

Syracuse University

SURFACE

Physics

College of Arts and Sciences

1992

An Algebraic Approach to the Quantization of Cosntrained Systems: Finite Dimensional Examples

Ranjeet S. Tate
Syracuse University

Follow this and additional works at: <https://surface.syr.edu/phy>



Part of the [Cosmology, Relativity, and Gravity Commons](#)

Recommended Citation

Tate, Ranjeet S., "An Algebraic Approach to the Quantization of Cosntrained Systems: Finite Dimensional Examples" (1992). *Physics*. 6.
<https://surface.syr.edu/phy/6>

This Working Paper is brought to you for free and open access by the College of Arts and Sciences at SURFACE. It has been accepted for inclusion in Physics by an authorized administrator of SURFACE. For more information, please contact surface@syr.edu.

An Algebraic Approach to the Quantization of Constrained Systems:
Finite Dimensional Examples
(Ph.D. dissertation, Syracuse University, August 1992)

Ranjeet S. Tate

Department of Physics, University of California - Santa Barbara, CA 93106-9530
e-mail: rstate@cosmic.physics.ucsb.edu

ABSTRACT

General relativity has two features in particular, which make it difficult to apply to its existing schemes for the quantization of constrained systems. First, there is *no background structure* in the theory, which could be used, e.g., to regularize constraint operators, to identify a “time” or to define an inner product on physical states. Second, in the Ashtekar formulation of general relativity, which is a promising avenue to quantum gravity, the natural variables for quantization are *not* canonical; and, classically, there are algebraic identities between them. Existing schemes are usually not concerned with such identities. Thus, from the point of view of canonical quantum gravity, it has become imperative to find a framework for quantization which provides a *general* prescription to find the physical inner product, and is flexible enough to accommodate non-canonical variables.

In this dissertation I present an algebraic formulation of the Dirac approach to the quantization of constrained systems. The Dirac quantization program is augmented by a general principle to find the inner product on physical states. Essentially, the Hermiticity conditions on physical operators determine this inner product. I also clarify the role in quantum theory of possible algebraic identities between the elementary variables.

I use this approach to quantize various finite dimensional systems. Some of these models test the new aspects of the algebraic framework. Others bear qualitative similarities to general relativity, and may give some insight into the pitfalls lurking in quantum gravity. The previous quantizations of one such model had many surprising features. When this model is quantized using the algebraic program, there is no longer any unexpected behaviour. I also construct the complete quantum theory for a previously unsolved relativistic cosmology. All these models indicate that the algebraic formulation provides powerful new tools for quantization.

In (spatially compact) general relativity, the Hamiltonian is constrained to vanish. I present various approaches one can take to obtain an interpretation of the quantum theory of such “dynamically constrained” systems. I apply some of these ideas to the Bianchi I cosmology, and analyze the issue of the initial singularity in quantum theory.

Contents

Preface	v
1 INTRODUCTION	1
1.1 Motivation	1
1.2 Chronology	6
1.3 Outline	7
2 ALGEBRAIC QUANTIZATION OF CONSTRAINED SYSTEMS	13
2.1 Introduction	13
2.2 Algebraic quantization	13
2.3 Summary of the program	18
2.4 Remarks	18
2.5 (†) Reduced space quantization	23
3 SIMPLE EXAMPLES	27
3.1 Introduction	27
3.2 Particle on a circle	28
3.2.1 (†) Fractional statistics on S^1	29
3.3 Harmonic oscillator in the (q, z) variables	31
3.4 Bianchi II model	33
3.4.1 Dirac quantization	35
3.4.2 (†) Reduced space quantization	38
3.5 Remarks	41
4 ASHTEKAR-HOROWITZ MODEL	45
4.1 Introduction	45
4.2 Dirac quantization	47
4.2.1 Remarks	53
4.3 (†) Reduced space quantization	55
5 COUPLED OSCILLATORS: CONSTRAINED ENERGY DIFFERENCE	61
5.1 Introduction	61
5.2 Dirac quantization	62
5.3 Classical expectations and quantum theory	67
5.4 FRW universe with conformally coupled scalar field	69

5.5	(†) Reduced space quantization	70
5.6	(†) Coupled oscillators: constrained energy sum	72
6	PHYSICAL INTERPRETATION FOR SYSTEMS WITH A CON-	
	STRAINED HAMILTONIAN	75
6.1	Introduction	75
6.2	Non-relativistic parametrized particle	79
	6.2.1 Kinematical quantum theory	79
	6.2.2 Dynamics and interpretation	82
6.3	Reduced space quantization and interpretation	83
6.4	Bianchi I model	86
	6.4.1 Physical interpretation	88
	6.4.2 The initial singularity in quantum cosmology	89
	6.4.3 (†) Expanding or contracting Universe, or both?	91
6.5	Discussion	92
7	DIALOGUE	99
A	QUANTIZATION OF SECOND CLASS CONSTRAINTS	111
	A.1 Holomorphic δ function	112
	A.2 Second class constraints in quantum theory	113
	Bibliography	117

Preface

Further work has been done on parts of this thesis. A preprint (on which chapter 2 and some of the examples are based) is in preparation (A. Ashtekar and R. S. Tate) on the algebraic approach to the quantization of constrained systems. The approach to deparametrization applied to the quantized Bianchi type I model has been improved upon, and the analysis of the singularity has been extended to a class of “solvable” Bianchi models, by A. Ashtekar, R. S. Tate and C. Uggla, see gr-qc/9302027.

ACKNOWLEDGEMENTS

First and foremost I would like to thank my thesis advisor, Prof. Abhay Ashtekar. He has been a very good advisor, in terms of the guidance and encouragement he has provided, both scientific and personal. Discussions with him are always exciting, and our collaboration has been very enjoyable. His detailed comments on this thesis –based on his uncanny ability to place himself in the shoes of the reader– have resulted in a much more readable thesis than the one I first presented to him.

Members of the relativity group at Syracuse University –faculty, post-docs, visitors and graduate students– foster an atmosphere which is both academically stimulating and personally friendly. All of them have always been willing to discuss things with me, even if the ideas were not of direct interest to them. Many ideas in my graduate work have arisen from discussions with various members of the group. I have enjoyed discussions with Bernd Brügmann, Josh Goldberg, Jorge Pullin, Joseph Samuel, Lee Smolin, Charles Torre and Claes Uggla; all of whom have also provided help on technical matters.

I thank Karel Kuchař and Carlo Rovelli for their patient explanations of their ideas.

Jorma Louko read preliminary drafts of my thesis very carefully; his criticisms and thought-provoking questions have clarified many conceptual and technical issues.

Most graduate students help each other out by reading first drafts, helping prepare talks, providing ideas or listening to them –and then helping to work them out. As my office-mates, (for four years and one year respectively) Joe Romano and Gabriela Gonzalez have always gone out of their way to provide such help.

I thank the Syracuse University Outing Club for providing wonderful alternatives to academics. The idea for at least one paper occurred to me on a club trip.

I thank HarperCollins Publishers for their permission to use Achilles and the Tortoise as characters in a dialogue.

I have been supported by funds provided by Syracuse University, a Syracuse University Graduate Fellowship and a research assistantship under NSF grants PHY86-12424 and PHY90-16733.

Chapter 1

INTRODUCTION

1.1 Motivation

For many physically interesting systems, not all points of the phase space are accessible. The allowed classical states of the system are confined to lie on a sub-manifold of the phase space, called the constraint surface. Now, all empirical evidence supports the widely held view that the fundamental behaviour of all systems must be quantum mechanical in nature, and not classical. As such, we are concerned with the *canonical quantization* of such *constrained systems*.

A pre-eminent constrained system –one that has withstood all assaults to quantize it through at least 4 decades [1]– is general relativity [2]. Of the difficulties related to quantizing gravity, a significant part arises from the fact that, in one way or the other, current approaches to the quantization of constrained systems have not been quite general enough to apply to general relativity. Almost all current approaches [3, 4, 5] rely on the presence of specific structures, on either configuration space or phase space; and a generic constrained system may or may not possess these structures. Certainly, it is not known whether these approaches can be taken to quantize general relativity.

Before I describe the features peculiar to general relativity, let us briefly recall gauge theories, to provide points of reference. Like general relativity, gauge theories are field theories with constraints on the phase space, (As fundamental theories of matter, they are of course important in their own right.)

Gauge field theories are defined on a background spacetime, usually taken to be Minkowski spacetime. The elementary configuration variable is a Lie algebra valued connection on spatial slices of the spacetime (Cauchy surfaces), and the canonical momentum is a triad which takes values in (the dual to) the Lie algebra. The constraint surface can be specified by the vanishing of the Gauss constraint functional. Dirac has pointed out [6] –in the general context of constrained systems– that due to the ambiguity in specifying the constraint function, one is forced to consider that canonical transformations generated by the constraint connect physically equivalent classical states. As we know, the Gauss constraint generates gauge transformations –i.e. rotations in the internal symmetry group– on the canonical variables. Dynamics is specified by a Hamiltonian, which is constructed however, not just from the canonical variables, but also

from the non-dynamical spatial metric. All progress in the quantization of gauge theories has made essential use of this background spacetime metric. The metric is used, e.g., to regularize operators (via point splitting or other means), to construct an inner product on physical quantum states, and even to define perturbation theory.

General relativity is markedly different from gauge theories. It is a theory of the structure of spacetime itself: in the geometrodynamical formulation the canonical variables [7] are the 3-dimensional spatial metric and its conjugate momentum, the extrinsic curvature of the spatial hypersurface. There are four constraints on the geometrodynamical phase space: the three independent vector constraints –which generate spatial diffeomorphisms of the canonical fields– and the scalar constraint. In the spacetime one can construct from any solution, the scalar constraint generates a time-like diffeomorphism of the canonical variables. Hence, in the spatially compact cases at least, the scalar constraint is the generator of dynamical evolution. This constraint is the primary source of difficulty, in both classical and quantum theory.

The most significant difference between general relativity and gauge theories is of course the complete absence in general relativity of any background fields: be they metrics or connections. As one can imagine, this absence of background structure has prevented the construction of universally accepted and well-defined regularizations of the constraints in quantum theory. Eventually, the absence of background structure will also make itself felt when one has quantum physical states and wishes to construct an inner product on them, *unless* one has a prescription –to find the physical inner product– which does *not* depend on the presence of background fields. Of course, the lack of a non-dynamical background will also cause difficulties in the construction of a physical interpretation of quantum gravity.

Recall that general relativity is the theory of *spacetime* itself, and hence there cannot be an external time parameter. In the Hamiltonian formulation, time is sometimes considered as “hidden” in the canonical variables themselves. However, there is no *preferred* internal time. This difficulty arises from the fact that, up to the possible addition of a surface term, the Hamiltonian of general relativity *is* the scalar constraint. Thus, on the one hand, the scalar constraint generates time evolution, where, classically, time can be identified as an affine parameter along the orbits of the canonical transformation generated by the scalar constraint. On the other hand, since it is after all a constraint, the canonical transformations it generates must be viewed as gauge; and since there is considerable ambiguity in defining the constraint function, there is at least that much ambiguity in identifying a time.

One is not used to dealing with time as a dynamical entity. In ordinary quantum mechanics and in field theories, the time parameter is available to us externally, from the background spacetime. Furthermore, time plays no role in constructing the kinematical quantum theory –i.e. in solving the constraints and finding the inner product on the space of physical states. From the point of view of canonical quantum gravity, an important issue then is whether or not “time” has first to be singled out from the other variables before one can proceed with the construction of the kinematical theory.

The difficulties associated with the canonical quantization of general relativity which I have discussed up to this point have been independent of any particular choice of canonical variables. Now, I will concentrate on a particular formulation of general relativity,

which appears to be the most promising for quantum gravity.

In 1986 Ashtekar [8] introduced new variables for general relativity, and formulated it as a theory of the dynamics of a certain connection. In terms of these variables, a fair amount of progress has been made towards a quantum theory of gravity¹. From the point of view of canonical quantization, there are some difficulties endemic to this connection dynamical formulation of general relativity.

- The new canonical variables are a complex $SU(2)$ connection A and a real triad E . For connections which describe real general relativity, the complex conjugate connection is given by the “reality condition”: $\bar{A} = 2\Gamma(E) - A$, where $\Gamma(E)$ is the spin connection of the triad. Immediately, a seeming difficulty presents itself: Consider e.g., the connection representation, in which states are (holomorphic) functions of the connection; \hat{A} , the operator corresponding to the connection, acts via multiplication and the canonically conjugate momentum \hat{E} is represented by a *holomorphic derivative operator*, symbolically $(\partial/\partial A)$. Now, the reality conditions on the classical variables imply Hermiticity conditions on the corresponding quantum operators. Thus, for real quantum gravity, \hat{E} should be a Hermitian operator. How though, can a *holomorphic derivative operator* be *Hermitian*? Thus, quite apart from the difficulties associated with the constraints of general relativity, within the contexts of the existing frameworks for quantization it is not immediately clear that a description in terms of such hybrid variables will lead to any consistent quantum theory.
- In the new variables, much of the progress towards a quantum theory of gravity has come about because the reformulation of general relativity as a connection-dynamical theory has allowed one to import and adapt techniques from Yang-Mills theory. Of particular interest for this discussion is the loop representation for a theory of a connection: quantum states are functionals of loops in the spatial manifold, and the action of various operators is to “break” and “join” the loops in the argument of the states. In some ways the loop representation is like the Fock representation for Maxwell theory: states are not functions on some configuration space, neither are they functions on the phase space which satisfy some polarization condition. Of course, operators on this space do correspond to functions on the phase space. However, the most natural, regularized operators on the loop states are not the canonically conjugate pair of (A, E) , but certain loop variables (see e.g [9, 10, 11]), built out of the holonomies of the connection around loops in the spatial manifold (the Wilson loops), with triads inserted in appropriate ways. These loop variables are not canonical coordinates on the phase space, though in a (reasonably) well-understood sense they do code the entire symplectic structure of the gravitational phase space. To *some* extent one is familiar with dealing with non-canonical coordinates in quantum theory. However, with the loop variables there is another difficulty: They are an *overcomplete* set of functions on the phase space –i.e., there are “too many” of them– and they satisfy certain non-trivial algebraic identities. How are these algebraic identities to be incorporated in quantum

¹For recent reviews of the new variables approach to quantum gravity, see [9, 10, 11].

theory?

