easily check that the set $(J_+, J_-)$ is by itself complete; $J_z$ is included in order that the set of observables is closed under the Poisson bracket.

Again, there is an algebraic relation between the overcomplete set of generators of $A_{phy}$ which fixes the value of a Casimir invariant of $A_{phy}$. Using the definitions of $\hat{J}_\pm$ and the commutation relations (4.4), one finds that

$$\hat{J}_2 := -\hat{J}_z^2 + \frac{1}{2} [\hat{J}_+ , \hat{J}_-]_+ \equiv \frac{1}{4} - \delta^2. \quad (4.24)$$

Equivalently, the algebraic identity can be expressed as

$$\hat{J}_+ \hat{J}_- = (\hat{J}_z - \frac{1}{2})^2 - \delta^2, \quad (4.24')$$

in which form it is clear that the condition on the operators is automatically satisfied due to (4.22).

The last step in the program is to select an inner product by requiring that the $\star$-relations on $A_{phy}$ become Hermitian adjointness relations on the resulting Hilbert space. As for the previous model, from the expressions for the physical operators in terms of the elementary quantum operators $\hat{a}_I, \hat{c}_I$ and the $\star$-relation (4.5), one obtains the $\star$-relation induced on $A_{phy}$:

$$\hat{J}_+^\star = \hat{J}_- \quad \text{and} \quad \hat{J}_z^\star = \hat{J}_z. \quad (4.25)$$

The Hermiticity condition on $\hat{J}_z$ requires that its eigenvalues $j$ must be real, and its eigenkets orthogonal to each other. As in the previous model, the representation (4.21) is reducible: the physical operators either leave the value of $j$ unchanged, or change it by an integer. Thus, the fractional part of $j$ —denoted by $\epsilon = \text{frac}(j)$— is invariant under the action of $\hat{J}_z, \hat{J}_\pm$. Consider $\mathcal{V}_{phy}^\epsilon$, the vector space of states with the same fixed value of $\epsilon$. Each $\mathcal{V}_{phy}^\epsilon$ carries an irreducible representation of the $SO(2,1)$ Lie algebra (1.20); however, the $\star$-relations on the algebra have not all been imposed.

Let us now return to the Hermiticity conditions. Let $j = n + \epsilon, n = \cdots -2, -1, 0, 1, 2, \cdots$. Each $\mathcal{V}_{phys}^\epsilon$ has a countable basis, labelled by $n$, the integer part of $j$, and it is on these irreducible representations that one implements the Hermiticity conditions on $A_{phys}$. Note that at this stage it appears that we have a 1-parameter family of ambiguities in quantization of the system, labelled by the parameter $\epsilon \in [0, 1)$.

Henceforth, for definiteness, let us consider a representation with a fixed value of $\epsilon$. The Hermiticity of $\hat{J}_z$ implies that on $\mathcal{V}_{phys}^\epsilon$ there exists an inner product in which
the above basis is orthogonal; without any loss of generality, we can choose it to be orthonormal. Hence the inner product can be chosen to be:

$$\langle j' = n' + \epsilon, \delta | j = n + \epsilon, \delta \rangle = \delta_{n',n},$$  \hspace{1cm} (4.26)

where both states on the left have the same fractional part of $j$. As in the case of the energy sum model, it is only because we implement the Hermiticity conditions on an irreducible sector —with a countable basis— that we can postulate a Kronecker-$\delta$ normalization on $V^k_{\text{phy}}$. On $V_{\text{phy}}$, we would be led to a Dirac-$\delta$ normalization.

Now, the first of the $\star$-relations (4.25) implies that $\kappa_+ + (j) = \kappa_- (j)$. Substituting this in (4.22), the condition on the undetermined coefficients, yields

$$|\kappa_+ (j)|^2 = j^2 - \delta^2.$$  \hspace{1cm} (4.27)

We can use the freedom in the phase of the kets $|j, \delta\rangle$ to make $\kappa_+ (j)$ real for all $j$, and solve (4.27). Then we have

$$\hat{J}_+ |j, \delta\rangle = (j + \frac{1}{2}) |j, \delta\rangle,$$

$$\hat{J}_- |j, \delta\rangle = \sqrt{(j + 1)^2 - \delta^2} |j + 1, \delta\rangle$$

and

$$\hat{J}_- |j, \delta\rangle = \sqrt{j^2 - \delta^2} |j - 1, \delta\rangle.$$  \hspace{1cm} (4.28)

For solutions to exist, we require that physical states satisfy

$$j^2 \geq \delta^2.$$  \hspace{1cm} (4.29)

However, we cannot simply begin with any state satisfying $j^2 \geq \delta^2$ and hope to obtain a genuine representation of the observable algebra. Consider for example a state $|j, \delta\rangle$ with arbitrary $j \geq \delta$. In the simplest cases (see the remark at the end of this section), using $\hat{J}_-$ repeatedly, one can lower $j$ until the condition $j^2 \geq \delta^2$ is violated, unless there exists a state $|j_0, \delta\rangle$ annihilated by $\hat{J}_-$. From (4.28), we see that this will occur if and only if $j_0 = \pm |\delta|$. Acting with $\hat{J}_+$ repeatedly on the “ground” state $|j_0 = |\delta|, \delta\rangle$, we see that an allowed representation consists of states labelled by

$$j = |\delta| + n, \hspace{0.5cm} n = 0, 1, 2 \cdots.$$  \hspace{1cm} (4.30)

This corresponds to a representation with a fixed value $\epsilon = \text{frac}(|\delta|)$.

Similarly, starting with arbitrary $j \leq -|\delta|$ one can use $\hat{J}_+$ repeatedly to raise $j$ until (4.23) is violated, unless there exists a “top” state, $|j_0, \delta\rangle$ which is annihilated by $\hat{J}_+$. This would happen if $j_0 = -|\delta| - 1$. One obtains a representation inequivalent to the previous one,

$$j = -|\delta| - 1 - n, \hspace{0.5cm} n = 0, 1, 2 \cdots,$$  \hspace{1cm} (4.31)

so that $\epsilon = 1 - \text{frac}(|\delta|)$. Thus for each value of the energy difference $\delta$ one obtains the two representations (4.30) and (4.31) of the algebra of observables.

As in the quantization of the energy sum model, the coefficients $\alpha_I, \gamma_I$ in (4.7) are left undetermined, and we have not obtained an inner product on the original representation space. However, (4.26) provides us with an inner product on $V_{\text{phy}}$. Note that
before imposing the reality conditions, there was considerable ambiguity in the choice of representation of the observable algebra. In the first place, there are representations in which $j$ is complex-valued; next, there is ambiguity in the choice of the coefficients $\kappa_\pm$ satisfying (4.22). Further, for fixed choices of $\kappa_\pm$, there is a 1-parameter family of irreducible representations of the observable algebra. Imposing the $\star$-relations had four consequences: i) We were restricted to representations with real valued $j$; ii) we found an inner product on physical states; iii) we found unique $\lambda_\pm$ satisfying (4.22); and, iv) in the simplest case considered above, for each choice of $\varrho$ we are left with only two irreducible representations, which can be distinguished by the value of $\epsilon$.

In contrast to the energy sum model, where one finds representations only for integer $E$, in this model there is no such constraint on $\varrho$. This difference between the two models is related to the fact that in the energy sum model the reduced phase space is compact ($S^2$) whereas for the energy difference model the reduced phase space is non-compact ($\mathbb{R}^2$). In quantum theory, this shows up as a difference between the conditions on the parameters labelling physical states: In the energy sum model $|m|$ is bounded, whereas in the energy difference model, $|j|$ is bounded only from below. Finally, whereas in the energy sum model there is a unique representation for each integer $E$, in this model we have two representations of the physical observable algebra for all real $\varrho$. Without further physical input, both are admissible quantum theories.

Other Representations:

The representations we considered above are “generic.” There are, in addition, some exceptional cases. From (4.28) we see that a “ground” state $|j_0, \varrho\rangle$ is annihilated by $\hat{J}_-$ if and only if $j_0 = \pm |\varrho|$. To construct the representation (4.30) we acted repeatedly with $\hat{J}_+$ on one choice of ground state, namely $|j_0 = +|\varrho|, \varrho\rangle$. Let us attempt to construct a representation by acting repeatedly with $\hat{J}_+$ on the other possible choice of “ground state”: $|j_0 = -|\varrho|, \varrho\rangle$. Then the allowed states are labelled by $j = -|\varrho| + n$. However, generically, this procedure does not lead to viable representations: in particular, the “first excited state” $|j = -|\varrho| + 1, \varrho\rangle$ violates (4.29) unless $|\varrho| \leq \frac{1}{2}$. Similarly, the alternate choice of “top state” $|j_0 = +|\varrho| - 1\rangle$ — i.e. a state annihilated by $\hat{J}_+$ — does not yield a new representation unless $|\varrho| \leq \frac{1}{2}$. However, if $0 < |\varrho| \leq \frac{1}{2}$ we do have the additional representations

$$j = -|\varrho| + n, \quad n = 0, 1, 2 \cdots \quad 0 < |\varrho| \leq \frac{1}{2}, \quad (4.32)$$

for which $\epsilon = 1 - \text{frac}(|\varrho|)$; and,

$$j = |\varrho| - 1 - n, \quad n = 0, 1, 2 \cdots \quad 0 < |\varrho| \leq \frac{1}{2}, \quad (4.33)$$

with $\epsilon = \text{frac}(|\varrho|)$.

In fact, as Louko has pointed out [24], for $|\varrho| \in \left[0, \frac{1}{2}\right)$, the above representations are only special cases. There is a whole slew of representations, one for each choice of $\epsilon \in [|\varrho|, \frac{1}{2}]$ or $\epsilon \in [-\frac{1}{2}, -|\varrho|]$. In each such representation, the basis states are labelled by all integers:

$$j = \epsilon + n, \quad n = \cdots -2, -1, 0, 1, 2 \cdots \quad |\varrho| \leq |\epsilon| \leq \frac{1}{2}, \quad (4.34)$$
not just the non-negative ones as in (4.30–4.33). These representations do not possess either a “ground state” or a “top state”. Note also that of the new representations we have just constructed, in all but the representation (4.32), \( j \) is unbounded below.

### 4.3 Remarks

The quantum theory of the “energy difference” model has a number of interesting features which we can now discuss.

**Inner product on \( V \):**

In the energy difference model, we imposed the Hermiticity conditions only on physical states. We could of course have imposed them already on the elementary operators, prior to solving the quantum constraint equation and obtained a “kinematic Hilbert space.” However, generically, we would have found that none of the solutions to the constraints are normalizable with respect to that inner product. To see this, note that, if the elementary operators are represented by Hermitian operators, then the number operators \( \hat{N}_1 \) and \( \hat{N}_2 \) would take on only integral values. Hence, if \( \delta \) is not an integer or half-integer, the only normalizable state in the kernel of the constraint operator would be the zero state. Thus, we would be forced to conclude that \( V_{\text{phy}} \) is zero dimensional. The resulting quantum theory is clearly incorrect since, in this case, the reduced phase space is a 2-dimensional non-compact manifold; the system has one “true” degree of freedom. Thus, our strategy of holding off the imposition of the \( \# \)-relations until after the physical states are isolated is essential to obtain an acceptable quantum theory.

**Energy:**

Recall that, in the case of two ordinary (i.e. unconstrained) oscillators, the function \( H(x_I, p_I) := \frac{1}{2}(x_1^2 + p_1^2 + x_2^2 + p_2^2) \) is the total energy. Let us therefore refer to the corresponding operator \( \hat{H} = \hat{2J}_z \) as the Hamiltonian (although it may have nothing to do with the actual dynamics of the constrained system). Now, in the classical theory, the total energy is non-negative, i.e. \( H \geq 0 \). In the quantum theory however, we have obtained representations (the ones other than (4.30, 4.32)) of \( A_{\text{phy}} \) in which the corresponding operator \( \hat{H} \) is unbounded below (with eigenvalues \(-2|\delta| - 2n - 1, n = 0, 1, 2 \cdots, \delta \in \mathbb{R}; 2|\delta| - 2n - 1, n = 0, 1 \cdots, |\delta| \leq \frac{1}{2}, \) or, \( 2\epsilon + 2n + 1, n = \cdots - 1, 0, 1 \cdots \)). Since \( \hat{H} \) is an elementary physical observable, it is not of the form \( \hat{O}^\dagger \hat{O} \) for any \( \hat{O} \in A_{\text{phy}} \); there is nothing to ensure its positivity. Thus, without additional physical input, we can not rule out these representations. However, in the representations corresponding to (4.31) and (4.33), there are no states with positive energy eigenvalues. Therefore, by requiring in addition that we obtain an acceptable classical limit, we can rule out the representations corresponding to \( m < 0 \).

Even if we restrict ourselves to the positive energy representations, the spectrum of the energy operator has a feature that is at first unexpected. Recall that, in the quantum theory of two oscillators, the eigenvalues of the total Hamiltonian can take only integral values. In the present case, on the other hand, we found that \( \hat{H} = 2\hat{J}_z \) whence its eigenvalues, \((2n + 2|\delta| + 1)\), are in general non-integral. How does this result come about? The answer is that it is forced on us by the constraint. In the usual quantum theory of an oscillator, it is the requirement of positivity of the energy and
the existence of an annihilation operator that forces the energy eigenvalues to be half-integral. Because the quantum constraint is already satisfied by the physical states, once the energy of the “lower” oscillator is positive, the constraint guarantees that the energy of the “higher” oscillator will also be positive; this is no longer an independent requirement! Hence the energy of the “higher” oscillator is not forced to be half-integer, whence the total energy is also not subject to that requirement.

Overcomplete algebra of observables:

In both the “energy sum” and the “energy difference” models, one can construct the reduced phase space \( \hat{\Gamma} \) in a straightforward manner \([10]\). It turns out, however, that \( \hat{\Gamma} \) does not naturally inherit a cotangent bundle structure. For the energy sum model, \( \hat{\Gamma} \) is \( S^2 \), which is compact. For the energy difference model, while \( \hat{\Gamma} \) is topologically \( \mathbb{R}^2 \), the symplectic structure is not the obvious one; it is more natural to think of \( \hat{\Gamma} \) as the positive mass-shell in a 3-dimensional Minkowski space \([10]\). A related interesting feature is that, although we began with algebraically independent elementary variables (and did not therefore have to impose the ACRs), the algebra of physical observables is overcomplete. This is particularly striking in the energy difference model where the topology of the reduced phase space is trivial. In both examples, it is the requirement that the set of generators of \( \mathcal{A}_{phy} \) be closed under the commutator Lie bracket that forces one to include an “extra” element in the set of generators of \( \mathcal{A}_{phy} \). Thus, there is an algebraic relation on the physical observables, the quantum version of which is satisfied on the physical states.

Discrete symmetries:

Recall that prior to imposing the Hermiticity conditions, for a fixed choice of \( \kappa_\pm \) satisfying \((4.22)\), we had a 1-parameter family, labelled by \( \epsilon \), of irreducible representations of the algebra of physical observables. It is natural to ask if the irreducible sectors \( \mathcal{V}_{phy}^\epsilon \) are the eigenspaces of an operator corresponding to some (discrete) symmetry. Let us begin with the classical theory. The constraint function \( \frac{1}{2}(z_1 \bar{z}_1 - z_2 \bar{z}_2) - \delta \) of \((4.18)\) as well as the physical observables \( \{ \frac{1}{2}(z_1 \bar{z}_1 + z_2 \bar{z}_2), z_1 z_2, \bar{z}_1 \bar{z}_2 \} \) of \((4.23)\), are all invariant under the discrete “parity” map \( (z_I) \mapsto -z_I \). Hence, although the set of observables \((4.23)\) is locally complete on the constraint surface \( \bar{\Gamma} \) (in the sense that their gradients span the cotangent space at each point of \( \bar{\Gamma} \)) they fail to capture certain global information about the constraint surface since they can not distinguish between the point labelled by \( z_I \) and that labelled by \(-z_I\). Let us now consider the quantum theory. In the Bargmann-type representation, this discrete symmetry corresponds to the operation \( \psi(z_I) \mapsto \psi(-z_I) \). Since \( \langle z_1, z_2 | j, m \rangle = z_1^j \bar{z}_2^{\bar{m}} \), it follows that in the \( | j, m \rangle \) representation, the action of the parity operator is given by

\[
| j, m \rangle \mapsto \hat{\mathcal{P}} | j, m \rangle := (-1)^{2j} | j, m \rangle,
\]

where, to evaluate the right hand side we will take the principal value, namely, \((-1)^{2j} = \exp(i2\pi \epsilon)\), and as before \( \epsilon = \text{frac}(j) \) is the fractional part of \( j \). Next, recall that since the physical operators change \( j \) only in integral steps they do not affect the fractional part \( \epsilon \). Consequently, \( \mathcal{V}_{phy}^\epsilon \) is reducible, and each eigenspace \( \mathcal{V}_{phy}^\epsilon \) of the parity operator provides an irreducible representation of the algebra \( \mathcal{A}_{phy} \). Thus, there is indeed a superselection.
The parity operator has an unexpected feature in quantum theory. Classically, the parity transformation \( P(z_I) = (-z_I) \) satisfies
\[
P^2 = 1.
\tag{4.36}
\]
irrespective of the precise value of \( \delta \in \mathbb{R} \). In quantum theory, on the other hand, the eigenvalues of \( \hat{P} \) are given by \( \exp(i2\pi \epsilon) \) (see (4.35)), where in the physical representation, \( \epsilon = \frac{\text{frac}(\delta)}{\text{int}(\delta)} \). Hence, on physical states, \( \hat{P}^2 = \exp(i4\pi \text{frac}(\delta)) \). Thus, we recover the classical behavior only if \( \delta \) is an integer or half integer. For other values, the classical behavior of the parity symmetry cannot be recovered. Within quantum mechanics, however, there seems to be no compelling reason to restrict ourselves to states with eigenvalues \( \pm 1 \) of \( \hat{P} \). On sectors with other eigenvalues, we have a situation that is rather similar to the one encountered in systems of identical particles in 2 space dimensions where the use of eigenvalues other than \( \pm 1 \) for the parity (or the permutation) operator leads to the interesting quantum phenomena of fractional statistics.

**FRW universe with conformally coupled scalar field:**

As we remarked earlier, the energy difference model arises in quantum cosmology. In the context of the algebraic program, this fact is mainly a mathematical curiosity since the program is not equipped to deal with the difficult interpretational issues faced by quantum cosmology. Nonetheless, it is useful to regard this minisuperspace as a toy model for full general relativity and see that the program does lead to mathematically complete quantum descriptions without, e.g., having to first solve the problem of time.

Let us begin by indicating how the cosmological model can be reduced to the energy difference model. The Ricci scalar for the closed \((k = +1)\) Friedman-Robertson-Walker universe is
\[
R = \frac{6}{a^2} \left( a \frac{\partial^2 a}{\partial \tau^2} + \left( \frac{\partial a}{\partial \tau} \right)^2 + 1 \right),
\tag{4.37}
\]
where \( a \) is the scale-factor of the universe and \( \tau \) is the proper time. Hence, the gravitational part of the Lagrangian (up to a factor of \( \frac{4\pi}{3} \), and after an integration by parts) is:
\[
\mathcal{L}_G = \frac{6}{G} \left( -a \left( \frac{\partial a}{\partial \tau} \right)^2 + a \right),
\tag{4.38}
\]
where \( G \) is the gravitational constant, and the action is \( S = \int \text{d} \tau \mathcal{L} \). The Lagrangian for the homogeneous, conformally coupled \((\xi = \frac{1}{6}, \text{massless})\) scalar field is
\[
\mathcal{L}_{KG} = 8\pi \left( a^3 \left( \frac{\partial \phi}{\partial \tau} \right)^2 + a \left( \frac{\partial a}{\partial \tau} \right)^2 \phi^2 + 2a^2 \phi \frac{\partial a}{\partial \tau} \cdot \frac{\partial \phi}{\partial \tau} - a \phi^2 \right).
\tag{4.39}
\]
Introduce a reparametrization of the time, \( \partial t = \partial \tau / N \), where \( N \) is the lapse. Let \( \dot{\cdot} \equiv (\partial/\partial t) \). Then the total Lagrangian is
\[
\mathcal{L} = -\frac{6}{GN} a \dot{a}^2 + \frac{6Na}{G} + \frac{8\pi a}{N} (a\dot{\phi})^2 - \frac{8\pi N}{a} (a\phi)^2.
\tag{4.40}
\]
Define the variables

\[ x_1 := \sqrt{\frac{12}{G}} a \]  \hspace{1cm} (4.41)

\[ x_2 := \sqrt{\frac{16\pi}{G}} a\phi. \]  \hspace{1cm} (4.42)

Now the Lagrangian takes the form

\[ \mathcal{L} = -\frac{1}{2N}a\dot{x}_1^2 + \frac{1}{2N}a\dot{x}_2^2 + \frac{6Na}{G} - \frac{N}{2a}\dot{x}_2^2. \]  \hspace{1cm} (4.43)

Performing the Legendre transform, we find the canonical momenta:

\[ p_1 := -\sqrt{\frac{12}{G}} \frac{a\dot{a}}{N} \]  \hspace{1cm} (4.44)

\[ \text{and } p_2 := \frac{4}{\sqrt{\pi N}} a (a\dot{\phi}). \]  \hspace{1cm} (4.45)

Since we are in a spatially compact situation, the Hamiltonian is constrained to vanish. Indeed, it has the form \( \mathcal{H} = \frac{2N}{x_1} C \), where the scalar constraint \( C \) is given by

\[ C = \frac{1}{4} (p_1^2 + x_1^2 - p_2^2 - x_2^2) \approx 0. \]  \hspace{1cm} (4.46)

We see that it is exactly of the form of (4.18), with \( \delta = 0 \).