- The new variables approach is a connection-dynamical reformulation of general relativity. There is the Gauss constraint of Yang-Mills theory, which generates transformations in the internal gauge group $-\mathbf{CSU}(2)$ in this case. In addition, there are the usual diffeomorphism and scalar constraints of general relativity. A salient feature of the new variables is that the scalar constraint is expressible in a very simple form. In terms of the loop variables, a well-defined, regularized operator corresponding to the scalar constraint has been constructed, and a large number of solutions to all the quantum constraints has been found [9-12]. An inner product on physical states is no longer of only conceptual interest in general relativity; due to the existence of the recent solutions, it has now become imperative to establish a criterion governing the completeness of a set of solutions to the constraint equations, and a criterion to select a physical inner product on these states.

Now, let us return to the problem of the canonical quantization of constrained systems in general. As we have seen, one of the most important potential applications of a quantization scheme will be to quantum gravity. Hence, we must take an approach which is general enough to include relativity in its framework.

A prominent approach to canonical quantization, which has proven successful in the quantization of many well known physical systems, is Dirac quantization, or the operator constraint method [6]. Here, one has to first choose a representation of quantum operators on some complex vector space, then solve the quantum constraints by finding states which are annihilated by the constraint operators and restrict attention to these *physical states*. Physically interesting observables correspond to operators that leave the space of physical states invariant. However, before one can calculate physical probabilities, expectation values or transition amplitudes one has to find an inner product and thus impose a Hilbert space structure on the physical quantum states. In this respect the original procedure outlined by Dirac is incomplete: no general principle is outlined to find the physical inner product.

Why has this problem not surfaced before, and how, within the framework of Dirac quantization, has one been able to successfully quantize a vast variety of physically interesting constrained systems? Though no general principle has been used, most theories have been quantized on a case by case basis, with very essential use being made of the symmetries of the background spacetime metric. For example, in Schrödinger particle mechanics one naturally uses the volume element of the background spatial metric to define an inner product on the states. In Minkowskian quantum field theories, the inner-product—or, equivalently, the vacuum state—is selected by making an appeal to Poincaré invariance (equivalently, Lorentz invariance on Fourier space): the vacuum is the unique Poincaré invariant state and the vacuum expectation values of all operators provide us with the inner product and the Hilbert space (e.g., through the Gelfand-Naimark-Segal construction [13]). When quantizing a field theory on a curved, stationary spacetime, on the other hand, one can use the time-like Killing vector field of the background spacetime metric to carry out a positive/negative frequency decomposition of the fields, and hence construct an inner product [14]. Even in linearized gravity, one uses the structure

of the background Minkowski spacetime to construct an inner product on the solutions to the linearized constraints.

None of the above techniques (mostly field theoretic) can be used to find an inner product for general relativity. In all the above cases, the availability of the *background* spacetime metric and the simplicity of its structure (flatness or stationarity) is essential to find the measure, and has been explicitly used to do so. In full general relativity, of course one does not have this luxury. The metric is now no longer a kinematical, background field but a *dynamical* entity. Except in reduced and simplified theories, one has to consider arbitrary positive-definite 3-metrics.

Consider the usual metric representation, in which quantum states are functions of 3-metrics. In this case, for the inner product on quantum states, one is concerned with the metric structure not of spacetime but of the superspace, i.e. the space of all 3-metrics. Now, the scalar constraint consists of two parts: the kinetic part, which is quadratic in momenta; and the potential term, which depends only on the configuration variables. (In the connection-dynamical formulation, there is no potential term.) The coefficient of the kinetic term in the scalar constraint defines a *supermetric* on the space of 3-metrics. One might be tempted to use the volume element of the supermetric to construct an inner product on quantum states, integrating over the configuration space, as one does in ordinary quantum mechanics. The first difficulty is field theoretic: there are an infinite number of degrees of freedom, and such infinite dimensional integrals are not, in general, well-defined. Next, consider spatially homogeneous cosmological models, in which the components of the metric are constants on the spatial manifold; and, since the resulting configuration space is finite-dimensional, one does not have to worry about the field degrees of freedom. Even in these simplified models of general relativity, since the superspace metric is of *Lorentzian signature*, its volume element cannot yield the correct inner product on physical states. By analogy with the relativistic particle, one might then consider the following alternative: foliate superspace with submanifolds which are space-like w.r.t. the supermetric; and use the volume element of the supermetric induced on these spatial slices (which is then positive definite) to define an inner product. For the spatially homogeneous cases, this *might* work, though there is no guarantee that it will. However, as a strategy for the full theory, this will run into the field theoretic difficulties we discussed before.

In the absence of a nondynamical background spacetime metric, can one use the *symmetries* of the supermetric instead, to construct an inner product or select a unique ground state? The analog of Poincaré invariance in field theories is diffeomorphism invariance in general relativity. Hence, one might imagine using the spatial diffeomorphism group to select the inner product on physical states: by requiring the (unique) vacuum state to be spatially diffeomorphism invariant. However, we cannot select the vacuum expectation value in this manner: now the vector constraint requires that *every* physical state be spatially diffeomorphism invariant! Are there other symmetries of the supermetric that one could use? In the geometrodynamical formulation, the supermetric has no symmetries which also appropriately scale the potential [15]. Specifically, the supermetric admits no conformal Killing vector field, along the integral curves of which the potential is rescaled by the same conformal factor. While conformal rescaling is a symmetry of the supermetric, it is not a physical operator, and thus it has limited

usefulness in singling out a ground state².

Apart from the lack of a general prescription for the inner product, there is another reason that the procedure outlined by Dirac is unsuitable for general relativity: it implicitly relies on *canonical* coordinates, and there is no discussion of the role, in quantum theory, of algebraic identities between non-canonical coordinates.

Due to the difficulties, which I have discussed, associated with quantizing general relativity, and the features peculiar to the new variables, the Dirac quantization program has to be supplemented. We need a *general principle* to select an inner product on a complete set of physical states. This principle should not rely on background kinematical structure, as there is none in general relativity. The new framework must be general enough to include non-canonical choices of elementary variables and must establish the role of any algebraic identities that the classical variables may satisfy. In addition, the framework should be able to deal with representation spaces which are not directly constructed on the phase space.

In order to find or state such a principle, we need to work with a specific technique to implement Dirac quantization. Several quantization schemes exist, like geometric quantization [3], group theoretic quantization [4] or Feynmann path integrals [5] which have been successful in many cases. Path integrals for example have been tremendously useful in perturbative approaches in field theory. However, as I mentioned earlier, these techniques are too specific, they rely on the presence of structure on the phase space which may or may not be present in general relativity. For example, both geometric quantization and path integrals rely too heavily on configuration space (or at least a polarization on phase space) to construct representations. While these techniques have worked very well for Yang-Mills theory, they are too restrictive for many constrained systems, and in particular for general relativity. Our interest here is to construct a general *framework* applicable at least in principle to all or most constrained systems; and encompassing some of the above techniques. The algebraic formulation of Dirac quantization [17, see Appendix 5], provides a good starting framework which we can extend and complete.

In this dissertation I will present the algebraic approach to the quantization of constrained systems, which is broad enough to apply to general relativity.

1.2 Chronology

A general framework is now available which establishes criteria and provides guidelines for the canonical quantization of constrained systems. At least as early as the Osgood Hill conference (Boston University 1987), Ashtekar [18, pp. 407-8] presented the essential steps. Based on an algebraic approach to Dirac quantization, a criterion for the choice of the physical inner product was established, which at the same time elucidated the role in quantum theory of the reality conditions on the new canonical variables for general relativity.

²For certain Bianchi cosmologies, the scalar constraint does admit causal symmetries which can be used to construct a physical inner product [16].

The general strategy outlined by Ashtekar –and the one I will present here– is to choose an inner product on the space of physical states such that with respect to it, physical operators corresponding to any two classical observables that are complex conjugates of each other become Hermitian adjoint operators of one another in the chosen representation. Though on the face of it this strategy appears obvious, recall that this is *not* one of the strategies commonly employed, as the preceding discussion shows. Typically, an inner product is found by other means, and then one checks that various operators are Hermitian with respect to it. Here, one *uses* the reality conditions on the physical operator algebra to *find* the inner product.

In addition, based on ideas from the quantum mechanics of a particle on a manifold (see e.g. [19] and [17, Appendix 2]) Ashtekar realized that the classical algebraic identities between functions on phase space have to be satisfied by the corresponding operators in quantum theory, in order to regain the correct physical sector.

The algebraic approach has now been adopted by leading researchers in the new variables, and the essential features have been discussed briefly in recent reviews (see [10, 11]), and in somewhat greater detail in various lecture notes [9]. The criterion to select the physical inner product has been applied successfully in the many field theories (e.g., Maxwell theory, 2+1 gravity and linearized gravity) which have been quantized using the loop representation as well as the connection representation. For full quantum gravity in the new variables, the loop representation has led to a number of major advances. Of the various techniques for quantization which are currently in use, the algebraic approach is the only one which is complete and general enough to encompass the loop representation.

I personally became involved with the algebraic approach when I tried quantizing a certain model (the coupled oscillators model solved in chapter 5). Since then, I have studied various other finite dimensional test models. Based on the difficulties and questions that arose in the quantization of these models, Ashtekar and I have completed the construction of a reasonably coherent algebraic framework for the canonical quantization of constrained systems [20].

The focus of this framework is the construction of the kinematical quantum theory, i.e. a unitary representation on physical states of a complete set of physical operators. Within the quantization program itself there is no discussion of either dynamics or physical interpretation. A further extension of the algebraic framework is required to extract dynamical information and physical interpretation from the quantum theory. Illuminating discussions, first with Rovelli [21], and soon after with Ashtekar [22], clarified many of these issues for me. Some of the essential steps in a particular approach to physical interpretation are present in Rovelli's work [23]. While my ideas –on the dynamical and physical interpretations of canonical quantum theories of constrained systems– are preliminary, and possibly ill-formed, I will discuss these issues too.

1.3 Outline

In chapter 2 I will present the algebraic approach to quantum mechanics, paying close attention to the two new features, namely the role of algebraic relations in quantum

theory, and the criteria for selecting an inner product on a complete set of physical states. Initially the approach will be somewhat heuristic, but in a later section I will also discuss various technical details.

An alternative approach to the canonical quantization of constrained systems is the reduced space approach (see e.g. [17, 24]). In this approach, the constraints are first solved classically, and then the reduced system is quantized. It is not always clear that the resulting theory is equivalent to the Dirac quantum theory; in fact there are interesting examples where they differ. In order to compare the results of these two approaches, I will reformulate the reduced space approach in the algebraic framework in chapter 2.

In chapters 3-5, I will construct the kinematical quantum theories for some finite dimensional systems. While many of the models share a number of features in common with general relativity, some models are included specifically to illustrate the new features of the quantization program.

- In chapter 3, I will first consider the quantization of a (free) particle moving on a circle. This is the simplest model in which non-trivial algebraic identities arise between the elementary operators, and so provides a good illustration of the absolute necessity of correctly taking these identities into account in the quantum theory. The next example, in section 3.2, is that of the 1-dimensional oscillator in a “hybrid” set of variables (one variable is real; and the canonically conjugate variable to this one is complex). This model illustrates the use of the Hermiticity conditions to find an inner product. Also, the hybrid variables are the simplest analogs of the new variables, and this example indicates that it is consistent to do quantum theory with such hybrid variables. In section 3.3 I will quantize the Bianchi II cosmology, which is a spatially homogeneous reduction of general relativity. We will see that even though the supermetric in the obvious polarization does not possess enough symmetries of the required kind, a complete set of physical operators exists, and can be used to construct an explicit physical inner product.
- The next model, introduced by Ashtekar and Horowitz [25], is somewhat more complicated, as one can see from some of the previous attempts to quantize it. The previous quantizations either displayed various unexpected features [25, 26] or were incomplete in some critical way [26]; in other quantum theories the classically unexpected behaviour was ruled out by fiat [27]. As we will see in chapter 4, algebraic quantization leads finally to a quantum theory which is complete and consistent in every way. The final quantum theory displays no strange features.
- In chapter 5, I will consider a model in which two oscillators are coupled to each other via a first class constraint. This is a model for a homogeneous, isotropic relativistic cosmology, and in addition shares qualitative features with full general relativity. From the point of view of the quantization program, this model illustrates again the role of algebraic identities on physical operators, the importance of the Hermiticity conditions, and the importance of discrete symmetries in pinning down a unique inner product. In the quantum theory of this model, there is an unavoidable violation of classical intuition.

There are many classical systems in which the dynamics is generated by a Hamiltonian which is constrained to vanish; general relativity in the spatially compact case, and in particular the homogeneous cosmologies, are prime examples. The non-relativistic parametrized particle is another such model, and in chapter 6 I will use it to illustrate the need for a framework to extract a physical interpretation from the quantum theory. I will present two such frameworks: one quantum mechanical, following Ashtekar [22], Kuchař [28] and Rovelli [21, 23]; and another “classical” framework, after Rovelli [21]. I will then apply this framework to the issue of the initial singularity in quantum cosmology.