Note, however, that there is a nonholonomic constraint, \( a \geq 0 \). One consistent approach to handle this would be to consider the physical scale factor to be defined by \( a := \frac{|x_1|}{\sqrt{12}} \), on the phase space defined by \((x_1, p_1)\). The solutions then describe a periodic, bouncing universe. One can use the representations obtained in section 4.2 as quantum descriptions of this model\(^6\).

### 5 Constrained rotor model

In this section we will quantize a model which mimics some of the features of general relativity. It was introduced by Ashtekar and Horowitz \cite{26} and was believed to display certain unexpected behaviour in the quantum theory. Since this behaviour arose from precisely those features of this model that it shares with general relativity, there was some concern that similar surprises might occur in a quantum theory of gravity. In \cite{26}, however, there were no guidelines to select the inner product on the physical states. By using the algebraic program, we can now select the “correct” inner-product and analyse the issues raised in \cite{26} within the resulting quantum representation. We will find that the unexpected features are in fact absent; they arose because of the use of a physically incorrect inner-product. The manner in which the correct inner product avoids the problems is quite subtle and, without the reality conditions to guide us, it would have been difficult to argue that this is the appropriate inner product to use. Thus, the example illustrates the power of the algebraic approach in addressing concrete physical issues.

\(^6\)This cosmological model has been quantized elsewhere, see e.g. \cite{25}, in which the quantum theory corresponds to the representation (4.30) and does not include any of the representations (4.34).
5.1 Motivation

Let us recall certain features of general relativity in the geometrodynamical variables. In the Arnowitt-Deser-Misner (ADM) formulation [27], the basic phase space variables are the 3-metric and its canonically conjugate momentum. The constraint surface is specified by the vanishing of the scalar constraint function. The scalar constraint is the sum of two terms: a kinetic term —quadratic in the momenta— the coefficient of which defines a “supermetric” on the configuration space; and a potential term —proportional to the 3-dimensional Ricci scalar— which depends only on the configuration variables. Due to the complicated form of the constraint, the geometry of the constraint surface, $\Gamma$, and the structure of the reduced phase space of general relativity are still not fully understood. There are, however, many features which are well known. Of interest to us are the following:

- First, the constraint surface defines a “classically forbidden” region in the configuration space. More precisely, the image in the configuration space of the constraint surface $\Gamma$ (under the natural projection map) is a proper subset of the configuration space $C$.
- Second, in the asymptotically flat case, the Hamiltonian is not constrained to vanish. On $\Gamma$, the Hamiltonian reduces to a surface integral at spatial infinity, called the ADM energy. The ADM energy depends only on the 3-metric and its spatial derivatives, and not on the canonically conjugate momenta.
- Finally, the positive energy theorems of classical general relativity state that on the allowed regions of $C$ defined by the projection of the constraint surface, the ADM energy is positive. In the “forbidden” regions, where the constraint cannot be satisfied, the ADM energy can be negative.

Ashtekar and Horowitz constructed a finite dimensional model which mimics the above features of general relativity. Consider a particle on a (unit) 2-sphere in 3-dimensional Euclidean space, subject to the constraint

$$C \equiv \ell_0^2 - R(\phi) = 0,$$

where $(\theta, \phi)$ are the usual spherical coordinates. The “potential”, $R(\phi)$, is a smooth function, which is not everywhere positive. As in general relativity, the constraint surface $\Gamma$ projects down to a proper subset of the configuration space $C$: the classically allowed region $\bar{C}$ corresponds to those sectors where $R(\phi) \geq 0$. Now introduce a Hamiltonian via

$$H = C + E(\phi), \quad \text{with} \quad E(\phi) \cdot R(\phi) \geq 0;$$

we assume that $E$ is bounded. On the constraint surface $C = 0$, the Hamiltonian reduces to the “ADM energy” $E(\phi)$, and depends only on the configuration variable $\phi$. Since

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7In these motivating remarks, the diffeomorphism constraint of general relativity plays no role and is therefore ignored.

8The inclusion or exclusion of the radial degree of freedom plays no significant role.
$E(\phi)$ is positive in the classically allowed regions, where $R(\phi)$ is positive, this function satisfies a classical positive energy theorem, as does the Hamiltonian in general relativity. We will henceforth refer to this model as the constrained rotor model.

Now consider the Dirac quantum theory of this model, say in the Schrödinger representation, where states are functions of the configuration variables. Ashtekar and Horowitz raised the following question: In the Dirac quantum theory, do there exist physical states that penetrate the classically forbidden region ($R < 0$)? Let us suppose that such states do exist. Now, physical states are solutions to the quantum constraint equation, and on these states the Hamiltonian acts via a multiplication by $E(\phi)$. (Note that — as in general relativity — in this model, the “ADM energy” $E$ is a function only of the configuration variables.) In this model $E$ is negative in the classically forbidden region $\tilde{C} = C - \bar{C}$. Thus, on some physical states which penetrate sufficiently into $\tilde{C}$, the energy will be negative. Due to the close analogy with general relativity, if such behaviour occurs in this model it would indicate that similar tunnelling can occur in quantum gravity as well.

We will re-analyse this problem in the context of the algebraic quantization program.

5.2 Dirac quantization

Let $(\theta, \phi)$ denote the usual spherical coordinates on $S^2$, and let $(p_\theta, p_\phi)$ be the canonically conjugate momentum operators. We choose the set $S$ of elementary variables to consist of all functions $f(\theta, \phi)$ on $S^2$ and the momentum variables $p_\theta, p_\phi$. The $\star$-algebra $A(\star)$ is straightforward to construct. An obvious choice for the vector space representation is provided by the availability of a configuration space. Here, the states are (complex-valued) functions on $S^2$, $\Psi = \Psi(\theta, \phi)$, and the elementary operators are represented by

\[
\hat{f} \circ \Psi(\theta, \phi) = f(\theta, \phi) \cdot \Psi(\theta, \phi)
\]

\[
\hat{p}_\theta \circ \Psi(\theta, \phi) = \frac{\hbar}{i} \left( \frac{1}{\sqrt{\sin \theta}} \frac{\partial}{\partial \theta} (\sqrt{\sin \theta} \Psi(\theta, \phi)) \right) \equiv \frac{\hbar}{i} \left( \frac{\partial}{\partial \theta} + \frac{1}{2} \cot \theta \right) \Psi(\theta, \phi)
\]
and

\[
\hat{p}_\phi \circ \Psi(\theta, \phi) = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Psi(\theta, \phi).
\]

(5.3)

These operators satisfy the usual CCRs, and although the set of elementary variables is overcomplete, all the resulting anticommutation relations are identically satisfied in this representation. Note that we do not require the Hermiticity of the elementary operators, and since we have no inner product, we could have left the familiar “divergence” term out of the representation of the momentum operator $\hat{p}_\theta$. We could define a kinder, gentler, representation by replacing $\sqrt{\sin \theta} \Psi$ by $\Psi$; then, for example, $\hat{p}_\theta \circ \Psi = (\hbar/i)(\partial/\partial \theta) \Psi$ and the forms of the constraint and the solutions are simplified considerably. However, we will use the above representation (5.3), as it is the one chosen by Ashtekar and Horowitz. The two representations are equivalent (see [10]). In the representation

\[\text{In fact, as we discuss briefly in section 5.3, requiring that the momentum operators be Hermitian on all states (as in [28]) leads to an inadequate space of physical states.}

\[\text{The vector field } \partial/\partial \theta \text{ is not globally defined on } S^2. \text{ However, this is not essential to the points we illustrate here, since in particular the analysis could be repeated by replacing } S^2 \text{ by a cylinder, where}
\]
the constraint equation satisfied by physical states $\psi$ is

$$\frac{\hbar^2}{\sqrt{\sin \theta}} \frac{\partial^2}{\partial \theta^2} \left( \sqrt{\sin \theta} \psi \right) + R(\phi) \psi = 0. \quad (5.4)$$

Although we assume for simplicity that $R(\phi)$ is smooth, discontinuities in $R$ will not matter.

Since this is a quadratic differential equation, there are two linearly independent sets of solutions

$$\psi_\pm = k_\pm(\phi) \cdot (\sin \theta)^{-\frac{1}{2}} \cdot \exp(\pm \frac{i}{\hbar} \sqrt{R} \theta) \quad (5.5)$$

where $\sqrt{R}$ denotes the principal value: $\sqrt{R} = +\sqrt{R}$, if $R > 0$, and $\sqrt{R} = +i\sqrt{|R|}$ if $R < 0$. The functions $k_\pm(\phi)$ are arbitrary and have support everywhere in configuration space, including the classically forbidden region $\bar{C}$. Let the linear vector space of physical states be denoted by $\mathcal{V}$. Then $\mathcal{V} = \mathcal{V}^+ \oplus \mathcal{V}^-$, where $\psi_\pm \in \mathcal{V}^\pm$ respectively, and we can write a general (physical) state as

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}. \quad (5.6)$$

Note that since we have not yet defined an inner product, this representation of $\psi$ does not provide us with an orthogonal decomposition of $\mathcal{V}$.

Let us construct the Dirac observables. Since the constraint is first class, there is one true degree of freedom, and thus we expect two independent Dirac observables. From their representations, it is clear that $\hat{p}_\theta, f(\phi)$ commute with the constraint and leave $\mathcal{V}$ invariant, their only effect on the physical states is to change the coefficients $k_\pm$ of the corresponding exponential terms. However, on the constraint surface $p_\theta = \pm \sqrt{R(\phi)}$, and thus $(p_\theta, f(\phi))$ is not a complete set. In order for the set to be complete, we need another observable. Ashtekar and Horowitz introduced a classical Dirac observable, $P^\pm_\phi = p_\phi \mp \frac{1}{2} \theta R' \sqrt{R}$. The set $(p_\theta, f(\phi), P_\phi)$ is now complete almost everywhere, in the required sense.

The quantum operator corresponding to $P^\pm_\phi$ is:

$$\hat{P}_\phi = \begin{pmatrix} \hat{P}_\phi^+ & 0 \\ 0 & \hat{P}_\phi^- \end{pmatrix}, \quad \text{where} \quad \hat{P}_\phi^\pm = \hat{p}_\phi^\pm \mp \frac{1}{2} \left( \frac{R'}{\sqrt{R}} \theta \right). \quad (5.7)$$

where $' \equiv \partial / \partial \phi$ denotes the partial derivative with respect to $\phi$. To see that this is a physical operator, let us concentrate on one component, acting on $\mathcal{V}^+$. Then,

$$\hat{P}_\phi^+ \circ \psi_+ = \frac{\hbar}{i} k'_+ (\sin \theta)^{-\frac{1}{2}} \cdot \exp(+ \frac{i}{\hbar} \sqrt{R} \theta) \in \mathcal{V}^+. \quad (5.8)$$

This subtlety is not encountered. Nonetheless, in order not to obscure the main point —the power of the algebraic approach to remove ambiguities— we will continue to use the original model discussed in the literature.

\footnote{It fails to be complete only at those points on the constraint surface where $R(\phi) = 0$. This fact plays a minor role in the Dirac quantization and will therefore be ignored in what follows. It is, however, quite significant in the construction of the reduced phase space quantum theory.}
Similarly, $\hat{P}_\phi^- \circ \psi_- \in \mathcal{V}^-$. Hence $\hat{P}_\phi$ as defined above is a physical operator. For future reference, note that

\[
\hat{P}_\phi^- \circ \psi_+ = \left( \frac{\hbar}{i} k'_+ + 2 \left( \sqrt{R} \right)' \theta k_+ \right) \cdot (\sin \theta) \cdot \frac{1}{2} \cdot \exp(\frac{i}{\hbar} \sqrt{R} \theta) \not\in \mathcal{V},
\]

is not a physical state, since the second term in the coefficient in the bracket is no longer a function only of $\phi$.

We now have to find the $\ast$-relations on the algebra of observables. Clearly, $\hat{p}_\phi^* = \hat{p}_\theta$, $\hat{f}(\phi)^* = \hat{f}(\phi)$ and are physical operators. In order to analyse the $\ast$-relation on $\hat{P}_\phi$, let us further decompose $\mathcal{V}^+$ into the set of states $\bar{\mathcal{V}}^+$ with support only on the classically allowed region $\bar{\mathcal{C}}$ and the set of states $\bar{\mathcal{V}}^+$ with support entirely in the classically forbidden region $\bar{\mathcal{C}}$. Now, on the sector of states $\bar{\mathcal{V}}^+$, $(\sqrt{R})^* = -\sqrt{R}$ and hence

\[
(\hat{P}_\phi^+)^* = \left( \hat{p}_\phi - \frac{1}{2} \left( \frac{\sqrt{R'}}{\sqrt{R}} \right) \theta \right)^* = \hat{p}_\phi - \frac{1}{2} \left( \frac{\sqrt{R'}}{\sqrt{R}} \theta \right) = \hat{P}_\phi^+
\]

is a physical operator on $\bar{\mathcal{V}}^+$. However, on the “forbidden sector” $\bar{\mathcal{V}}^+$, $(\sqrt{R})^* = -\sqrt{R}$ and hence

\[
(\hat{P}_\phi^-)^* = \left( \hat{p}_\phi - \frac{1}{2} \left( \frac{\sqrt{R'}}{\sqrt{R}} \theta \right) \right)^* = \hat{p}_\phi + \frac{1}{2} \left( \frac{\sqrt{R'}}{\sqrt{R}} \theta \right) = \hat{P}_\phi^-,
\]

which, as we see from (5.9), is not a physical operator. In the matrix notation, since $(\hat{P}_\phi^\pm)^* = \hat{P}_\phi^\mp$ on the sector of “classically allowed” states $\bar{\mathcal{V}}^+$, $\hat{P}_\phi^* = \hat{P}_\phi$ is a physical operator. On the other hand, since on the sector of “classically forbidden states” $\bar{\mathcal{V}}^-$,

\[
(\hat{P}_\phi)^* = \begin{pmatrix} (\hat{P}_\phi^+)^* & 0 \\ 0 & (\hat{P}_\phi^-)^* \end{pmatrix} = \begin{pmatrix} \hat{P}_\phi^- & 0 \\ 0 & \hat{P}_\phi^+ \end{pmatrix},
\]

it does not leave the space of physical states invariant.

Clearly something peculiar is happening here. We have a complete set of physical states which carry a representation of an (almost) complete algebra $\mathcal{A}_{\text{phy}} \subset \mathcal{A}$ of physical operators generated by $\{\hat{p}_\theta, \hat{f}(\phi), \hat{P}_\phi\}$. Further, the $\ast$-involution on $\mathcal{A}$ has a well-defined action on $\mathcal{A}_{\text{phy}}$ and induces a map from $\mathcal{A}_{\text{phy}}$ into $\mathcal{A}$. What fails however, is that the induced $\ast$ is not an involution on $\mathcal{A}_{\text{phy}}$; its action on one of the generators of $\mathcal{A}_{\text{phy}}$, namely $\hat{P}_\phi$, takes it out of $\mathcal{A}_{\text{phy}}$. (This can be understood in terms of the Hamiltonian vector field of the classical observable $P_\phi$, see [10].) The algebra of physical observables, $\mathcal{A}_{\text{phy}}$, does not admit a $\ast$-involution induced from $\mathcal{A}(\ast)$. Thus there is no sensible way to formulate the Hermiticity conditions on physical operators in terms of an inner product on physical states.

On the face of it, due to the above mathematical inconsistency, i.e. the lack of a $\ast$-involution on $\mathcal{A}_{\text{phy}}$, one cannot proceed with the quantization program. Since the difficulty arises due to the sector of “forbidden” states, one way out would be to discard them on mathematical grounds. However, this is somewhat unsatisfactory since there appears to be no compelling physical reason to do so. We would be ruling out, by fiat, precisely the “tunnelling” states whose existence is the issue under investigation.
An alternative approach would be to try and implement the $\star$-relations on the other physical observables, and then see if it leads to a mathematically and physically sensible framework. As we will see in detail, we will find that the resulting measure is such that the forbidden region $\mathcal{C}$ is a set of measure zero, and $\hat{P}_\phi^\star$ is an observable. Thus, it is not that the solutions can not have support on the classically forbidden regions. Rather, the forbidden region does not “contribute” because it is simply a set of measure zero.

For the purposes of the analysis above, we had decomposed $\mathcal{V}$ into two linearly independent parts $\mathcal{V}^+$ and $\mathcal{V}^-$. Each of these sectors carries an irreducible representation of $\mathcal{A}_{phy}$, and one might be tempted to consider an inner product in which $\mathcal{V}^+$ and $\mathcal{V}^-$ are mutually orthogonal. This would be justified if we knew that $\mathcal{V}^\pm$ were the eigenspaces of some operator which is expected to be Hermitian or unitary. In the absence of an obvious candidate for such an operator, let us consider, as an ansatz, a general inner product of the form

$$\langle \psi_1 | \psi_2 \rangle = \int_\mathcal{C} d\theta \wedge d\phi \left( \mu_+ k_1^+ k_2^+ + \mu_- k_1^- k_2^- + \mu_+ k_1^+ k_2^- + \mu_- k_1^- k_2^+ \right)$$

$$+ \int_\mathcal{C} d\theta \wedge d\phi \left( \bar{\mu}_+ k_1^+ k_2^+ + \bar{\mu}_- k_1^- k_2^- + \bar{\mu}_+ k_1^- k_2^+ + \bar{\mu}_- k_1^+ k_2^- \right). \quad (5.13)$$

The $\mu = \mu(\theta, \phi)$ are arbitrary functions on $S^2$ and we have absorbed an overall factor of $\sin^{-1} \theta$ into their definitions. Extra factors of $\exp(-\frac{2\mu}{\hbar}\sqrt{|R|\theta})$, $\exp(-\frac{\mu}{\hbar}\sqrt{|R|\theta})$, and $\exp(\frac{2\mu}{\hbar}\sqrt{|R|\theta})$ have been absorbed into $\mu_{+-}$, $\bar{\mu}_+$ and $\bar{\mu}_-$ respectively. The inner product is positive definite if and only if the “diagonal” measures are positive and the “off-diagonal” measures satisfy

$$|\mu_{+-}| < \sqrt{\mu_+ \mu_-} \quad \text{and} \quad |\bar{\mu}_{+-}| < \sqrt{\bar{\mu}_+ \bar{\mu}_-}. \quad (5.15)$$

Now let us impose the Hermiticity conditions on the observables. Clearly, all $\tilde{f}(\phi)$ are Hermitian. Next, consider $\hat{p}_\theta$. We will carry-out a straightforward analysis which shows that $\hat{p}_\theta$ can be Hermitian only if $\tilde{\mu}_+ = \tilde{\mu}_- = \bar{\mu}_{+-} = 0$.