In chapter 7, I will discuss –in the form of a dialogue– the lessons we have learned about the quantization program from the various models to which it has been applied, and some of the implications for quantum gravity.

In the main portion of the dissertation I deal only with first class constraints, since as is widely known, second class constraints have to be solved classically, before the quantum theory is constructed. In Appendix A, however, I will present a way to “quantize and solve” second class constraints, using a certain “holomorphic δ -function”. The applications of this are not immediately obvious, but some possibilities do exist.

I will assume that the reader is familiar with the following topics: *i*) symplectic formulation of classical constrained systems [3, 9, 29] *ii*) construction of the abstract Poisson algebra of functions on phase space and the algebraic approach to quantum mechanics [19, 17, (see appendices 2,4)], and *iii*) elementary representation theory of (Lie) algebras. While some knowledge of these topics is helpful to understand details of the program, I hope that the various models will enable even readers unfamiliar with the above topics to grasp the ideas and concepts behind the approach. Sections and subsections marked with a ‘(†)’ may be skipped on a first reading, without much loss of continuity.

Bibliography

- [1] Isham C J, Penrose R and Sciama D W (eds) 1981 *Quantum Gravity 2: A Second Oxford Symposium* (Clarendon Press Oxford); see in particular the overview by Isham C J
- [2] Wald R M 1984 *General Relativity* (University of Chicago Press, Chicago)
- [3] Woodhouse N J M 1981 *Geometric Quantization* (Oxford University Press, Oxford)
Sniatycki J 1980 *Geometric Quantization and Quantum mechanics* (Springer-Verlag, New York)
Ashtekar A and Stillerman M 1986 *J. Math. Phys.* **27** 1319
- [4] Isham C J 1984 in *Relativity, Groups and Topology II, Les Houches 1983*, DeWitt B S and Stora R (eds) (North-Holland Amsterdam)
- [5] Feynmann R P and Hibbs A R 1965 *Path Integrals and Quantum Mechanics* (McGraw Hill, New York)
- [6] Dirac P A M 1964 *Lectures on Quantum mechanics, Belfer Graduate School Monograph Series No. 2* (Yeshiva University New York)
- [7] Arnowitt R, Deser S and Misner C W 1962 *Gravitation: An Introduction to Current Research* Witten L (ed) (Wiley New York) and references therein
- [8] Ashtekar A 1986 *Phys. Rev. Lett.* **57** 2244
_____ 1987 *Phys. Rev.* **D36** 1587
- [9] Ashtekar A 1991 *Lectures on Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore)
- [10] Rovelli C 1991 *Class. Quantum Grav.* **8** 1613-75
- [11] Smolin L 1992 in *Proc. XXII Gift Intl. Seminar on Theo. Phys., Quantum Gravity and Cosmology, June 1991 Catalonia Spain* (World Scientific, Singapore)
- [12] Brüggman B, Gambini R and Pullin J 1992 *Phys. Rev. Lett.* **68** 431-4
- [13] Gelfand I M and Naimark M A 1943 *Mat. Sobornik* **12** 197
Segal I E 1947 *Bull. Amer. Math. Soc.* **53** 73

- [14] Ashtekar A and Magnon A 1975 *Proc. R. Soc. (Lond.)* **A346** 375
_____1982 *Comm. Math. Phys.* **86** 55-68
- [15] Kuchař K 1981 *J. Math. Phys.* **22** 2640-54
_____1982 *J. Math. Phys.* **25** 1647-61
- [16] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print No. SU-GP-92/2-5
- [17] Ashtekar A and Geroch R 1974 *Rep. Prog. Phys.* **37** 1211-56
- [18] Ashtekar A 1989 in *Conceptual Problems in Quantum Gravity* Ashtekar A and Stachel J (eds) (Birkhäuser Boston)
- [19] Ashtekar A 1980 *Comm. Math. Phys.* **71** 59
- [20] Ashtekar A and Tate R S 1992 Syracuse University pre-print, in preparation
- [21] Rovelli C 1992 *private communication* Pittsburgh January 1992
- [22] Ashtekar A 1992 *private communication* Syracuse February 1992
- [23] Rovelli C 1991 *Phys. Rev.* **D43** 442-56
- [24] Romano J D and Tate R S 1989 *Class. Quantum Grav.* **6** 1487-500
- [25] Ashtekar A and Horowitz G H 1982 *Phys. Rev.* **D26** 3342-53
- [26] Boulware D G 1983 *Phys. Rev.* **D28** 414-16
- [27] Gotay M J 1986 *Class. Quantum Grav.* **3** 487-91
- [28] Kuchař K 1992 *private communication* Cincinatti March 1992
- [29] Tate R S 1992 *Constrained systems and Quantization, Lectures at the Advanced Institute for Gravitation Theory, Session: December 91 Cochin* Syracuse University pre-print No SU-GP-92/1-4

Chapter 2

ALGEBRAIC QUANTIZATION OF CONSTRAINED SYSTEMS

2.1 Introduction

In this chapter I will present an algebraic approach to the quantization of constrained systems which is based on the representation of an algebra of functions on the phase space. In the section 2 I will present the details of the program, following [1, 2, 3, (see chapter 10)]. I will concentrate on the definitions that are used in the context of algebraic quantization [4, 5], and heuristically establish the criteria to be satisfied by the choices one has to make at various stages. In section 3, I will summarize the quantization program, condensing it into an itemized step-by-step outline. I will then make some technical remarks about various steps (section 4), and postpone a general discussion about the program until the concluding chapter, *after* the illustrative examples and physical models have been solved.

Primarily, the approach is an extension and generalization of the *Dirac quantization program* (or the operator constraint method), in the sense that the operator equations corresponding to the constraints are solved in quantum theory [6]. An alternate approach to the quantization of constrained systems is to first solve the constraints classically, and then quantize the resulting theory free of constraints. In general, the two approaches are inequivalent (see e.g. [7, 8, 9]), and then it is of interest to compare the resulting quantum theories. Hence, in section 5 I will reformulate *reduced space quantization* [4, 8] in the algebraic framework, and discuss possible sources of difference from the operator constraint approach.

2.2 Algebraic quantization

Consider a classical system described by a *phase space* Γ , a real (finite-dimensional) symplectic manifold. In many physical systems, not all points of Γ are accessible to the system, only those points which lie on a *constraint surface* $\bar{\Gamma}$ —described by the vanishing of some (constraint) functions on Γ —are allowed classical states for the system. Recall that in the terminology of Dirac ([6], see also [10]), the set of constraints is *first class* if

and only if their mutual Poisson brackets vanish on the constraint surface. Classically, this ensures that the “gauge” orbits, of the canonical transformations generated by the constraints, lie in the constraint surface. As Dirac concluded after a careful analysis [6], points on $\bar{\Gamma}$ that lie on the same gauge orbit describe equivalent physical configurations of the classical system. i.e. as “gauge” equivalent. Thus the “true” degrees of freedom of the classical system can be represented by the space of orbits of the canonical transformations generated by the constraints. This space, which has a natural symplectic structure induced on it, is the *reduced phase space*, $\hat{\Gamma}$.

We are interested in a general approach to the quantization of such first class constrained systems¹. The steps in the canonical quantization of a (first-class) constrained system are as follows:

1: Set of elementary functions on phase space

In order to eventually construct the quantum theory, we want to start with an optimum description of the classical system. Let us therefore consider the vector space \mathcal{S} generated by a suitable subset of the space of (complex valued) functions on the phase space Γ . This space has to satisfy three conditions:

1. In order to capture all the classical physics, this set of elementary functions 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} . This is ensured by requiring that at each point of the phase space Γ , \mathcal{S} should contain a subset of functions which are coordinate functions in an open neighbourhood of the point. Technically, \mathcal{S} is (locally) complete if and only if the gradients of the functions F in \mathcal{S} span the cotangent space of Γ at each point; that is, we require that

$$\text{Rank} \left(d_\mu F^{(i)} \right) = 2n \quad (2.1)$$

where $d_\mu F^{(i)}$ are the components in some chart of the elementary variables generating \mathcal{S} and the phase space is $2n$ dimensional.

2. In order to construct the (Poisson bracket) algebra of functions on phase space, we require that \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 one of the functions in \mathcal{S} .
3. 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 \mathcal{S} represents an elementary classical variable which is to have an unambiguous quantum analog.

In general, \mathcal{S} may be *overcomplete*, i.e., the number of generators of \mathcal{S} (not including the constant function, the gradient of which vanishes) may be larger than $2n$, the

¹Dirac has pointed out [6] that second class constraints, i.e. those constraints not of first class, cannot be solved in quantum theory (see, however, Appendix A) and have to be eliminated classically. Therefore, I will henceforth assume that such a reduction has been carried out and we are left with a first class constrained system.

dimension of phase space. In this case, the set of generators of \mathcal{S} will satisfy some *algebraic identities*. Are there any situations where one is forced to consider such genuinely overcomplete sets? Clearly, if the phase space is \mathbb{R}^{2n} , then the global Cartesian coordinates (and the constant function) are a suitable choice for \mathcal{S} . However, it is when the phase space is a nontrivial manifold that the point about overcompleteness becomes important. There exist *no* global coordinates, and unfortunately, one does not know how to do quantum mechanics “in coordinate patches”. One might attempt to construct a quantum theory on a specific coordinate patch; however, since for e.g. one may not know the “correct” boundary conditions, in general the quantum theory will not be well defined. Furthermore, there is no way to “patch together” the quantum theories on overlapping coordinate patches. Therefore, an *overcomplete* set of globally defined functions becomes necessary. One can then think of the identities as arising from the overlap regions between two open neighbourhoods with different sets of coordinates.

Consider for example the case when the phase space is the unit 2-sphere in Euclidean space (say centered at the origin). (This phase space arises in the classical description of internal spin [11, 12].) There are no global coordinates on S^2 : the pullbacks to S^2 of the Cartesian coordinates (x, y) fail to be coordinates on S^2 at the equator $z = 0$; similarly, (the pullbacks of) (θ, ϕ) are bad coordinates at the poles. However, at each point of S^2 one can find a subset of (x, y, z) which does coordinatize an open neighbourhood. For example, as we just saw, in the neighbourhood of the $z = 0$ equator the set (x, y) is a bad set of coordinates. However, at all points of the $z = 0$ equator (except where $y = 0$), (x, z) is a good set of coordinates. Thus, the set (x, y, z) is complete on S^2 , as we can also verify directly using (2.1). But now, since Γ is a 2-manifold, the set of *three* functions (x, y, z) is *overcomplete*: we know that on S^2 one cannot specify arbitrary values for the functions $(1, x, y, z)$, they have to satisfy the algebraic identity $x^2 + y^2 + z^2 - 1 = 0$. The vanishing of the function $x^2 + y^2 + z^2 - 1$ specifies the embedding of S^2 into \mathbb{R}^3 .

Thus we see that in some cases at least, the algebraic identities between elements of \mathcal{S} can be derived from the vanishing of the functions which specify the embedding of the phase space Γ into some $\mathbb{R}^{>2n}$. In the general finite dimensional case, simple counting will usually indicate the number of such algebraic relations that should be identified.

2: Commutator algebra of functions on phase space

From the Poisson bracket relations on \mathcal{S} , we want to construct the abstract commutator algebra of quantum operators. Following e.g. [4, (appendices 4,5)] and [5], associate with each element F in \mathcal{S} an abstract operator \hat{F} . Construct the free associative algebra generated by these elementary quantum operators. Impose on this algebra the *canonical commutation relations* (CCRs): for all F and G in the set \mathcal{S} , impose

$$[\hat{F}, \hat{G}] := \hat{F} \cdot \hat{G} - \hat{G} \cdot \hat{F} = i\hbar \widehat{\{F, G\}}, \quad (2.2)$$

where $\widehat{\{F, G\}}$ denotes the operator corresponding to the function $\{F, G\}$. If \mathcal{S} is overcomplete, then as we just saw there are algebraic relations between its elements. Thus, also impose the *anti-commutation relations* (ACRs) which capture the algebraic identities between the elementary classical variables: e.g., if all three functions F, G and

$H := F \cdot G$ belong to \mathcal{S} , then in the algebra impose the condition

$$\hat{F} \cdot \hat{G} + \hat{G} \cdot \hat{F} = 2\hat{H}. \quad (2.3)$$

Denote the resulting algebra by \mathcal{A} .

3: \star -relations on the algebra

On \mathcal{A} , introduce an involution operation² 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 $\hat{F}^\star \equiv \hat{G}$ in \mathcal{A} . The properties of the involution operation then define \star on the rest of the algebra. Denote the resulting \star -algebra by $\mathcal{A}^{(\star)}$. The \star -relation on $\mathcal{A}^{(\star)}$ reflects just the complex conjugation relations between the functions in \mathcal{S} .

4: Linear representation of \mathcal{A}

Ignore for now the \star relation we just constructed on \mathcal{A} .

In order to construct the quantum theory, we want a representation of the abstract algebra \mathcal{A} via linear operators on some complex vector space \mathcal{V} . As in standard quantum mechanics, the canonical commutation relations (2.2) should be faithfully represented. In addition, the representation should be such that the anticommutation relations (2.3) should also be satisfied. Note that for now the \star -relations on $\mathcal{A}^{(\star)}$ are to be ignored.