Since physical states are specified entirely by their coefficients $k_\pm$, we can represent operators by their action on $k_\pm$. In particular,

$$\hat{p}_\theta \circ \begin{pmatrix} k_+ \\ k_- \end{pmatrix} = \begin{pmatrix} +\sqrt{|R|k_+} \\ -\sqrt{|R|k_-} \end{pmatrix} \quad \text{on} \quad \mathcal{C}$$

$$= \begin{pmatrix} +i\sqrt{|R|k_+} \\ -i\sqrt{|R|k_-} \end{pmatrix} \quad \text{on} \quad \mathcal{\bar{C}}. \quad (5.16)$$

---

\[\text{In terms of the matrix notation, the inner product corresponds to}\]

$$\langle \psi_1 | \psi_2 \rangle = \begin{pmatrix} k_1^+ \\ k_1^- \end{pmatrix} \left( \begin{array}{cc} \mu_+ & \mu_{+-} \\ \mu_+ & \mu_- \end{array} \right) \begin{pmatrix} k_2^+ \\ k_2^- \end{pmatrix} \quad (5.14)$$

Suppose we write a general physical state as $\psi = \psi_+ + \psi_-$, and postulate the seemingly natural inner product $\langle \psi_1 | \psi_2 \rangle = \int_\mathcal{C} \bar{\mu} \psi_1 \psi_2 + \int_{\mathcal{\bar{C}}} \bar{\mu} \psi_1 \psi_2$. In the above notation, this corresponds to choosing a matrix all of whose components are equal up to phase. A short calculation, attempting to impose the Hermiticity conditions on $\hat{p}_\theta$, shows that there is in fact no such inner product. Therefore one is forced to work with the more general form (5.13) or (5.14).
We want to find an inner product such that \( \langle \psi_1 | \hat{p}_\theta | \psi_2 \rangle = \langle \psi_1 | \hat{p}_\theta^\dagger | \psi_2 \rangle \) for all \( \psi_1, \psi_2 \).
Consider states in \( V_+ \), i.e. \( k_1^- = k_2^- = 0 \). Then
\[
\langle \psi_1 | \hat{p}_\theta | \psi_2 \rangle = \int_C \mu_+ k_1^+ \sqrt{R} \, k_2^+ + i \int_C \bar{\mu}_+ k_1^+ \sqrt{|R|} \, k_2^+. \tag{5.17}
\]
On the other hand, by definition
\[
\langle \psi_1 | \hat{p}_\theta^\dagger | \psi_2 \rangle := \langle \psi_2 | \hat{p}_\theta | \psi_1 \rangle = \int_C \mu_+ k_1^+ \sqrt{R} \, k_2^+ - i \int_C \bar{\mu}_+ k_1^+ \sqrt{|R|} \, k_2^+. \tag{5.18}
\]
Clearly, \( \hat{p}_\theta \) can be Hermitian on \( V_+ \) only if \( \bar{\mu}_+ = 0 \). Similarly, one can conclude that \( \bar{\mu}_- = 0 \). Thus, both the diagonal terms in the forbidden region vanish. But now, due to the condition (5.15), in the forbidden region the cross term also vanishes, \( \bar{\mu}_{+-} = 0 \). In the inner product (5.13), the only terms that survive are the integrals over the classically allowed region! Thus, while physical solutions can indeed have support in the classically forbidden region \( \bar{C} \), this support is of measure zero in the physical inner product.

Let us return to the Hermiticity of \( \hat{p}_\theta \). Consider states \( \psi_1 = \psi_{1+} \) and \( \psi_2 = \psi_{2-} \), i.e. \( k_1^- = k_2^+ = 0 \). Then,
\[
\langle \psi_1 | \hat{p}_\theta | \psi_2 \rangle = \int_C \mu_{+-} k_1^+ (-\sqrt{R}) k_2^- . \tag{5.19}
\]
However,
\[
\langle \psi_1 | \hat{p}_\theta^\dagger | \psi_2 \rangle := \langle \psi_2 | \hat{p}_\theta | \psi_1 \rangle = \int_C \mu_{+-} k_2^- (\sqrt{R}) k_1^+ . \tag{5.20}
\]
Equating the two, we find that \( \hat{p}_\theta \) is Hermitian if and only if \( \mu_{+-} = 0 \). Thus, it is the Hermiticity of a continuous operator which implies that the subspaces \( V_+ \) and \( V_- \) are orthogonal. (Since they are in fact orthogonal, clearly the system admits another discrete symmetry, albeit a hidden one.)

Imposing the \( \star \)-relations on \( \hat{p}_\theta, \hat{\phi} \) as Hermiticity conditions on the representation, we have reduced the form of the physical inner product (5.13) to
\[
\langle \psi_1 | \psi_2 \rangle = \int_C (\mu_+ k_1^+ k_2^+ + \mu_- k_1^- k_2^-), \tag{5.21}
\]
where \( \mu = \mu(\theta, \phi) \). Since the measure in the classically forbidden region vanishes, as elements in the Hilbert space physical states can be specified entirely by their support on \( \bar{C} \). In other words, by restricting the support of physical states to the classically allowed region \( \bar{C} \), in this problem we do not lose any elements of the physical Hilbert space. Thus, as we saw earlier (5.8), on states with support only on \( \bar{C} \), \( \bar{P}_\phi \) is a physical operator, in fact \( \bar{P}_\phi^* = \bar{P}_\phi \). Now, since in terms of \( k_\pm \), the action of \( \bar{P}_\phi \) on physical states is
\[
\bar{P}_\phi \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial \phi} k_\pm . \tag{5.22}
\]
it is trivial to check that \( \bar{P}_\phi \) is symmetric if and only if \( \partial \mu_\pm / \partial \phi = 0 \).

Thus, the measure depends only on \( \theta \), and furthermore, this dependence is not determined by any Hermiticity conditions. Now, since the coefficients \( k_\pm \) do not depend
on $\theta$ either, the integral over $\theta$ can be performed trivially, and the inner product is thus reduced to
\[
\langle \psi_1 | \psi_2 \rangle = \mu_+ \int_\phi d\phi \overline{k_1^+} k_2^+ + \mu_- \int_\phi d\phi \overline{k_1^+} k_2^- ,
\] (5.23)
where $\overline{\phi}$ indicates that the integral is performed only over classically allowed values of $\phi$, and $\mu_{\pm}$ are positive numbers which are the results of the $\theta$-integration, or the total measure on $\theta$.

Is there a criterion that will fix the relative weights of the two terms? Recall that all the (continuous) physical observables we have considered so far are diagonal in the representation (5.6), i.e. their action leaves each of the physical subspaces $V^\pm$ invariant. In order to fix the relative weights of the two terms in the inner product, we are led to look for a physical operator whose action on physical states is not diagonal in the representation (5.6); requiring it to be Hermitian or unitary would then fix the inner product. It is natural to suppose that such an operator corresponds to a discrete symmetry of the constraint.

An obvious symmetry is reflection in the $x$-$y$ plane, $I_z : \theta \mapsto \pi - \theta$. In quantum theory, the corresponding operator is represented by $\hat{I}_z \circ \Psi(\theta, \phi) = \Psi(\pi - \theta, \phi)$. It is manifestly a physical operator, and since classically $I_z^2 = 1$, it should be both Hermitian and unitary, and its eigenspaces should be orthogonal. The even and odd physical eigenstates (with eigenvalues $+1$ and $-1$ respectively) are of the form
\[
\psi_e = \begin{pmatrix}
\frac{1}{2} k_e(\phi) \exp \left(-\frac{i\pi}{2\hbar} \sqrt{R} \right) (\sin \theta)^{-\frac{1}{2}} \cdot \exp\left(\frac{i}{\hbar} \sqrt{R} \theta\right) \\
\frac{1}{2} k_e(\phi) \exp \left(+\frac{i\pi}{2\hbar} \sqrt{R} \right) (\sin \theta)^{-\frac{1}{2}} \cdot \exp\left(-\frac{i}{\hbar} \sqrt{R} \theta\right)
\end{pmatrix},
\]
(5.24)
\[
\psi_o = \begin{pmatrix}
\frac{1}{2} k_o(\phi) \exp \left(-\frac{i\pi}{2\hbar} \sqrt{R} \right) (\sin \theta)^{-\frac{1}{2}} \cdot \exp\left(+\frac{i}{\hbar} \sqrt{R} \theta\right) \\
-\frac{1}{2} k_o(\phi) \exp \left(+\frac{i\pi}{2\hbar} \sqrt{R} \right) (\sin \theta)^{-\frac{1}{2}} \cdot \exp\left(-\frac{i}{\hbar} \sqrt{R} \theta\right)
\end{pmatrix},
\]
(5.25)
where $k_e$ and $k_o$ are arbitrary functions of $\phi$. The eigenspaces $V_e, V_o$ (5.24,5.25) are orthogonal if and only if $\mu_+ = \mu_-$. Thus we can choose $\mu_+ = \mu_- = 1$, and the final form for the inner product is
\[
\langle \psi_1 | \psi_2 \rangle = \int_\phi d\phi \overline{[k_1^+ k_2^+ + k_1^- k_2^-]}.
\] (5.26)

Is $\hat{I}_z$ “super-selected” in the sense that it commutes with all other observables? If it were, then its eigenspaces would carry irreducible representations of the algebra $A_{phy}$ of (continuous) Dirac operators. However, while it does commute with $\hat{f}(\phi), \hat{P}_\phi$, it does not commute with $\hat{p}_\theta$ (In fact, they anticommute, $[\hat{p}_\theta, \hat{I}_z] = 0$.) and hence $\hat{p}_\theta$ is not diagonal in the even/odd decomposition.

## 5.3 Remarks

Let us first briefly review the process by which we obtained a complete quantum theory for this model. We chose a representation of the elementary operators, on some vector space of complex valued functions on the configuration space. In this representation,
the constraint equation is a second order partial differential equation, which we solved explicitly. This set of solutions is “large” in the sense that it includes the tunnelling solutions, which penetrate the classically forbidden region. Next, we constructed a set of generators of $A_{phy}$, the algebra of physical observables. These operators act on the “large” space of solutions and leave it invariant. Then we attempted to induce the $\star$-involution on $A_{phy}$, from $A$. The $\star$s of most of the generators of $A_{phy}$ were also in $A_{phy}$. However, the $\star$ (evaluated in $A$) of one of the physical operators was no longer a physical operator itself. Thus, we were unable to induce on $A_{phy}$ the structure of a $\star$-algebra. This appeared to be an impassè, in terms of constructing the physical inner product via the prescription of the algebraic approach.

At this point we attempted to implement part of the $\star$-relations as Hermiticity conditions on some of the physical operators. Quite unexpectedly, these conditions led us to the conclusion that mathematically distinct solutions to the constraint equation can lead to the same physical state: the measure ignores the part of the wavefunctions that corresponds to the tunnelling solutions. Finally, the algebra of operators on the space of physical states—which effectively ignores the tunnelling solutions—does admit a $\star$-involution. Hence we were able to complete the quantization program. Finally, let us consider the Hamiltonian (5.2) in the quantum theory we have constructed. It is manifestly positive. On physical states the Hamiltonian operator is $\hat{H} \psi = E(\phi) \psi$. Since the states have (measurable) support only in $\bar{C}$, where $E(\phi) \geq 0$, $\langle \hat{H} \rangle \geq 0$ for all physical states.

A key result of the Ashtekar-Horowitz quantization was that the Dirac quantum theory does possess physical quantum states which tunnel into the forbidden region $\tilde{C}$. Further, some states had support entirely in $\tilde{C}$! This led to the further conclusion that a large number of physical quantum states possess negative energies: for this model the classical positive energy theorem was violated in quantum theory. These results were arrived at by using the “obvious” choice of measure: the Euclidean measure on $\mathbb{R}^3$. What we have shown here is that the choice of the measure—and hence of the physical inner product—is severely limited by the reality conditions. The “obvious” choice is in fact incorrect.

A careful re-analysis of the problem has thus removed the exotic features that were present in the previous quantization. While the final result seems somewhat disappointing (in the sense that the quantum theory does not display any exotic features), this example serves to demonstrate the power of the quantization program of section 2. In retrospect our final result could have been obtained by a number of other quantization procedures. However, in other schemes the elimination of the spurious tunnelling states would have probably been an ad hoc step.

In fact, based on an analysis of a similar model, which is perhaps even more peculiar than the A-H model, Gotay [29] proposed exactly such a requirement for quantum theory: by fiat the measure is restricted to the classically allowed region. On the other hand; in the algebraic approach to quantization, this result is derived from a general principle (which is not expressly invented for this example just to satisfy our classical intuition): real physical operators should be Hermitian with respect to the physical inner product.

In another re-analysis of this model, Boulware [28] assumed the usual Euclidean inner product on the representation space, and required that $p_\theta$ be a symmetric operator on
the space of all $L^2(S^2)$ states before solving the constraint equation and isolating the physical states. Then, physical states have support only on the classically allowed region, and there is no tunnelling in this theory. As in the case of Gotay’s analysis, the absence of tunnelling is simply an input. Furthermore, now a new problem arises: the resulting Hilbert space of physical states is only finite dimensional, and therefore represents zero degrees of freedom! However, the reduced phase space is a perfectly well-defined cotangent bundle over $S^1$. Thus the quantum theory of $[28]$ does not capture all the physics in the model.

In the quantum theory we constructed here, since $\hat{p}_\theta$ is an observable, we too required it to be Hermitian, but only on physical states. Since on physical states $\hat{p}_\theta = \sqrt{R(\phi)}$ one might wonder whether it is necessary to include $p_\theta$ in a set of generators of the physical observable algebra. However, it is a physical quantity, and one might wish to measure it. In the context of the algebraic approach, the mathematically important facet of the Hermiticity of $\hat{p}_\theta$ is the following: as we saw in (5.11), unless we impose the Hermiticity of $\hat{p}_\theta$, the rest of the formulation is not mathematically well-defined.

The quantization of a constrained system is inherently an ambiguous process. One can only require that the final quantum theory is “complete and consistent” in the sense that one has a faithful $\star$-representation of a suitably large algebra of observables and that one recover the classical description in a suitable limit. To achieve this end, one is justified in riding roughshod over the initial stages of the road to quantization. Thus, one can view the quantization of the rigid rotor model in the following way: In the beginning of this section, we exploited the freedom to define the representation space and the operators, and were intentionally obscure about the specification of $\mathcal{V}$. We then made some choice of factor-ordering for the constraint and solved it on this space. On physical states, we defined the actions of operators which formally had vanishing commutators with the constraint. Then we imposed reality conditions on these and found appropriate Hermitian physical operators, completing the quantization program.

Finally, one can construct the reduced space quantum theory for this model. The reduced phase space constructed in $[26]$ appears to consist of two halves $\hat{\Gamma}_\pm$, each coordinatized respectively by $(\hat{\phi}, P_{\hat{\phi}}^\pm)$, where $\hat{\phi}$ indicates the classically allowed values of $\phi$. The resulting reduced space quantum theory corresponds to the quantization of a particle whose phase space is the cotangent bundle over two disconnected intervals, and it is relatively easy to see that it is unitarily equivalent to the Dirac theory we have constructed above. However, there is a subtlety in the construction of the reduced phase space which arises due to the fact that the this “naive” reduced phase space is constructed using the functions $(p_\phi, f(\phi), P_{\phi}^\pm)$; these are the classical analogs of the Dirac observables constructed above, and as we noted earlier, they fail to be a complete set. Recall that this incompleteness occurs at points where $R(\phi) = 0$. An analysis of the constraint surface in the vicinity of these points shows that the two “halves” $\hat{\Gamma}_\pm$ of the reduced phase space are smoothly joined at these points and the reduced phase space is in fact a cotangent bundle over $S^1$. What is the relation between the two quantum theories? As we have seen, the Dirac quantum theory corresponds to the quantization

\[\text{The reduced configuration space may consist of multiple copies of } S^1, \text{ depending on the number of nodes of } R(\phi).\]
of a particle whose phase space is the cotangent bundle over two disconnected intervals. This “incorrect” phase space can be thought of as the cotangent bundle over $S^1$, but with two diametrically opposite points removed. To illustrate the relation, we can construct a momentum operator, which in the Dirac theory has a doubly degenerate spectrum with even eigenvalues, whereas in the reduced space theory this operator has a nondegenerate spectrum with all integer eigenvalues. Thus the two quantum theories are inequivalent, and there appear to be no obvious means to make them equivalent.

6 Issue of time and deparametrization

For ordinary constrained systems, such as gauge theories, the Hamiltonian—which generates dynamics—is distinct from the constraint functions and therefore does not vanish on the constraint surface. On the other hand, there are theories in which the vanishing of the Hamiltonian is itself a first class constraint function. We will refer to such theories as dynamically constrained systems since the generator of the dynamical trajectories is now constrained to vanish. General relativity in the spatially compact case is an outstanding example of such systems.

In dynamically constrained systems, to begin with, the notions of gauge and time evolution are entangled. To bring out the resulting difficulties, let us first recall some features of ordinary constrained systems. In such systems, solving the constraints—either classically, by constructing the reduced phase space (or, equivalently, a cross-section of the gauge orbits), or in quantum theory, by constructing the physical states, an operator algebra of observables and an inner product on these states—is a purely kinematical procedure. Conceptually, this construction is divorced from the dynamical structure of the theory which is dictated by the Hamiltonian. In the classical theory, the Hamiltonian can be projected unambiguously to the reduced phase space, and all physically interesting dynamics can be considered to occur there. In the quantum theory, the corresponding Hamiltonian operator generates (unitary) evolution on the Hilbert space of physical states.

In contrast, for systems in which the Hamiltonian is constrained to vanish, kinematical considerations are intimately linked with the dynamical structure of the theory. (For a more complete discussion of the problems in quantum theory, see [30, 31].) If one proceeds as one does for ordinary constrained systems, one ends up with a “frozen formalism.” Classically, each point in the reduced phase space corresponds to an entire dynamical trajectory. Quantum mechanically, solutions to the constraints can be found and represent physical states, but they do not evolve. To obtain evolution, one must re-interpret the constraint as telling us that how the “true degrees of freedom” change with respect to an appropriate canonical variable which can then be taken to represent time. Thus, for these systems, “time” is not an external parameter; it has to be singled out from among the canonical variables.

In section 6.1, we will discuss the simplest of such systems in the framework of algebraic quantization. We will see that one can follow the program step by step and arrive at the inner product on the space of physical states without having to single out time. In section 6.2, we will discuss the issue of dynamics and interpretation. The choice of our model was motivated by simplicity; we wish to illustrate the ideas in as simple a
setting as possible. For models which are physically more interesting, see, e.g., [11].

6.1 Non-relativistic parametrized particle

Consider a non-relativistic particle moving in a potential \(V(q_i)\) in Euclidean space. Dynamics is specified by the Hamiltonian \(H(q_i, p_i) = \frac{1}{2m} \sum p_i p_i + V(q_i)\). This simple system can be “parametrized” by adding to the 3-dimensional configuration space the time variable. Thus, the (enlarged) configuration space, \(C\), is now 4-dimensional, coordinatized by \((q_0, q_i)\); and the phase space is 8-dimensional. There is one (first class) constraint:

\[ C(q, p) := p_0 + H(q_i, p_i) = 0, \] (6.1)

where \(q\) and \(p\) stand for \((q_0, q_i)\) and \((p_0, p_i)\) respectively. The constraint reduces the fictitious 4 degrees of freedom to the original 3 “true degrees”: classically, the constrained system is equivalent to the original system evolving in the 6 dimensional phase space spanned by \((q_i, p_i)\) via the Hamiltonian \(H(q_i, p_i)\).

Let us now carry out the quantization program step by step. Let the space \(S\) of elementary observables be the complex vector space spanned by the 9 functions \((1, q, p)\) on the phase space \(\Gamma\), with the usual commutation relations. Choose for the representation space \(V\) the space of smooth functions on the 4-dimensional configuration space \(C\), and represent the operators by the usual multiplication and partial derivative operators.

The quantum constraint is now given by:

\[ \hat{C} \circ \Psi(q) \equiv \frac{\hbar}{i} \frac{\partial \Psi(q)}{\partial q^0} + \hat{H} \circ \Psi(q) = 0. \] (6.2)

(Although (6.2) has the form of the Schrödinger equation if \(q^0\) is identified as the “internal time,” in this subsection we will ignore this aspect and regard (6.2) simply as the quantum constraint equation as in the previous examples.) The space of physical states, \(V_{phy}\), now consists of solutions of this equation. A technically convenient way to write them (formally) is:

\[ \Psi(q) = e^{-\frac{i}{\hbar} \hat{q}^0 \circ \psi(q^i)} , \] (6.3)

where the \(\psi(q^i)\) are arbitrary functions of \(q^i\). Note that the solutions \(\Psi(q)\) to the quantum constraint are complex valued functions on the 4-dimensional configuration space \(C\); they are not functions of \(q_i\) alone as they necessarily depend on \(q^0\) as well. In this sense, they are “covariant”. However, since the \(q^0\) dependence is fixed by the exponential term, physical states are completely determined by the functions \(\psi(q^i)\), which we can think of as the “initial data” for the first order (in \(q^0\)) differential equation (6.2).