5: Physical states

Up to this point, the constraints of the classical theory have been ignored. We now want to solve the constraints and isolate the *physical states* of the quantum theory. Thus we have to obtain explicit operators \hat{C} on \mathcal{V} , representing the quantum constraints. In the chosen representation, if e.g. the constraints are quadratic or higher order in momenta, one has to suitably factor order them: while the functions in the set \mathcal{S} have unambiguous quantum analogs, operators corresponding to products of the elementary ones will in general *not* have unambiguous quantum analogs. The space of physical states \mathcal{V}_{phy} is the kernel of the constraint operators, i.e. the set of states annihilated by the constraints. Thus $|\psi\rangle$ is a physical state if and only if

$$\hat{C}|\psi\rangle = 0. \quad (2.4)$$

This is the quantum constraint equation which has to be *solved* to yield the physical states.

6: Physical operator algebra

Recall that in classical theory, the allowed physical states of the system (solutions to the constraint) are points that lie in the constraint surface $\bar{\Gamma}$. As Dirac noted, physically

²An involution is a map from an algebra to itself, satisfying the following properties. If \hat{A}, \hat{B} are in the algebra and λ is a complex number: *i)* $(\hat{A} + \lambda\hat{B})^\star = \hat{A}^\star + \bar{\lambda}\hat{B}^\star$; *ii)* $(\hat{A}\hat{B})^\star = \hat{B}^\star\hat{A}^\star$; and *iii)* $(\hat{A}^\star)^\star = \hat{A}$.

interesting functions are ones which generate canonical transformations which leave invariant $\bar{\Gamma}$, the space of classical physical states. These functions are the classical Dirac observables. Similarly, in the quantum theory, we are interested only in those operators which leave invariant \mathcal{V}_{phy} , the space of quantum physical states. Not all operators in \mathcal{A} are of this type. An operator \hat{A} in \mathcal{A} will leave \mathcal{V}_{phy} invariant if and only if \hat{A} commutes weakly with the constraints, i.e.

$$[\hat{A}, \hat{C}_I] = \sum_J \hat{f}_I^J \hat{C}_J. \quad (2.5)$$

Note that \hat{f}_I^J are operator valued “structure functions”, i.e. they may not all be proportional to the identity operator. Furthermore, it is important that various factor-ordering choices be made such that on the RHS of the above equation, the constraint operators always stand to the right. This guarantees that $\hat{C}_I(\hat{A}|\psi\rangle) = 0$ for all physical states $|\psi\rangle$, i.e. that $\hat{A}|\psi\rangle$ is a physical state if $|\psi\rangle$ is one³. The collection of all such operators forms a sub-algebra of \mathcal{A} , the algebra of physical observables. We denote it by \mathcal{A}_{phy} .

From the \star -relation on $\mathcal{A}^{(\star)}$, we *induce an involution* (denoted again by \star) on the physical algebra \mathcal{A}_{phy} (see the final remark in section 4). Denote the resulting \star -algebra of physical operators by $\mathcal{A}_{phy}^{(\star)}$.

7: Physical inner product

In order to answer or even pose physically relevant questions in the quantum theory (say about various transition amplitudes, expectation values or spectra of interesting physical observables), we need an inner product on the space of physical states. The general idea is to fix this inner product by requiring that various operators are Hermitian with respect to it. However, since arbitrary operators in \mathcal{A} are not operators on the space of physical states, we cannot require that they satisfy Hermiticity conditions with respect to an inner product on \mathcal{V}_{phy} . On the other hand, operators in \mathcal{A}_{phy} are operators on physical states. Hence, we fix the physical inner product in the following manner:

Introduce on \mathcal{V}_{phy} a Hermitian inner product so that the abstract \star -relations on $\mathcal{A}_{phy}^{(\star)}$ –which have been ignored so far– are represented as Hermitian adjoint relations on the resulting Hilbert space.

In other words, if $\hat{F}^\star = \hat{G}$ in the abstract algebra $\mathcal{A}_{phy}^{(\star)}$, 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. In the Dirac bra-ket notation:

$$\langle \psi | \hat{G} | \phi \rangle = \langle \psi | \hat{F}^\dagger | \phi \rangle := \overline{\langle \phi | \hat{F} | \psi \rangle} \quad \forall \psi, \phi \in \mathcal{V}_{phy}. \quad (2.6)$$

This is a key step in the algebraic quantization of constrained systems, which distinguishes it from previous approaches. It establishes a clear criterion for the selection of

³Since we are interested only in physical states, I will henceforth drop the qualifier “weakly” when applied to the vanishing of the commutator of physical operators with the constraints.

an inner product on physical states (based on the algebra of physical observables), and thus completes the Dirac program. Note that unlike in group theoretic quantization [13], no group theoretic or symmetry considerations are explicitly involved here. Neither do we invoke specific techniques to find the inner product, such as Kähler structures in geometric quantization [14].

2.3 Summary of the program

Now that we have considered the program in detail, and have also provided the required definitions and established various criteria to guide our choices at the various stages, I will summarize the steps in the algebraic approach to the quantization of constrained systems. This summary can serve as a ready reference for the reader through the following chapters.

1. Choose a complete set of (complex valued) functions on Γ such that the vector space they generate is closed under both Poisson brackets and complex conjugation. Identify all algebraic relations that may exist between its elements.
2. Construct the associative algebra \mathcal{A} generated by the elementary variables in \mathcal{S} , with the canonical commutation relations and the anticommutation relations imposed.
3. On this algebra, identify the \star -involution, corresponding to the classical complex conjugate relations on \mathcal{S} .
4. Find a linear representation of \mathcal{A} on a vector space \mathcal{V} . (Ignore the \star -relations in this and the next step.)
5. Solve the constraint equations and obtain the space of physical states, \mathcal{V}_{phy} .
6. Construct the \star -algebra $\mathcal{A}_{phy}^{(\star)}$ of physical observables.
7. Introduce on \mathcal{V}_{phy} a Hermitian inner product so that the abstract \star -relations on $\mathcal{A}_{phy}^{(\star)}$ are represented as Hermitian adjoint relations on the resulting Hilbert space.

2.4 Remarks

Remark 1: Inputs to the program

At the outset I should point out that the above “program” is *not* a constructive technique to quantize constrained systems. As a leading researcher in the field has so eloquently stated [15], “*This program is not a meat-grinder, into one end of which we can stick a classical system, turn the crank, and then expect to get a quantum sausage out the other end.*” When following this program, there are various stages at which *choices* have to be made. The first crucial choice is that of the set of elementary functions \mathcal{S} . A poor choice of \mathcal{S} may make it difficult to either represent the constraints, or solve them, or

find observables. While there is no prescription to make a good choice, (which after all depends largely on the intuition one has for the problem) minimum requirements that \mathcal{S} should satisfy have been established: These requirements are essential in order that the quantum theory capture all the physics.

The second crucial choice is that of the representation of \mathcal{A} on a complex vector space \mathcal{V} . A poor choice of representation may again make it difficult to solve the constraints. If the representation is not “general enough” in some loose sense, it may be impossible to find a physical inner product. Again, there is no prescription to avoid such bad choices. However, once a representation has been chosen and the constraints solved, the program specifies the criteria that should be used to select a physical inner product.

Remark 2: Algebraic identities and quantum theory

There may exist algebraic identities between the elementary functions which are of a more general form than the simple quadratic case we considered in step 2. There is a generalization of (2.3). Consider the case when there are N sets of up to m elementary functions, the (i) th set denoted by $(F_1^{(i)}, \dots, F_m^{(i)})$, which satisfy the identity $\sum_{(i)} F_1^{(i)} \cdot F_2^{(i)} \cdots F_m^{(i)} = 0$. On the commutator algebra constructed from \mathcal{S} , one should impose

$$\hat{\mathcal{F}} := \sum_{(i)} \hat{F}_{(1)}^{(i)} \cdot \hat{F}_2^{(i)} \cdots \hat{F}_m^{(i)} = 0, \quad (4.1)$$

where as usual $(1\dots m)$ denotes $1/m!$ times the sum of all the permutations.

Note that even though we are imposing anti-commutation relations, there is nothing fermionic about the system. Further, I should emphasize that the purpose of (2.3) is *not* to resolve any factor ordering ambiguity in the definition of the operator $\widehat{FG} \equiv \hat{H}$: since $H = FG$ is, by assumption, an elementary variable, \hat{H} is already an unambiguous and well-defined quantum operator. Rather, the role of the ACRs is to eliminate possible spurious sectors in the final quantum description. How do these spurious sectors arise? In simple cases, the left hand sides of the ACRs (e.g. the operator $\hat{\mathcal{F}}$ in (4.1)) are *super-selected* operators in the associative algebra, i.e., they commute with all the elementary operators⁴. Thus, in these cases, had we not imposed the ACRs, the representation of \mathcal{A} would be reducible, the irreducible representations would be carried by the eigenspaces of the operators $\hat{\mathcal{F}}$. We would obtain the correct classical limit *only* in the sector on which $\hat{\mathcal{F}}$ takes the value zero. By imposing (4.1), we ensure that the spurious sectors are avoided.

The algebraic identities arise due to a “failure of coordinatization” of the phase space. As we saw in the S^2 example considered earlier, we cannot classically solve the algebraic identity for and eliminate one of the elementary functions *globally* on the phase space. The identity then has to be appropriately incorporated in quantum theory.

Given a classical identity $F \cdot G = H$, is there any ambiguity in the quantum condition that we wish to impose? As we will see, rather than *solving* a factor-ordering problem,

⁴More generally, they constitute a Lie ideal in the commutator algebra. Thus, technically, the imposition of the ACRs amounts to taking the quotient of the commutator algebra by this ideal. The result is the required algebra of quantum operators. I do not know the *most* general statement about the role of the ACRs in the algebra.

as one might have initially thought, the algebraic identities *create* one. *A priori*, in the quantum theory, one does not know what condition to impose. Suspend for a moment the ACR (2.3) and consider instead a nonsymmetric condition of the form

$$\alpha \hat{F} \cdot \hat{G} + \beta \hat{G} \cdot \hat{F} = (\alpha + \beta) \hat{H}. \quad (4.2)$$

If we define $\delta = i \frac{\alpha - \beta}{\alpha + \beta}$ and re-arrange terms, we can write this as

$$\hat{F} \cdot \hat{G} + \hat{G} \cdot \hat{F} + \delta \hbar \{\widehat{F}, \widehat{G}\} = 2\hat{H}. \quad (4.3)$$

Since in the limit $\hbar \rightarrow 0$ the extra term on the LHS vanishes, independent of the value of δ we obtain the correct classical limit. Hence, there is a genuine ambiguity in the condition we wish to impose in quantum theory. In ordinary quantum mechanics, the factor ordering ambiguity is often resolved by invoking the Hermiticity of the new operator. In the algebraic framework, we would similarly require that the quantum condition corresponding to the classical identity be compatible with the \star -relation. Assuming in the simplest case that F, G, H are real functions, this implies only that $\delta \in \mathbb{R}$.

In the quantization program we spelled out in section 2, we made the specific symmetric choice $\delta = 0$ (and hence refer to the quantum condition as an anticommutation relation). The justification for this comes from ordinary quantum mechanics on a manifold (see [5] or [2, appendix C]), where the representation *identically* satisfies the quantum condition in the specific, symmetrized form (2.3). One could work with a family of algebras, parametrized by as many δ s as there are algebraic identities. However, it is much simpler to work with a specific choice, meanwhile retaining the existence of ambiguity in the back of one's mind, in case e.g. there are subtle topological issues involved, and one wants to relax the condition $\delta = 0$. Henceforth, in this thesis, I will always work with the symmetric choice.

Remark 3: Inner product

Note that for constrained systems the above quantization program neither requires nor introduces an inner product on the large representation space \mathcal{V} . (In step 4, the \star -relations are ignored.) From a physical point of view, we need to introduce a Hermitian inner-product *only* on the physical subspace. Indeed, as simple examples show, physical states in \mathcal{V}_{phy} are often *not* normalizable in the fiducial inner product one may be tempted to introduce on \mathcal{V} . For example, if one considers a constraint linear in momenta, defined by a vector field on configuration space, physical states are constant along the vector field. If the vector field is, say, a translational vector field in \mathbb{R}^3 , then physical states do not fall-off in those directions (unless the states are identically zero) and then, with respect to the usual Euclidean measure, they are not normalizable. On the other hand, consider a constraint which is a function only of the configuration variables. This defines a surface in the configuration space. In the configuration representation, physical states have support only on the sub-manifold defined by the constraint in configuration space. Thus, they are either of zero norm with respect to the usual Euclidean measure, or, they are all “normalizable” to Dirac δ -distributions, in which case the quantum theory is not well-defined unless one introduces a *new* inner product.

Hence, for constrained systems, it seems inappropriate to attempt to introduce a preferred inner product on all of \mathcal{V} (except perhaps as a technical device, e.g., for regularization of the constraint operators in field theories).

Remark 4: Quantum observables

Quantum mechanically, the true degrees of freedom of the constrained system are coded in \mathcal{A}_{phy} , the algebra of observables. Recall that in classical theory there is gauge freedom on the constraint surface: not all points on $\bar{\Gamma}$ are physically distinguishable. A somewhat similar situation occurs in the quantum theory too. To see this, let us explore the space of physical operators. An operator \hat{A} in \mathcal{A} will leave \mathcal{V}_{phy} invariant if and only if it commutes with the constraints (see (2.5)). Let \hat{A} and \hat{B} be physical operators: $[\hat{A}, \hat{C}] = \hat{f}_A \hat{C}$ and $[\hat{B}, \hat{C}] = \hat{f}_B \hat{C}$. Then

$$\begin{aligned} [\hat{A}\hat{B}, \hat{C}] &= \hat{A}\hat{f}_B\hat{C} + \hat{f}_A\hat{C}\hat{B} \\ &= \hat{A}\hat{f}_B\hat{C} + \hat{f}_A(\hat{B}\hat{C} - \hat{f}_B\hat{C}) \\ &= (\hat{A}\hat{f}_B + \hat{f}_A\hat{B} - \hat{f}_A\hat{f}_B)\hat{C}. \end{aligned} \tag{4.4}$$

Thus, $\hat{A}\hat{B}$ also commutes weakly with the constraint: the physical operators constitute an associative sub-algebra of \mathcal{A} , with the induced commutator bracket. Denote this sub-algebra by \mathcal{A}_{phy}' .

Since the constraints are by assumption first class, the constraint operators belong to \mathcal{A}_{phy}' too. This represents the gauge freedom quantum mechanically. However, 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 constraints⁵. One then takes the quotient of \mathcal{A}_{phy}' by this ideal: $\mathcal{A}_{phy} := \mathcal{A}_{phy}'/\mathcal{I}_C$. For physical operators quadratic or higher order in momenta, one first makes a factor-ordering choice and then quotients by \mathcal{I}_C .

One may be tempted to shorten the procedure and quotient by the ideal generated by the constraints in the “large” algebra \mathcal{A} itself. However, it is easy to see that this ideal is too large. In simple cases, it is the whole algebra. Consider the constraint $\hat{p} = 0$. Since \hat{q} is in \mathcal{A} and $[\hat{q}, \hat{p}] = \hat{1}$, $\hat{1}$ must belong to the ideal \mathcal{I}_p . But now, since $[\hat{A}, \hat{1}] = \hat{A}$ for all $\hat{A} \in \mathcal{A}$, $\mathcal{I}_p = \mathcal{A}$. Thus the quotient is just the identity operator, and all physical information has been lost.

How do we know that the set of physical operators captures *all* the physical degrees of freedom? To answer this question, one has no recourse but to resort to the classical theory. Consider the classical functions (classical Dirac observables) corresponding to the generators of \mathcal{A}_{phy} . These are functions on the constraint surface $\bar{\Gamma}$ which are Lie-derived along the orbits generated by the constraints, and are thus isomorphic to functions on the reduced phase space $\hat{\Gamma}$. Since $\hat{\Gamma}$ represents the true classical degrees of freedom, we can require that the set of functions corresponding to \mathcal{A}_{phy} should be complete on $\hat{\Gamma}$. As

⁵In general an ideal in an associative algebra generated by a set $\{\hat{C}\}$ consists of elements of the form $\hat{A}\hat{C}\hat{B}$ for all \hat{A}, \hat{B} in the algebra. However, due to (2.5), in \mathcal{A}_{phy}' the ideal can equivalently be considered to consist of elements of the form $\hat{A}\hat{C}$ for all $\hat{A} \in \mathcal{A}_{phy}'$.

in the definition of completeness of \mathcal{S} (see (2.1)), this means that the gradients of the functions on $\hat{\Gamma}$ (corresponding to the generators of the physical operator algebra) should span the cotangent space of the *reduced* phase space, at every point on $\hat{\Gamma}$.

However, in the Dirac theory, one is not necessarily interested in constructing the reduced phase space; indeed, it may be quite difficult to do so. In the absence of $\bar{\Gamma}$, we would like to formulate the condition for completeness on the constraint surface itself. First consider the simplest case when the constraint surface is of codimension 1, i.e. there is only one first class constraint. On $\bar{\Gamma}$, the gradients of the Dirac observables are orthogonal to the Hamiltonian vector field of the constraint function. Hence, the pull-backs of the gradients of the observables to $\bar{\Gamma}$ span a $2n - 2$ dimensional subspace of the cotangent space to $\bar{\Gamma}$. In practice, it may not be possible to coordinatize the constraint surface, and thus one may not be able to evaluate the pull-backs in a straightforward fashion. Thus, a more practical strategy is to explicitly include the constraint function in the set (thus the set corresponds to the set of generators of \mathcal{A}_{phy}' , as opposed to \mathcal{A}_{phy}), and then require that at each point of $\bar{\Gamma}$ the gradients of this set span a $2n - 1$ dimensional space, which is automatically orthogonal to the gauge vector fields. Since the pull-back of the gradient of the constraint (which is normal to the constraint surface) vanishes, this condition is clearly equivalent to the previous one. In the general case, when the constraint surface is of codimension m , we require that

$$\text{Rank} \left(d_\mu O^{(i)} \right) \Big|_{\bar{\Gamma}} = 2n - m, \quad (4.5)$$

where ($\mu = 1 \dots 2n$) $d_\mu O^{(i)}$ are the $2n$ components of the gradients of the functions corresponding to the generators of \mathcal{A}_{phy}' , labelled by (i) .

This condition is perhaps easier to visualize in terms of the Hamiltonian vector fields of the observables: we require them to span the tangent space to $\bar{\Gamma}$. However, since there is no natural subspace of the tangent space *orthogonal* to the gauge vector fields, one has to explicitly include the gauge vector fields. Since the symplectic structure is nondegenerate, it is easy to see that the condition (4.5) is equivalent to

$$\text{Rank} \left(X_{O^{(i)}}^\mu \right) \Big|_{\bar{\Gamma}} = 2n - m, \quad (4.6)$$

where $X_{O^{(i)}}^\mu$ is the Hamiltonian vector field of the function corresponding to the (i) th generator of \mathcal{A}_{phy}' .

As in the case of Γ itself, if the generators of \mathcal{A}_{phy} are overcomplete, or if one is unable to properly factor out the constraints classically, then there are algebraic relations between the physical observables.

Remark 5: Physical states

Since there is no inner product on the representation space \mathcal{V} , how does one know in step 5 that one has a “sufficiently large” set of solutions to the constraints? We now have the machinery to formulate a criterion: *the space of physical states \mathcal{V}_{phy} should be large enough to carry a faithful representation of \mathcal{A}_{phy}* . This is already an indication that the program cannot always be implemented as sequentially as it has been presented, since for some systems one may have to find the full physical algebra and then go back and check that \mathcal{V}_{phy} is large enough.

Remark 6: \star -involution on \mathcal{A}_{phy}

In step 7, we find the physical inner product using the \star -relations on $\mathcal{A}_{phy}^{(\star)}$, and it is necessary and sufficient to implement the Hermiticity conditions on only a set of generators of \mathcal{A}_{phy} .

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. 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. Are there physical systems for which the above condition is guaranteed to be satisfied? The answer is in the affirmative. Consider, in particular, the case when the constraint operators satisfy: $\hat{C}_I^\star = \hat{C}_I, \forall I$. 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. 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} .

2.5 (†) Reduced space quantization

As I mentioned in the introduction, there is an alternative approach to the quantization of (first class) constrained systems. In *reduced space quantization* one first solves the constraints classically and restricts attention to the allowed states, which lie in the constraint surface $\bar{\Gamma}$. Recall that since the constraint surface is first class, not all points in it are physically distinguishable: points related to each other by a canonical transformation generated by the constraints are *gauge equivalent*. Thus one has to find the orbits of the canonical transformations, by integrating the gauge flats spanned by the Hamiltonian vector fields of the constraints. The space of gauge orbits $\hat{\Gamma}$ represents classically the true degrees of freedom of the system.

Now one can construct a quantum theory on $\hat{\Gamma}$. Namely, as in step 1, introduce a subspace $\mathcal{A}_{red}^{(\star)}$ of the space of complex-valued functions on $\hat{\Gamma}$: $\mathcal{A}_{red}^{(\star)}$ is overcomplete on $\hat{\Gamma}$, and closed under Poisson brackets and complex conjugation. The variables in $\mathcal{A}_{red}^{(\star)}$ will have unambiguous quantum analogs. As in steps 2 and 3 above, one now constructs the abstract \star -algebra $\mathcal{A}_{red}^{(\star)}$. Since there are no longer any constraints to worry about, the final step here is to find a linear representation of the above algebra, and to select an inner product such that the \star -relations on $\mathcal{A}_{red}^{(\star)}$ are represented by Hermitian adjoint relations in the representation.

One is naturally led to ask for the relationship between the two quantum theories. In general this is a difficult problem, complicated by the fact that the answer is not unique and depends on precisely how the question is framed. However, the algebraic approach to quantization is a natural arena in which to consider this issue, and it does provide

some answers. Since the generators of the physical operator algebra \mathcal{A}_{phy} correspond to a complete set of functions on $\hat{\Gamma}$ (e.g. the generators of $\mathcal{A}_{red}^{(*)}$) one is naturally led to expect that there is some correspondence between \mathcal{A}_{phy} and \mathcal{A}_{red} . If there is a complete correspondence between the *generators* of \mathcal{A}_{phy} and \mathcal{A}_{red} , then one expects at least the “local” kinematical structure of the two quantum theories to be identical.

There are, however, a number of potential ambiguities. First, while there is a correspondence at the classical level, there is no guarantee that such a correspondence exists at the level of the abstract operator algebras. Remember that the operators in \mathcal{A}_{phy} are obtained by first factor-ordering in \mathcal{A}_{phy}' and then quotienting by the constraints. Thus there is a *factor-ordering ambiguity*. Second, while the overcompleteness of \mathcal{A}_{phy} is *necessary*, it is *not sufficient* to pick out a unique inner product in all cases, precisely because it is a local condition on $\bar{\Gamma}$ and not sensitive to any *large* canonical transformations on the constraint surface. For most simple systems the generators of \mathcal{A}_{phy} and \mathcal{A}_{red} may still be in 1 – 1 correspondence with each other in spite of the above observation. However, there do exist counter-examples. Some of the systems we will examine admit *discrete physical operators* (corresponding to large canonical transformations on $\bar{\Gamma}$) which have *no action* on $\hat{\Gamma}$ whatsoever. Such “superselected” discrete operators belong to \mathcal{A}_{phy} and not to \mathcal{A}_{red} . Therefore, even kinematically, there is no guarantee that the two quantization procedures yield equivalent results.

Are there *any* situations in which the two quantum theories are *equivalent*? Consider the case when Γ has the structure of a cotangent bundle. Then, if *all* the generators of the observable algebra are linear or independent of momenta, there is no factor ordering ambiguity and the theories are kinematically equivalent: there is a unitary transformation between the two Hilbert spaces which preserves the action of the *generators* of the two observable algebras \mathcal{A}_{red} and \mathcal{A}_{phy} . However, interesting dynamical variables, such as the Hamiltonian, may be quadratic or higher order in momenta. For these, in general there will be a factor-ordering ambiguity, and depending on how it is resolved the two methods may lead to *dynamically inequivalent* theories. In fact, in a number of examples, the prescriptions for factor-ordering which are natural to each approach do lead to such an inequivalence [8].

Bibliography

- [1] Ashtekar A 1989 in *Conceptual Problems in Quantum Gravity* Ashtekar A and Stachel J (eds) (Birkhäuser Boston)
- [2] Ashtekar A 1991 Lectures on *Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore)
- [3] Ashtekar A and Tate R S 1992 Syracuse University pre-print (in preparation)
- [4] Ashtekar A and Geroch R 1974 *Rep. Prog. Phys.* **37** 1211-56
- [5] Ashtekar A 1980 *Comm. Math. Phys.* **71** 59
- [6] Dirac P A M *Lectures on Quantum mechanics, Belfer Graduate School Monograph Series No. 2* (Yeshiva University New York)
- [7] Ashtekar A and Horowitz G H 1982 *Phys. Rev.* **D26** 3342-53
- [8] Romano J D and Tate R S 1989 *Class. Quantum Grav.* **6** 1487-500
- [9] Loll R 1990 *Phys. Rev.* **D41** 3785
- [10] Tate R S 1992 *Constrained systems and Quantization* Lectures at the Advanced Institute for Gravitation Theory, Session: December 91, Cochin
- [11] Stillerman M 1985 *Ph.D. thesis* Syracuse University
- [12] Ashtekar A and Stillerman M 1986 *J. Math. Phys.* **27** 1319
- [13] Isham C J 1984 in *Relativity, Groups and Topology II, Les Houches 1983*, DeWitt B S and Stora R (eds) (North-Holland Amsterdam)
- [14] Woodhouse N J M 1981 *Geometric Quantization* (Oxford University Press Oxford); Sniatycki J 1980 *Geometric Quantization and Quantum mechanics* (Springer-Verlag New York)
- [15] Traveska H A 1991 *private communication* Krapulho

Chapter 3

SIMPLE EXAMPLES

3.1 Introduction

The algebraic approach to quantization that I presented in the previous chapter has several new features. In this chapter I will quantize some simple models, each of which allows us to focus on and understand one of these new features, in a familiar setting.

In step 1 of the quantization program, one has to select a complete set of functions on the phase space. As I explained in the previous chapter, one is forced to consider *overcomplete* sets –i.e., sets in which there are more functions than the number of dimensions of the phase space– if the phase space is a non-trivial manifold, which does not admit global coordinates. This overcompleteness leads to certain algebraic identities between the elementary functions, which cannot be solved globally on the phase space. The algebraic relations are incorporated in quantum theory, via (2.2.3). In section 1 I will consider the simplest non-trivial manifold, S^1 , as the configuration space for a particle, and explicitly find the algebraic relation. We will see that the algebraic relation has to be appropriately incorporated in the quantum theory, in order to eliminate unphysical sectors.