Our next task in the quantization program is to isolate physical observables. None of the elementary quantum operators, \(\hat{q}^0, \hat{q}^i\) or \(\hat{p}_i\), corresponding to the set \(S\), is a physical operator since the action of any of them maps one out of the set of physical states.

\[14\] Note that for what follows, in the choice of representation it is essential only that \(\hat{q}^0\) be a multiplication operator. One is free to choose any representation of the \(\hat{q}^i, \hat{p}_i\) operators, depending on the specific form of the Hamiltonian.
Fortunately, it is not difficult to construct, at least formally, a complete set of physical operators. They are given by:

\[ \hat{Q}^i(0) \circ \Psi := \hat{U}(0) \hat{q}^i \hat{U}^{-1}(0) \circ \Psi = e^{-\frac{i}{\hbar} \hat{H} q^0} \hat{q}^i \circ \psi \equiv e^{-\frac{i}{\hbar} \hat{H} q^0} \circ q^i \psi(q^i) \quad \text{and} \]
\[ \hat{P}_i(0) \circ \Psi := \hat{U}(0) \hat{p}_i \hat{U}^{-1}(0) \circ \Psi = e^{-\frac{i}{\hbar} \hat{H} q^0} \hat{p}_i \circ \psi \equiv e^{-\frac{i}{\hbar} \hat{H} q^0} \circ \frac{\hbar}{i} \frac{\partial}{\partial q^i} \psi(q^i), \]

where
\[ \hat{U}(0) := e^{-\frac{i}{\hbar} \hat{H} q^0}. \]

Here, since \( \hat{q}^0 \) acts by multiplication, it has been replaced by \( q^0 \) and the operator \( \hat{H} \) is given by \( \hat{H} = H(\hat{q}^i, \hat{p}_i) \). (The reason for the notation \( \hat{U}(0) \) will become clear in the next subsection.) From the last step in \( (6.4) \), it is obvious that \( \hat{Q}^i(0) \circ \Psi \) and \( \hat{P}_i(0) \circ \Psi \) are again solutions to the quantum constraints; \( \hat{Q}^i(0) \) and \( \hat{P}_i(0) \) are physical operators. Indeed, a simple algebraic calculation shows that these six operators, \( \hat{Q}^i \) and \( \hat{P}_i \), commute with the constraint, and furthermore, are their own *'s. Since the reduced phase space is 6-dimensional, and the above Dirac operators are independent, they form a complete set. Hence we can now look for an inner product on \( \mathcal{V}_{phy} \) with respect to which these operators are Hermitian. For this, let us begin by introducing a measure \( \mu(q) \) on the configuration space and set:

\[ \langle \Psi(q) | \Phi(q) \rangle = \int \mathcal{C} \, d^4 q \, \mu(q) \, \overline{\Phi}(q) \, \Phi(q), \]

for all physical states \( \Psi(q) \) and \( \Phi(q) \). To determine the measure, we impose the Hermiticity requirements. The condition that \( \hat{Q}^0 \) be Hermitian does not constrain the inner product in any way. The condition that \( \hat{P}_i \) be Hermitian requires that the measure be independent of \( q_i \). (In the general case, when the “true” configuration space is a non-trivial manifold or the coordinates are not Cartesian, the Hermiticity conditions on \( \hat{P}_i \) determine the dependence of \( \mu \) on \( q^i \). The important point is that the dependence of \( \mu \) on \( q^0 \) is left undetermined.) Thus, the inner-product can now be calculated:

\[ \langle \Psi(q) | \Phi(q) \rangle = \int d^4 q \, \mu(q^0) \, \overline{\Phi}(q) \, \Phi(q) \]
\[ = \int dq^0 \, \mu(q^0) \int d^3 q^i \, \overline{\Phi}(q^0, q^i) \, \Phi(q^0, q^i) \]
\[ = \int dq^0 \, \mu(q^0) \int d^3 q^i \, \overline{\psi}(q^i) \, \phi(q^i) \]
\[ = K \int d^3 q^i \, \overline{\psi}(q^i) \, \phi(q^i) \equiv K \int d^3 q^i \, \overline{\Phi}(q^0, q^i) \, \Phi(q^0, q^i) \]

(6.7)

where the constant \( K \) is given by \( K = \int dq_0 \, \mu(q_0) \). Here, in the third step, we have used the fact that \( \Psi(q_0, q_i) \) and \( \Phi(q_0, q_i) \) are physical states, i.e., they satisfy \( (6.2) \). Thus, the second integral in the second line is independent of \( q_0 \). Since \( \mu(q^0) \) is not constrained in any way by the Hermiticity of the observables, we can choose it so that \( K \) is finite, say \( K = 1 \). Thus, the reality conditions do indeed select a unique inner product on \( \mathcal{V}_{phy} \) (up to the usual overall constant) and the resulting quantum description is completely equivalent to the quantum theory of the original unconstrained particle moving in a potential \( V \) in the Euclidean space.
The final picture is the following: the physical Hilbert space consists of solutions to the constraint equation \( (6.2) \), with the Hermitian inner product given by \( (6.7) \). Up to this point, the physical operators \( (6.4) \) were formal constructs, used to find an inner product. Now, however, we can use the physical inner product to rigorously define the unitary operator \( (6.5) \), and hence the physical observables. This completes the quantization program.

We conclude this subsection with two remarks.

Note first that the Hermitian inner product is defined on \( V_{\text{phy}} \), i.e., on the space of solutions \( \Psi(q^0, q^i) \) to \( (6.2) \). That in the final step we can perform the integral on a constant \( q^0 \) surface is “accidental”; it is only a calculational device. The situation is rather similar to that encountered in the covariant symplectic description of fields on Minkowski space \( [32] \) where the expression of the symplectic structure involves an integration over a spatial slice although the structure itself is defined on the space of solutions to the field equations on the entire space-time. In this sense, the above quantum description of the parametrized particle is also “covariant”.

In the main construction above, we have been dealing essentially with the covariant states \( \Psi(q) \). Note, however, that these covariant solutions are in 1-1 correspondence with the \( q^0 \) independent (“initial data”) states \( \psi(q^i) \). In fact, there is an obvious unitary transformation, given by \( (6.3) \), between the covariant states \( \Psi(q) \) and the states \( \psi(q^i) \equiv \psi_0(q^i) \). The inverse of the unitary transformation is given by:

\[
\psi_0(q^i) := e^{\frac{i}{\hbar} H q^0} \circ \Psi(q) \equiv \Psi(q)|_{q^0=0}.
\]

With \( K = 1 \), the inner product on these states is simply \( (6.7) \). Clearly, the states \( \psi_0(q^i) \) are not the solutions of any constraint equation. However, they carry a faithful representation of the observable algebra. Let \( z \) denote any operator in the set \( (q^i, p_i) \); and let \( Z \) denote the corresponding operator in the set \( (Q^i, P_i) \). Under the action of the unitary transformation, the representation of the observables \( (6.4) \) is simply

\[
\hat{Z}(0) \circ \psi_0(q^i) = \hat{z} \circ \psi_0(q^i).
\]

The physical observables have a simple action on the space of initial states for the constraint equation. Now, the intuitive meaning of these operators is clear: Since the constraint generates dynamical evolution, we know that the physical observables correspond to constants of motion, which in turn can be identified with the position and momentum at some initial time. Hence, a set of Dirac operators can be obtained by “evolving the covariant states \( \Psi \) back to \( q^0 = 0 \)” (or, via \( (6.8) \), evaluating them at \( q^0 = 0 \)), acting with the usual “instantaneous” operators on the initial state \( \psi(q^i) \), and then “evolving the resulting initial state forward to \( q^0 \)”, using the constraint equation. This is exactly the procedure we have carried out, as is obvious also from the second equalities in \( (6.4) \).

### 6.2 From frozen formalism to dynamics

We now wish to extract dynamics from the framework constructed above. The main idea of course is to regard \( q^0 \) as the internal clock, \( q^i \) as the “true degrees of freedom,”
and interpret the constraint equation as telling us how the functional dependence of the physical states $\Psi$ on $q^i$ changes as we go from one $q^0 = \text{constant}$ slice in the configuration space to another.

More precisely, to introduce the notion of evolution, it is necessary to foliate the 4-dimensional covariant configuration space by $q^0 = \text{constant}$ surfaces. Then, each covariant state $\Psi(q)$ defines a 1-parameter family of “Schrödinger states” $\psi_\tau(q^i)$:

$$\psi_\tau(q^i) := e^{i\hbar \hat{H}(q^0 - \tau)} \circ \Psi(q) \equiv \Psi(q)|_{q^0=\tau}. \quad (6.10)$$

Note that this correspondence exists only because the states $\Psi(q)$ satisfy the constraint equation. Let us now turn to observables. If $\hat{z}$ is a “Schrödinger observable,” the foliation naturally provides us with a 1-parameter family of physical observables $\hat{Z}(\tau)$ via the inverse of the unitary transformation (6.11):

$$\hat{Z}(\tau) \circ \Psi(q) = \hat{U}(\tau) \hat{z} \hat{U}^{-1}(\tau) \circ \Psi(q) = e^{i\hbar \hat{H}(\tau - \tau_0)} \hat{z} \circ \psi_\tau(q^i), \quad (6.11)$$

where

$$\hat{U}(\tau) = e^{-i\hbar \hat{H}(q^0 - \tau)} \quad (6.12)$$

is the unitary transformation defined in (6.11). It is now manifest from this analogy that we can identify $q^0$ with the time in the quantum theory and that the $\hat{Z}(\tau)$ are the “evolving” Heisenberg operators. In fact since the effect of the unitary evolution is simply to evaluate the covariant state at $q^0 = \tau$, i.e.,

$$\hat{U}^{-1}(\tau) \circ \Psi(q) := \psi_\tau(q^i) \equiv \Psi(q^0 = \tau, q^i) \quad (6.13)$$

the above rule to calculate the $\hat{Z}(\tau)$ operators states that their action is the following: Evaluate the covariant physical states $\Psi(q^0, q^i)$ at $q^0 = \tau$, act with the corresponding $\hat{z}$ operators, and then evolve forward to $q^0$ again. Thus, for $\hat{q}^0(\tau)$ the above rule yields

$$\hat{q}^0(\tau) \circ \Psi(q) = \hat{U}(\tau) \circ \tau \psi_\tau(q^i) = \tau \cdot \Psi(q). \quad (6.14)$$

Of course, if we desire, we can also evaluate the action of the operators $\hat{Z}(\tau)$ on a fixed Schrödinger Hilbert space, say corresponding to $q^0 = \tau_0$:

$$\hat{Z}(\tau) \circ \psi_{\tau_0}(q^i) = e^{i\hbar H(\tau - \tau_0)} e^{-i\hbar H(\hat{z})(\tau - \tau_0)} \circ \psi_{\tau_0}(q^i). \quad (6.15)$$

As expected, we have lost all reference to $q^0$, and have obtained the complete de-parametrization of the theory to the usual text-book picture.