Another new feature is the use of the Hermiticity conditions on observables to *select* an inner product on physical states. As I discussed in chapter 1, this extension of Dirac quantization was motivated by the hybrid nature of the new variables for general relativity (see e.g. [1]), where one variable is real and the other is complex. The canonically conjugate variables are a real triad, E , and a complex connection, A , which satisfies the reality condition

$$\bar{A} = 2\Gamma(E) - A. \tag{1.1}$$

Therefore, an immediate question that had arisen was whether the connection representation is consistent: can the momentum conjugate to a complex variable be itself Hermitian? (The gravitational phase space is constrained, and the new canonical variables are not observables; however, the above question is about *mathematical* consistency, and hence still important.) In section 2 we will consider the harmonic oscillator in hybrid variables analogous to the new variables for general relativity. I will quantize the oscillator in these variables (following [1, (chapter 10)]), and we will find that implementing the Hermiticity conditions leads to a quantum theory unitarily equivalent to the usual

one. Thus there is no *a priori* obstruction to using hybrid variables.

In section 3 I will apply the approach to a more physically motivated problem: the quantization of the Bianchi type II cosmology. This is a constrained system, and is exactly soluble. In the usual metric variables, a set of solutions to the quantum constraint has long been available [2, see Table III.1, pp. 91]. However, to my knowledge there has not been a full discussion of the completeness of the set of solutions, a physical inner product or the Dirac observables. I believe that at least in part this is due to a poor choice of the elementary variables. In terms of certain new geometrodynamical variables introduced by Uggla [3, 4], which are adapted to the symmetries of the problem, and using the quantization program, one can find the physical inner product and the above issues can be understood. This example illustrates the importance of a good choice of elementary variables and subsequent representation. Since this is a constrained system, one can compare the Dirac and reduced space quantum theories. As it turns out, in the representation we have chosen, the Dirac quantum theory is kinematically equivalent to the reduced space theory.

3.2 Particle on a circle

Consider a particle whose configuration space is the unit circle S^1 in the Euclidean plane. The phase space is just the cotangent bundle over S^1 , and thus the symplectic structure is given by $\Omega = dp \wedge d\theta$, where p is the momentum variable. Note that even though θ is *not* a well-defined function on S^1 , the 1-form $d\theta$ is globally defined, and so is the symplectic structure.

Since $\Gamma = T^*S^1$ is a nontrivial manifold, there is no global chart. However, one can choose the following overcomplete set of elementary functions: $\mathcal{S} = (1, q_1 := \sin \theta, q_2 := \cos \theta, p)$. The commutation relations between the corresponding operators are:

$$[\hat{q}_1, \hat{p}] = i\hat{q}_2, \quad [\hat{q}_2, \hat{p}] = -i\hat{q}_1 \quad \text{and} \quad [\hat{q}_1, \hat{q}_2] = 0. \quad (2.1)$$

Note that these are the commutation relations of the 2-dimensional Euclidean group. Classically, the functions q_1 and q_2 satisfy $q_1^2 + q_2^2 = 1$. Due to the nontriviality of the manifold, this equation cannot be solved globally for one variable. We impose the ACR:

$$(\hat{q}_1)^2 + (\hat{q}_2)^2 - \hat{1} = 0 \quad (2.2)$$

on the quantum operators. Note that the operator on the LHS, which we wish to set to zero, commutes with all the generators of the algebra, and hence with any Hamiltonian that one may construct. $(\hat{q}_1)^2 + (\hat{q}_2)^2$ is the Casimir invariant of the above algebra, and the ACR requires that we restrict ourselves to the sector on which its value is 1.

Let us choose as our representation space the space of (smooth) functions $\psi(\theta)$ on a circle of radius r . A representation of the commutation relations (2.1) is given by:

$$\begin{aligned} \hat{q}_1 \circ \psi(\theta) &= r \sin(\theta) \psi(\theta) \\ \hat{q}_2 \circ \psi(\theta) &= r \cos(\theta) \psi(\theta) \\ \hat{p} \circ \psi(\theta) &= \frac{\hbar}{i} \frac{\partial}{\partial \theta} \psi(\theta). \end{aligned} \quad (2.3)$$

Note again that while the “coordinate” θ is bad, the vector field $\partial/\partial\theta$ is well-defined. However this representation is still manifestly wrong, e.g. the spectrum of \hat{q}_1 lies between $\pm r$, while classically $|q_1| \leq 1$. In order to obtain a quantum theory with the correct classical limit, we have to satisfy the algebraic relation, and choose the $r = 1$ representation only. Thus, while the commutator algebra is correctly represented on functions on *any* S^1 , the correct quantum theory corresponds to a representation only on the functions on the *unit* S^1 . Finally, the inner product is simply $\langle \psi | \phi \rangle = \int_{S^1} d\theta \bar{\psi} \phi$.

One could have represented the commutator algebra on the space of functions on the two plane. While this representation contains the physical one, it also contains infinitely many spurious sectors, unless the algebraic condition is also imposed. The representation is reducible, and since the LHS of the algebraic relation (2.2) is a superselected operator, its eigenspaces carry the irreducible representations. Note that this representation points out the importance of imposing the algebraic condition *before* selecting an inner product. For, suppose that we assume an inner product of the form $\langle \psi | \phi \rangle = \int_{\mathbb{R}^2} \mu(r, \theta) \bar{\psi} \phi$. Then the Hermiticity conditions on \hat{p} imply that $\partial\mu/\partial\theta = 0$ i.e., $\mu = \mu(r)$. Now, however, to regain the physical sector, the support of the wavefunctions has to be restricted to $r = 1$, and the corresponding states are not normalizable, unless we choose μ to be a *distribution*, $\mu = \delta(r - 1)$.

3.2.1 (†) Fractional statistics on S^1

In group theoretic quantization [5], one constructs (a unitary representation of) a certain group with a *global* action on the phase space Γ . The global properties of Γ are built into the procedure right from the start. In algebraic quantization, on the other hand, one represents the Poisson bracket algebra of a set of functions on Γ . This algebra “knows” only the (local) symplectic geometry of Γ , and *a priori*, is not always sensitive to the global properties of Γ . Thus, even after imposing the correct ACRs, and the Hermiticity conditions on an (over)complete set of observables, there may still remain some ambiguity in the quantum theory. An example is provided by the quantum theory of the particle on S^1 , if we choose a more general representation space than the space of functions on the unit circle. In this case, as we will see, the new sectors at least have a simple physical interpretation.

In step 4 of the quantization program, the only requirement is that we find *a* representation of \mathcal{A} . Instead of choosing, as before, the carrier space of the representation to be the space of smooth complex functions on the unit circle, I will now make an alternate choice.

Consider the (non-trivial) Z_2 *bundle over* S^1 (see Fig3.1) [6, pp. 362]; call it B . The group Z_2 consists of two elements: the identity $\mathbf{1}$, and “parity” \mathbb{P} , with the group law $\mathbb{P}^2 = \mathbf{1}$. The base space is S^1 and the fibre over any base point on S^1 consists of just two points. Note that because of the “twist”, the bundle is topologically S^1 , and not $S^1 \oplus S^1$. Let $\phi \in [0, 4\pi)$ denote a point on the bundle. The action of \mathbb{P} is given by:

$$\mathbb{P} \circ \phi = \phi + 2\pi. \quad (2.4)$$

The projection mapping Π from the bundle to the base space S^1 ‘coordinatized’ by

Figure 3.1: B : Z_2 bundle over S^1

$\theta \in [0, 2\pi)$ is simply

$$\theta = \Pi \circ (\phi) := pr.val.(\phi) \quad (2.5)$$

where $pr.val.(\phi)$ denotes the principal value of ϕ . Thus the two points ϕ and $\mathbb{P} \circ \phi = \phi + 2\pi$ in the bundle are mapped to the same point in the base space.

Let us use the space of functions on B as the carrier space \mathcal{V} , and represent the operators by:

$$\begin{aligned} \hat{q}_1 \circ \Psi(\phi) &= \sin \phi \cdot \Psi(\phi) \\ \hat{q}_2 \circ \Psi(\phi) &= \cos \phi \cdot \Psi(\phi) \\ \hat{p} \circ \Psi(\phi) &= \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Psi(\phi). \end{aligned} \quad (2.6)$$

These are representations of the commutation relations (2.1). Note that since the base space is the unit circle, the ACR plays no further role. The inner product on \mathcal{V} is $\langle \Psi | \chi \rangle = \frac{1}{4\pi} \int_B d\phi \bar{\Psi} \chi$. With respect to this inner product, a convenient o.n. basis is $\{|m\rangle = e^{im\phi/2}\}$, $m \in integers$. The spectra of \hat{q}_1, \hat{q}_2 are the expected ones. However, the spectrum of \hat{p} , which is diagonal in this basis, is $\{m/2\}$, $\forall m \in integers$. We obtain not only the expected integer eigenvalues, but also *half*-integer eigenvalues in the spectrum of \hat{p} . Let us see how this arises.

First, notice that the representation defined above is *reducible*. There exists a *super-selected operator*

$$\hat{\mathbb{P}} \circ \Psi(\phi) := \Psi(\phi + 2\pi) \quad (2.7)$$

which is the quantum analog of the parity element in Z_2 . $\hat{\mathbb{P}}$ commutes with all the elementary observables, i.e., the elementary variables are *even* under parity. Each eigenspace of $\hat{\mathbb{P}}$ will carry an irreducible representation of the algebra (2.1,2.2). Since $\hat{\mathbb{P}}^2 = \hat{1}$, its eigenvalues are just ± 1 , and the respective eigenspaces are

$$\mathcal{V}_+ = \{|2m\rangle\}, \quad \forall m \in integer \quad (2.8)$$

$$\text{and } \mathcal{V}_- = \{|2m+1\rangle\}, \quad \forall m \in integer. \quad (2.9)$$

On the ‘bosonic’ sector \mathcal{V}_+ , \hat{p} has integer eigenvalues, whereas on the ‘fermionic’ sector \mathcal{V}_- , \hat{p} has half-integer eigenvalues. Each of these sectors carries a unitarily inequivalent representation of the 2-dimensional Euclidean algebra (2.1). Note that the even representation is naturally isomorphic to the one considered in the first part of this section, since the parity even functions on B satisfy $\Psi(\phi + 2\pi) = \Psi(\phi)$ and are thus projectible to functions on S^1 itself.

Since the spectra of \hat{p} in the two representations are just ‘shifted’ w.r.t. each other, one could argue that they are physically indistinguishable. In the first place, however, one can easily construct a ‘parity even’ operator. say $H = p^2/2m$, whose spectra in the two representations are not related by just a shift. Furthermore, these representations are distinguishable if, e.g, the Hamiltonian contains an interaction term corresponding to a magnetic field coupled to the ‘spin’. *A priori* one must consider both representations, and allow an experiment to pick the correct physical sector.

There is a straightforward generalization of the above effect. One can construct a representation of the algebra (2.1) on the Z_n bundle over S^1 . Since in this case $\hat{\mathbb{P}}^n = \hat{1}$, there are n irreducible representations, labelled by the n th roots of unity. In each sector, the eigenvalues of \hat{p} are integer plus $\frac{k}{n}$, $k < n$. Clearly, this is a description of ‘fractional statistics’ for the particle.

Thus, exploiting the fact that in the algebraic approach to quantization the representation need not be tied to the phase space, we have obtained new representations in the quantum theory for the above system. This occurs inspite of the facts that: *i*) it is a finite dimensional system; *ii*) there is a faithful representation of the algebraic relations; and *iii*) all Hermiticity conditions have been satisfied. These new representations are not just of mathematical interest, but they enable one to obtain physically important sectors of the theory, corresponding to particles with fractional statistics. In a canonical approach to quantum gravity based on the new variables, the most useful representation appears to be one which is not based on a polarization of phase space, but in which the states are labelled discretely by loops. “New” sectors of the theory, analogous to those in the above example, could play an important role.

3.3 Harmonic oscillator in the (q, z) variables

Consider the phase space of a harmonic oscillator of unit mass and spring constant. Γ is coordinatized by the real functions (q, p) and the symplectic structure is given by $\Omega = dp \wedge dq$. In analogy with general relativity in the connection variables, let us introduce the complex variable $z = q - ip$. Note that the phase space is still real, and that (q, z) are *not* coordinates on Γ . However, we choose as \mathcal{S} the vector space spanned by the (complex) functions $(1, q, z)$. Note that this is complete and closed under Poisson brackets. \mathcal{S} is also closed under complex conjugation, since $\bar{q} = q$ is real and $\bar{z} = 2q - z \in \mathcal{S}$. These hybrid \star -relations are analogous to the ones (1.1) for the new variables. The canonical commutation relations between the corresponding operators are

$$[\hat{q}, \hat{z}] = 1, \tag{3.1}$$

and the \star -relations are:

$$\hat{q}^\star = \hat{q}, \quad \hat{z}^\star = 2\hat{q} - \hat{z}. \quad (3.2)$$

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 *holomorphic* functions of one complex variable. Note that we have introduced complex coordinates on Γ in order to define z , and we can use holomorphic functions on Γ since the notion $\partial\psi/\partial\bar{z}$ would be well-defined. However, this might be confusing since \bar{z} is *not* one of the elementary variables in \mathcal{S} . In order to avoid this possible source of confusion, and to further emphasize the independence of the representation space from the phase space, we can consider a fiducial 1-dimensional complex space with coordinates $(\zeta, \bar{\zeta})$. Let \mathcal{V} be the space of holomorphic functions $\psi = \psi(\zeta)$ (i.e., $\partial\psi/\partial\bar{\zeta} = 0$), and represent the operators by:

$$\hat{z} \circ \psi(\zeta) = \zeta\psi(\zeta) \quad \text{and} \quad \hat{q} \circ \psi(\zeta) = \frac{d}{d\zeta}\psi(\zeta) \quad (3.3)$$

(Since \hat{z} is diagonal in this representation; one can loosely identify ζ with z .)