Finally, note that it is trivial to extend this discussion to allow for a $q_0$-dependence in the expression of the Hamiltonian (by appropriately time-ordering the $\hat{U}(\tau)$) or to replace the Euclidean space by an $n$-manifold.

We conclude this subsection with three remarks.

In retrospect we see that we could have worked always in the covariant picture, with the $\tau$-dependent Heisenberg operators defined in (6.11). However, we would then have lost both the interpretation of $q^0$ as time as well as the motivation for the introduction of the “evolving” observables. It is in order to see the unfolding of the dynamics which
is hidden in the frozen formalism that we have to break the covariance of the space of solutions and introduce on this space a “foliation” corresponding to time evolution and the resulting sequence of Schrödinger states.

Recall that nowhere in the kinematical construction to find the inner product was it necessary to treat $q^0$ in a special manner. We found the inner product without explicitly eliminating the “time” $q^0$. That is, contrary to what is commonly done in the literature, we did not integrate only over the true degrees of freedom $q^i$. Rather, we used the the reality conditions on the space $V_{phy}$ of solutions to the constraint to obtain the inner product. This is an important point, since it illustrates that it is not necessary to isolate time in order to construct the Hilbert space of physical states. In this simple example, the form of the constraint immediately suggests that we treat $q^0$ as the internal clock and $q^i$ as the true degree of freedom. Hence we could also have first singled out the time variable and then found the inner product. However, in more interesting examples of dynamically constrained theories such as 3-dimensional general relativity, the constraints do not provide an obvious internal clock and, except in the simplest spatial topology, we do not yet know how to find a convenient deparametrization. One can, however, impose the reality conditions directly and the strategy does yield an unique inner product. (For a more complete discussion of this aspect of the issue of time in quantum gravity, see [33, §12].)

However, to complete the analysis and make physical predictions, as in the Schrödinger picture, one may need to find explicit solutions by diagonalizing the “true” Hamiltonian $\hat{H}$. In addition to the states, one has to construct explicit expressions for a complete set of interesting operators. In Bianchi models [11] of 4-dimensional general relativity, for example, while the reality conditions lead one directly to the inner product on the physical Hilbert space, deparametrization is necessary to answer physically interesting questions concerning the fate of classical singularities in quantum theory. Furthermore, even from a mathematical viewpoint, the availability of deparametrization simplifies the quantization program significantly. In particular, it provides a direct route to the problem of finding a complete set of physical observables.

7 Conclusion

In this paper, we have illustrated various features of the algebraic quantization program of [6] through a number of examples. The fact that the program could be carried out to completion in all these examples provides confidence in the viability of the strategies involved.

The main lessons of this study can be summarized as follows:

i) Overcompleteness of elementary classical variables can be incorporated into quantum theory through appropriate algebraic conditions on the elementary quantum operators. Thus, it is not necessary to eliminate these relations classically. Indeed, in the case when the phase space is a non-trivial manifold, it is in principle impossible to do so. This point is conceptually important for a number of systems being investigated in the literature, including lattice gauge theories, where the Wilson loop functionals form an overcomplete set on the configuration space and in continuum Yang-Mills theories and general relativity, where the “loop variables” of Gambini
and Trias [34] and Rovelli and Smolin [35] also form an over-complete set almost everywhere on the phase space.

ii) Even when there are no obvious symmetries present, the inner product on physical states can be singled out using the “reality conditions,” i.e., by demanding that real classical observables be represented on the physical Hilbert space by self-adjoint operators. In the constrained rotor model, in particular, this procedure clarified an important conceptual point thereby resolving a controversy.

iii) The issue of completeness of physical observables is subtle. Even when the set of observables is “locally complete,” superselection sectors can arise due to global ambiguities. This issue is important for general relativity where the Rovelli-Smolin loop variables fail to constitute a complete set on sets of measure zero [36].

iv) Deparametrization of a dynamically constrained is not essential to obtain a mathematically complete quantum description, including the inner product on the space of physical states. However, to display dynamics explicitly and extract physical information from the theory, one may have to deparametrize the theory at least approximately. Furthermore, if an exact deparametrization happens to be available, it can be used to find a complete set of (“time dependent”) Dirac observables and these in turn can be used to obtain the inner product on the space of physical states.

The program and the examples were motivated primarily by various problems one encounters in quantization of general relativity. Some of the points listed above have already played an important role in the quantization of 3-dimensional general relativity [1, §17], and various mini-superspace models [11, 12, 13, 15] of 4-dimensional gravity. We expect that these points are all significant to the quantization of full, 4-dimensional general relativity.

The program, however, has a much broader range of applicability; it is not tied to general relativity. Indeed, since it is formulated rather loosely, it serves more as an umbrella that brings together the ideas underlying various approaches to the quantization of constrained systems such as the group theoretic approach [3] and geometric quantization [22, 16]. Thus, the large class of examples in which these methods have been successful also provide illustrative applications of the program. However, because it is formulated somewhat loosely, it allows more general strategies. For example, unlike geometric quantization, it can be used to construct “exotic” representations that do not directly arise from polarizations of the phase space. An important example is provided by the loop representations of gauge theories [34].

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42
References

[1] P. A. M. Dirac, *Lectures on quantum mechanics* (Yeshiva University, New York, 1964).

[2] K. Kuchař, J. Math. Phys. **22**, 2640 (1982).

[3] C. G. Torre and I. Anderson, Phys. Rev. Lett. **70**, 3525 (1993).

[4] F. Barbero-Gonzalez, in preparation (1994).

[5] C. J. Isham, in *Relativity, Groups and Topology II, Les Houches 1983*, edited by B. S. DeWitt and R. Stora (North Holland, Amsterdam, 1984).

[6] A. Ashtekar, *Lectures on nonperturbative canonical gravity* (World Scientific, Singapore, 1991).

[7] A. Rendall, Class. Quantum Grav. **10**, 2261-69 (1993), [gr-qc/9303026](https://arxiv.org/abs/gr-qc/9303026); erratum: [gr-qc/9403001](https://arxiv.org/abs/gr-qc/9403001).

[8] A. Ashtekar and R. Geroch, Rep. Prog. Phys. **37**, 1211 (1974).

[9] A. Ashtekar, Commun. Math. Phys. **71**, 59 (1980).

[10] R. S. Tate *Ph.D. Dissertation* Syracuse University (1992), [gr-qc/9304043](https://arxiv.org/abs/gr-qc/9304043).

[11] A. Ashtekar, R. S. Tate and C. Uggla, Int. J. Mod. Phys. D**2**, 15-50 (1993), [gr-qc/9302027](https://arxiv.org/abs/gr-qc/9302027).

[12] G. A. Mena Marugán, Class. Quantum Grav. **11**, 589 (1994), [gr-qc/9309024](https://arxiv.org/abs/gr-qc/9309024); Int. J. Mod. Phys. D, (to appear, 1994), Pennsylvania State University preprint CGPG-93/11-2, [gr-qc/9311020](https://arxiv.org/abs/gr-qc/9311020); PSU preprint CGPG-94/2-2, [gr-qc/9402034](https://arxiv.org/abs/gr-qc/9402034).

[13] G. Gonzalez, G. A. Mena Marugán, and R. S. Tate, (in preparation) 1994.

[14] P. Hajicek, In: *The Canonical formalism in classical and quantum gravity*, edited by J. Ehlers and H. Friedrichs (Springer-Verlag, Berlin, 1994, in press).

[15] C. Rovelli, Phys. Rev. D**35**, 2987 (1987).

[16] A. Ashtekar and M. Stillerman, J. Math. Phys. **27**, 1319 (1986).

[17] A. Ashtekar, Phys. Rev. Lett. **57**, 2244 (1986).

[18] A. Ashtekar and J. Lee, Int. J. Mod. Phys. D, (to appear).

[19] K. Kuchař, In: *General Relativity and Gravitation 1992*, edited by R. J. Gleiser, C. N. Kozameh and O. M. Moreschi (IOP, Bristol, 1993).

[20] K. S. Narain, *Ph.D. Dissertation*, Syracuse University (1982).

[21] C. Rovelli, Phys. Rev. D**42** 2638, (1990); D**43**, 442 (1991).
[22] N. J. M. Woodhouse, *Geometric Quantization* (Oxford University Press, Oxford, UK, 1981).

[23] M. Stillerman, *Ph.D. Dissertation*, Syracuse University (1985).

[24] J. Louko, *private communication* (1992); Phys. Rev. D48, 2708 (1993), gr-qc/9305003.

[25] G. A. Mena Marugán, PSU preprint CGPG-94/5-2, gr-qc/9405027.

[26] A. Ashtekar and G. T. Horowitz, Phys. Rev. D26 3342-53 (1982).

[27] R. Arnowitt, S. Deser and C. W. Misner, in *Gravitation: an introduction to current research*, edited by L. Witten (Wiley 1962); K. Kuchař, in *Quantum Gravity 2*, edited by C. J. Isham, R. Penrose and D. Sciama (Oxford University Press, Oxford, 1981).

[28] D. G. Boulware, Phys. Rev. D28, 414-16 (1983).

[29] M. J. Gotay, Class. Quantum Grav. 3, 487-91 (1986).

[30] K. Kuchař, In: *Proceedings of the 4th Canadian Conference on general relativity and relativistic astrophysics*, edited by G. Kunstatter, D. E. Vincent and J. G. Williams, (World Scientific, Singapore, 1992).

[31] C. J. Isham, In: *Proceedings of the NATO Advanced Studies Institute, Salamanca, June 1992*, (Kluwer Academic Publishers, London, 1993).

[32] A. Ashtekar, L. Bombelli and O. Reulla, In: *Mechanics, analysis and geometry: 200 years after Lagrange*, edited by M. Francaviglia, (Elsevier, Amsterdam, 1991).

[33] A. Ashtekar, In: *Conceptual Problems in Quantum Gravity*, edited by A. Ashtekar and J. Stachel, (Birkhäuser, Boston, 1989).

[34] R. Gambini and A. Trias, Nucl. Phys. B278, 436 (1986).

[35] C. Rovelli and L. Smolin, Nucl. Phys. B331, 80-152 (1990).

[36] J. Goldberg, J. Lewandowski and C. Stornaiolo, Commun. Math. Phys. 148, 377 (1992).