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

$$\langle \psi | \chi \rangle = \int \frac{d\zeta \wedge d\bar{\zeta}}{2\pi i} e^{\mu(\zeta, \bar{\zeta})} \bar{\psi} \chi, \quad (3.4)$$

where $\mu = \bar{\mu}$ is some as yet undetermined measure. We now have to impose the Hermiticity conditions (3.2) on these operators. This is the crucial step: it is quite counter-intuitive to have a real momentum conjugate to a complex variable; the whole formalism could fall apart right here. However, we have

$$\begin{aligned} \langle \psi | \hat{q}^\dagger | \phi \rangle &= \int e^\mu \left(\frac{d}{d\bar{\zeta}} \bar{\psi}(\bar{\zeta}) \right) \phi = - \int e^\mu \left(\frac{d}{d\bar{\zeta}} \mu \right) \bar{\psi} \phi \\ \text{and } \langle \psi | \hat{q} | \phi \rangle &= \int e^\mu \bar{\psi} \frac{d}{d\zeta} \phi = - \int e^\mu \left(\frac{d}{d\zeta} \mu \right) \bar{\psi} \phi, \end{aligned} \quad (3.5)$$

where we have used the holomorphicity of the wavefunctions to integrate by parts. Thus the Hermiticity condition on \hat{q} is solved by $\mu = \mu(\zeta + \bar{\zeta})$. Similarly, the Hermiticity condition on \hat{z} yields a differential equation for μ :

$$\frac{d}{d\zeta} \mu = -\frac{1}{2}(\zeta + \bar{\zeta}), \quad (3.6)$$

which is solved by:

$$\mu(\zeta, \bar{\zeta}) = -\frac{(\zeta + \bar{\zeta})^2}{4}. \quad (3.7)$$

The Hermiticity conditions do determine the measure uniquely. Note that even though the measure does not “fall-off” as expected, there exist normalizable states, which are of the form $\psi(\zeta) = e^{\frac{\zeta^2}{4}} f(\zeta)$, where $f(\zeta)$ are polynomials in ζ . Now, if we note that the z we have defined is $\sqrt{2}$ times the usual Bargmann variable, and identify $f(\zeta)$ with

the Bargmann states, the unitary equivalence of the two quantum theories is easily established¹.

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

3.4 Bianchi II model

For a certain class of spatially homogeneous (SH) models (see [7, 2, 8]) one can choose a “diagonal” gauge in which the spacetime metric is given by

$$ds^2 = -(N(t))^2 dt^2 + \sum_{i=1}^3 q_{ii}(t) (\omega^i)^2, \quad (4.1)$$

where $N(t)$ is the lapse function; q_{ii} , $i = 1, 2, 3$ are the diagonal components of the spatial metric and the ω^i are basis 1-forms. The components of the metric depend only on the time coordinate t . The homogeneous basis forms ω^i are Lie-derived by the generators of the spatial homogeneity group, and satisfy $d\omega^i = -\frac{1}{2}C_{jk}^i \omega^j \wedge \omega^k$, where C_{jk}^i are the structure constants of the spatial homogeneity group.

For the above class of diagonal SH models, the scalar constraint can be obtained directly by applying the ADM procedure [9], assuming that the spatial manifold is compact. The diffeomorphism constraint is automatically solved, in the gauge in which the metric is diagonal. Thus there is a single first class constraint.

For Bianchi type II models, one can choose a basis in the Lie algebra such that the only non-vanishing structure constants are $C_{12}^3 = -C_{21}^3 = 1$. One can make certain initial choices of variables to simplify the expression of the scalar constraint. Starting with the Misner parametrization of the metric components [7], one can make a point transformation, and thus parametrize the metric in the following manner [10]. Let $q_{ii} = \exp(2\beta^i)$, $i = 1, 2, 3$. Define new variables $\bar{\beta}^A$, $A = 0, +, -$ by

$$\begin{pmatrix} \bar{\beta}^0 \\ \bar{\beta}^+ \\ \bar{\beta}^- \end{pmatrix} = \frac{1}{2\sqrt{3}} \begin{pmatrix} 1 & 1 & 2 \\ 0 & 0 & -2 \\ 1 & -1 & 0 \end{pmatrix} \begin{pmatrix} \beta^1 \\ \beta^2 \\ \beta^3 \end{pmatrix}. \quad (4.2)$$

For reference, the inverse of this transformation is given by

$$\begin{pmatrix} \beta^1 \\ \beta^2 \\ \beta^3 \end{pmatrix} = \sqrt{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} \bar{\beta}^0 \\ \bar{\beta}^+ \\ \bar{\beta}^- \end{pmatrix}. \quad (4.2^{-1})$$

To further simplify matters, one usually chooses the “Taub time gauge”, i.e., one chooses the lapse function $N_T = 12 \exp(2\sqrt{3}\bar{\beta}^0 + \sqrt{3}\bar{\beta}^+)$ [11]. (This time gauge is also

¹Alternately, one could have represented \hat{q} by $\hat{q} \circ \psi(\zeta) = (\frac{d}{d\zeta} + \frac{\zeta}{2})\psi(\zeta)$. Then, the commutation relations are still satisfied, but the inner product is the usual Bargmann inner product $e^{-\frac{\zeta\bar{\zeta}}{2}}$. The unitary equivalence is then manifest.

known as Misner's supertime gauge [7].) With this choice the scalar constraint for Bianchi II takes the form:

$$C = \frac{1}{2}(-\bar{\pi}_0^2 + \bar{\pi}_+^2 + \bar{\pi}_-^2) + 6e^{-4\sqrt{3}\bar{\beta}^+} \quad (4.3)$$

where the $\bar{\pi}_A$ are the momenta canonically conjugate to $\bar{\beta}^A$; the Poisson brackets are given by $\{\bar{\beta}^A, \bar{\pi}_B\} = \delta_B^A$. In these variables, the model is kinematically equivalent to a relativistic particle moving in 3-dimensional Minkowski space under the influence of a potential. (Of course, interesting physical and dynamical observables will be completely different.) Clearly, the constraint is separable. One could now choose $(1, \bar{\beta}^A, \bar{\pi}_A)$ as the set of elementary variables and proceed with the quantization of the model. While it is by no means trivial, the quantum constraint (in the $\bar{\beta}^A$ representation) *can* be solved by elementary methods [2]. However, there is no obvious inner product on the space of solutions (but see [12]), and one has to resort to the algebraic approach to find one. It is here that a poor choice of elementary variables makes further progress difficult. First, a complete set of observables is not easy to find. Second, the complicated form of some of the observables makes it difficult, if not impossible, to factor-order them in this representation; one cannot therefore hope to impose Hermiticity conditions.

However, Uggla [3] noticed that this model admits a canonical transformation, under the action of which the Hamiltonian constraint is in the form of that of a relativistic *free* particle. This is achieved by absorbing the potential, which depends on only $\bar{\beta}^+$, into a new momentum. I will first outline his canonical transformation and then use the new variables for quantization of the model.

Postulate a new momentum, defined by

$$\tilde{\pi}_+ = +\sqrt{\bar{\pi}_+^2 + 6e^{-4\sqrt{3}\bar{\beta}^+}}. \quad (4.4)$$

Note that, by definition, $\tilde{\pi}_+ > 0$. We would now like to find the canonically conjugate variable. Consider first the intermediate canonical transformation $(\bar{\beta}^+, \bar{\pi}_+) \mapsto (\bar{\beta}^+, \tilde{\pi}_+)$. In terms of these variables, the symplectic structure is

$$\Omega = d\tilde{\pi}_+ \wedge d\bar{\beta}^+ = \frac{\tilde{\pi}_+}{(\tilde{\pi}_+^2 - 6e^{-4\sqrt{3}\bar{\beta}^+})} \cdot d\tilde{\pi}_+ \wedge d\bar{\beta}^+. \quad (4.5)$$

Now we would like to perform a second canonical transformation, $(\bar{\beta}^+, \tilde{\pi}_+) \mapsto (\tilde{\beta}^+, \tilde{\pi}_+)$, such that $(\tilde{\beta}^+, \tilde{\pi}_+)$ are canonical variables. Thus we want

$$d\tilde{\pi}_+ \wedge d\tilde{\beta}^+ = d\tilde{\pi}_+ \wedge \left(\frac{\partial \tilde{\beta}^+}{\partial \tilde{\pi}_+} \cdot d\tilde{\pi}_+ + \frac{\partial \tilde{\beta}^+}{\partial \bar{\beta}^+} \cdot d\bar{\beta}^+ \right) = \frac{\partial \tilde{\beta}^+}{\partial \bar{\beta}^+} \cdot d\tilde{\pi}_+ \wedge d\bar{\beta}^+ \equiv \Omega. \quad (4.6)$$

Comparing with (4.5), we obtain a differential equation for $\tilde{\beta}^+$:

$$\frac{\partial \tilde{\beta}^+}{\partial \bar{\beta}^+} = \frac{\tilde{\pi}_+}{(\tilde{\pi}_+^2 - 6e^{-4\sqrt{3}\bar{\beta}^+})}. \quad (4.7)$$

Since there is no condition on $\partial \tilde{\beta}^+ / \partial \tilde{\pi}_+$, the above p.d.e. can be readily solved:

$$\tilde{\beta}^+ = -\frac{1}{2\sqrt{3}}(\ln[-\tilde{\pi}_+ + \sqrt{\tilde{\pi}_+^2 + 6e^{-4\sqrt{3}\bar{\beta}^+}}] - \ln[\sqrt{6}e^{-2\sqrt{3}\bar{\beta}^+}]). \quad (4.8)$$

Thus (4.4) and (4.8) together define a canonical transformation which yields a constraint of the desired form. The inverse of this canonical transformation is given by

$$e^{-2\sqrt{3}\tilde{\beta}^+} = \frac{\tilde{\pi}_+}{\sqrt{6} \cosh(2\sqrt{3}\tilde{\beta}^+)}, \quad \bar{\pi}_+ = \tilde{\pi}_+ \tanh(2\sqrt{3}\tilde{\beta}^+), \quad (4.9)$$

from which we can see that the canonical transformation is globally defined on the phase space, since $\bar{\pi}_+$ takes all values.

Since the other variables are invariant under the transformation, ($\tilde{\beta}^0 = \bar{\beta}^0, \tilde{\beta}^- = \bar{\beta}^-, \tilde{\pi}_0 = \bar{\pi}_0, \tilde{\pi}_- = \bar{\pi}_-$). the constraint now takes the simple form

$$C = \frac{1}{2}(-\tilde{\pi}_0^2 + \tilde{\pi}_+^2 + \tilde{\pi}_-^2) = 0. \quad (4.10)$$

However, as mentioned above, this canonical transformation leads to a nonholonomic constraint

$$\tilde{\pi}_+ > 0. \quad (4.11)$$

on the new momentum. (As before $\tilde{\pi}_0 < 0$ since the Taub time has been chosen to be future directed.)

3.4.1 Dirac quantization

In the quantum theory the presence of the non-holonomic constraint $\tilde{\pi}_+ > 0$ and the requirement that $\tilde{\pi}_0 < 0$ means that the phase space cannot be considered as the cotangent bundle over the configuration space $\{(\tilde{\beta})\}$, and thus makes it inconvenient to use the $\tilde{\beta}^A$ -representation. The form of the Hamiltonian constraint function naturally suggests that we view the $\{\tilde{p}_A\}$ as the configuration variables since this leads to a constraint function which is independent of the momenta $\tilde{\beta}^A$. Since the constraint is quadratic in the configuration variables, which form a vector space, it naturally defines a *covariant* metric on the configuration space. The phase space again has a cotangent bundle structure, and the configuration space is the 3-dimensional Minkowski space M^3 , coordinatized by $\{\tilde{p}_A\}$.

We choose for \mathcal{S} the set of all functions on phase space independent of or linear in the momenta $\tilde{\beta}^A$. The set of elementary quantum operators is constructed as follows [13, 14, (see appendix 2)]: With any function $f(\tilde{\pi})$ on the configuration space M^3 associate the configuration operator $\hat{Q}(f)$. Functions linear in momenta $\tilde{\beta}^A$ are determined by a vector field $V^A(\tilde{\pi})$ on M^3 ; we associate with V^A the momentum operator $\hat{P}(V) := \sum_A V^A \tilde{\beta}^A$. The above set of operators satisfy the commutation relations:

$$\begin{aligned} [\hat{Q}(f(\tilde{\pi})), \hat{Q}(g(\tilde{\pi}))] &= 0, \\ [\hat{P}(V), \hat{Q}(f(\tilde{\pi}))] &= i\hbar \hat{Q}(\mathcal{L}_V f)(\tilde{\pi}), \\ [\hat{P}(U), \hat{P}(V)] &= i\hbar \hat{P}([U, V]), \end{aligned} \quad (4.12)$$

which can be obtained from the classical Poisson brackets. They also satisfy the anti-commutation relations:

$$\{\hat{Q}(f(\tilde{\pi})), \hat{Q}(g(\tilde{\pi}))\}_+ - 2\hat{Q}(f \cdot g(\tilde{\pi})) = 0$$

$$\text{and } \{\hat{Q}(f(\tilde{\pi})), \hat{P}(V)\}_+ - 2\hat{P}(fV) = 0, \quad (4.13)$$

which follow from the algebraic relations between functions and vector fields on \mathcal{C} . One can easily check that the LHS of the above relations constitute a Lie ideal in \mathcal{A} . For steps 1-5 in the quantization program, we could have chosen $(1, \tilde{\pi}, \tilde{\beta})$ as the set of elementary variables. It is to implement step 6 –i.e., to find a complete set of Dirac observables– that I have chosen a more general set of elementary operators than the set $(1, \tilde{\pi}, \tilde{\beta})$.

Let the representation space \mathcal{V} consist of functions on M^3 , $\Psi = \Psi(\tilde{\pi})$. The action of the above operators on these wavefunctions is given by:

$$\begin{aligned} \hat{Q}(f(\tilde{\pi})) \circ \Psi(\tilde{\pi}) &:= f(\tilde{\pi}) \cdot \Psi(\tilde{\pi}) \\ \text{and } \hat{P}(V) \circ \Psi(\tilde{\pi}) &:= i\hbar \left(\mathcal{L}_V \Psi(\tilde{\pi}) + \frac{1}{2} \xi(V) \Psi(\tilde{\pi}_A) \right), \end{aligned} \quad (4.14)$$

where $\xi(V)$ is a real function on \mathcal{C} , linear in the vector field V , i.e. $\xi(U + V) = \xi(U) + \xi(V)$. In order to satisfy the CCRs (4.12) and the ACRs (4.13), $\xi(V)$ also has to satisfy the following conditions:

$$\xi([U, V]) = \mathcal{L}_U \xi(V) - \mathcal{L}_V \xi(U) \quad (4.15)$$

$$\text{and } \xi(fV) = \mathcal{L}_V f + f \cdot \xi(V) \quad (4.16)$$

Note first that since (4.16) is *not* linear in ξ , the inclusion of the multiplicative term $\xi(V)$ is *necessary* to satisfy (4.13). Second, we have not yet introduced any inner product on \mathcal{V} . However, in order to *eventually* find an inner product on the physical states, the “extra” term $\xi(V)$ in the representation of the momentum operators (4.14) is again crucial.

The constraint is easily solved in this representation. Physical wavefunctions, i.e. solutions to the quantum constraint

$$\hat{C} \circ \Psi(\tilde{\pi}) := \frac{1}{2} (-\tilde{\pi}_0^2 + \tilde{\pi}_+^2 + \tilde{\pi}_-^2) \Psi(\tilde{\pi}) = 0, \quad (4.17)$$

(as well as the nonholonomic constraints) are simply those wavefunctions with support only on the right half ($\tilde{\pi}_+ > 0$) of the past ($\tilde{\pi}_0 < 0$) null cone \mathcal{L}_R^- . Let us denote physical states by ψ and the vector space of solutions by \mathcal{V}_{phy} . Next we find the Dirac observables, i.e. those operators which commute weakly with the constraint. Configuration observables correspond to functions on \mathcal{L}_R^- ; a complete set consists of $\hat{\mathbb{P}}^\pm \circ \psi := \hat{Q}(\tilde{\pi}_\pm) \circ \psi = \tilde{\pi}_\pm \psi(\tilde{\pi})$. Momentum observables correspond to vector fields on \mathcal{L}_R^- . Note that since \mathcal{L}_R^- is a manifold with boundary, one must be careful to select only those vector fields which are tangential to the boundary. Any such vector field corresponds to a momentum observable which leaves the space of physical states invariant, and is a good Dirac operator. In order that the corresponding momentum operators form an overcomplete set closed under Poisson brackets, the vector fields should form a Lie algebra, and span the tangent space to \mathcal{L}_R^- (almost) everywhere. In order to select an inner product, I will make a specific choice of physical momentum observables.

Two vector fields, which span the tangent space to \mathcal{L}_R^- everywhere, and happen to commute with each other, are:

$$V_-^A = \left(\frac{\partial}{\partial \tilde{\pi}_-} \right)^A + \frac{\tilde{\pi}_-}{\tilde{\pi}_0} \left(\frac{\partial}{\partial \tilde{\pi}_0} \right)^A$$

$$V_+^A = \tilde{\pi}_+ \left(\frac{\partial}{\partial \tilde{\pi}_+} \right)^A + \frac{\tilde{\pi}_+^2}{\tilde{\pi}_0} \left(\frac{\partial}{\partial \tilde{\pi}_0} \right)^A. \quad (4.18)$$

Note that V_-^A is proportional (by a factor of $1/\tilde{\pi}_0$) to the boost vector field in the $\tilde{\pi}_-$ direction and is the “lift” to \mathcal{L}_R^- of the *translational* vector field $(\partial/\partial\tilde{\pi}_-)$ (see (4.34)). V_+^A , on the other hand, is more complicated. It is the lift to \mathcal{L}_R^- of the *dilation* vector field in the $\tilde{\pi}_+$ direction. In place of V_\pm , we might have been tempted to choose the usual Lorentz vector fields corresponding to a rotation and two boosts. However, unlike V_\pm^A , the Lorentz vector fields are *not* tangential to the $\tilde{\pi}_+ = 0$ boundary of \mathcal{L}_R^- , and thus the corresponding momentum operators do not leave the space of physical states invariant.

Thus, a complete set of momentum observables is generated by the operators:

$$\begin{aligned} \widehat{\mathbb{B}}_- &:= \hat{P}(V_-) \equiv \tilde{\beta}^- + \frac{\tilde{\pi}_-}{\tilde{\pi}_0} \tilde{\beta}^0 \\ \text{and } \widehat{\mathbb{B}}_+ &:= \hat{P}(V_+) \equiv \tilde{\pi}_+ \tilde{\beta}^+ + \frac{\tilde{\pi}_+^2}{\tilde{\pi}_0} \tilde{\beta}^0, \end{aligned} \quad (4.19)$$

which are represented by (4.14). The algebra \mathcal{A}_{phy} of Dirac operators is then given by the commutation relations

$$\begin{aligned} [\widehat{\mathbb{B}}_-, \widehat{\mathbb{P}}^-] &= i\hbar \\ \text{and } [\widehat{\mathbb{B}}_+, \widehat{\mathbb{P}}^+] &= i\hbar \widehat{\mathbb{P}}^+. \end{aligned} \quad (4.20)$$

Since the physical states are functions with support only on \mathcal{L}_R^- , a natural ansatz for the physical inner product is

$$\langle \psi | \phi \rangle := \int_{\mathcal{L}_R^-} \mu \bar{\psi} \phi, \quad (4.21)$$

for some two-form μ on \mathcal{L}_R^- . We now require that all physical operators be self-adjoint. Since the $\widehat{\mathbb{P}}^\pm$ are already symmetric, the only nontrivial condition is that the momentum observables (4.19) be represented by self-adjoint operators. This condition is satisfied if and only if, in the representation of the momentum operators (4.14),

$$\xi(V) = \text{Div}_\mu V, \quad (4.22)$$

where $\text{Div}_\mu V$ is the divergence of the vector field V with respect to to the measure μ . Note that the Hermiticity conditions have *not* fixed the inner product. However, the *relation* between the representation and the inner product has been fixed. Alternate choices of μ yield unitarily equivalent theories. One way to fix the inner product is to require that the vector fields (4.18) be divergence free. This yields a set of differential equations which can be solved for the measure

$$\mu = \frac{1}{\tilde{\pi}_+} d\tilde{\pi}_+ \wedge d\tilde{\pi}_-. \quad (4.23)$$

With this choice of μ , the momentum observables (4.19) are represented by just the Lie derivative terms in (4.14).

Thus, a good choice of elementary variables and representation has enabled us to complete the (kinematical) quantization of this model. We have found a complete set of Dirac observables, and an inner product on physical states such that the observables are Hermitian operators.

At this stage, I would like to emphasize again the importance of the choice of elementary variables. To find the Dirac operators in the “old” variables $(\bar{\beta}^A, \bar{\pi}_A)$, one would have to formally solve the Heisenberg equations of motion (with the constraint as the generator of evolution) and find the constants of motion, either classically or quantum mechanically. Assuming this could have been done, the formal operators would then have to be factor-ordered. The enormity of this task can be seen by using the Dirac observables $(\widehat{\mathbb{P}}^\pm, \widehat{\mathbb{B}}_\pm)$ (4.19) and expressing them in terms of $(\bar{\beta}^\pm, \bar{\pi}_\pm)$ by substituting the inverse (4.9) of the canonical transformation.

3.4.2 (†) Reduced space quantization

In chapter 2.4 I outlined an alternative approach to the quantization of constrained systems. Recall that to construct the reduced space quantum theory, we have to find the space of the true degrees of freedom of the system, and then quantize. In the Dirac quantum theory we constructed in the previous section, we viewed the $\tilde{\pi}$ as the configuration variables. Thus the constraint was independent of momenta. As was pointed out in section 2.5, for a constraint of this form, the two quantum theories are kinematically equivalent. In this section, as an example I will explicitly construct the reduced space theory, and demonstrate the unitary equivalence to the Dirac theory of the previous section.

Obviously, it is most convenient to use the “tilde” variables introduced earlier. To construct the reduced phase space, we have to solve the constraint (4.10) and find the constants of motion classically. The constraint is most easily solved for $\tilde{\pi}_0$

$$\tilde{\pi}_0 = -\sqrt{\tilde{\pi}_+^2 + \tilde{\pi}_-^2}. \quad (4.24)$$

Let τ be an affine parameter along the dynamical trajectories generated by the Hamiltonian constraint in the Taub time gauge. (τ is a “time” function on $\bar{\Gamma}$ rather than on spacetime. In each solution, τ can be identified with the Taub time in the spacetime picture.) The Hamiltonian equations of motion, for any function f on the constraint surface are given by $\frac{\partial f}{\partial t} \equiv \dot{f} = \{f, C\}$. Due to the simple form of the constraint, these can be readily solved to yield

$$\begin{aligned} \tilde{\pi}_\pm &= p^\pm & \text{and} & & -\tilde{\pi}_0 &= p^0 := \sqrt{(p^+)^2 + (p^-)^2}, \\ \tilde{\beta}^\pm &= b_\pm + p^\pm \tau & \text{and} & & \tilde{\beta}^0 &= p^0 \tau + \tilde{\beta}^0(0), \end{aligned} \quad (4.25)$$

where $(p^\pm, b_\pm, \tilde{\beta}^0(0))$ are five constants of motion which correspond to the initial values of $(\tilde{\pi}_\pm, \tilde{\beta}^\pm, \tilde{\beta}^0)$ respectively. Since the space of orbits is only 4-dimensional, the five constants of motion are not all independent. Clearly, of the five constants of motion, one should be chosen as a parameter which serves only to fix the “initial time”. This corresponds to fixing a particular cross-section of the gauge orbits on which the rest of

the initial data is specified. Of all the constants of motion, let us select $\tilde{\beta}^0(0)$ as the “gauge-fixing” parameter, since the constraint is solved for its conjugate momentum. Without any loss of generality, I will set $\tilde{\beta}^0(0) = 0$. Now we can consider the five functions (p^\pm, b_\pm, τ) as coordinates on the constraint surface: four of them (p^\pm, b_\pm) are coordinates on the reduced phase space which label the orbits, and τ is by definition the affine parameter along the orbits. We can invert (4.25) and explicitly obtain these five functions on $\bar{\Gamma}$. Substituting (4.25) into the canonical symplectic structure one sees that the p^\pm are canonically conjugate to the b_\pm :

$$\{b_{\hat{A}}, p^{\hat{B}}\} = \delta_{\hat{A}}^{\hat{B}}, \quad (4.26)$$

where $\hat{A}, \hat{B} = +, -$ are indices on $\hat{\Gamma}$. The nonholonomic constraint (4.11) implies that $p^+ > 0$.

Now we want to quantize the system whose phase space is $\hat{\Gamma}$, with the Poisson brackets (4.26). Note that due to the presence of the nonholonomic constraint on p^+ , it is convenient to choose p^+ (and p^-) as the configuration observables. The reduced phase space $\hat{\Gamma}$ is then a cotangent bundle over the half plane $\Sigma_R = \{(p^+ > 0, p^-)\}$, with the b_\pm as the new momenta (note that an upper (lower) index position is used for configuration (momentum) observables). Momentum observables $B(v) = v^{\hat{A}} b_{\hat{A}}$ correspond to vector fields $v^{\hat{A}}(p)$ on the reduced configuration space Σ_R . Note however that since Σ_R is a manifold with boundary, it admits only one translational vector field, (the vector field $(\partial/\partial p^+)^{\hat{A}}$ is incomplete) and thus momentum variables are somewhat trickier to select. We need a Lie algebra of vector fields which span the tangent space to Σ_R everywhere. Such an algebra (which happens to be Abelian) is generated by the translational vector field in the p^- direction and a dilation in the p^+ direction:

$$v_{(-)}^{\hat{A}} := \left(\frac{\partial}{\partial p^-} \right)^{\hat{A}} \quad \text{and} \quad v_{(+)}^{\hat{A}} := p^+ \left(\frac{\partial}{\partial p^+} \right)^{\hat{A}}. \quad (4.27)$$

Note that these are just the projections to Σ_R of the vector fields $V_{\pm}^{\hat{A}}$ on \mathcal{L}_R^- considered in the Dirac theory. While one could have chosen any pair of linearly independent vector fields which are tangential to the boundary, I have selected this pair in order to make the isomorphism with the Dirac theory manifest (see (4.34)).

With these particular vector fields, we associate the momentum observables

$$B_- = b_- \quad \text{and} \quad B_+ = p^+ b_+ \quad (4.28)$$

The commutation relations can be easily obtained from the Poisson brackets (4.26), the algebra \mathcal{A}_{red} of Dirac observables is given by

$$[\hat{B}_-, \hat{p}^-] = i\hbar \quad \text{and} \quad [\hat{B}_+, \hat{p}^+] = i\hbar \hat{p}^+. \quad (4.29)$$

Note that this algebra is isomorphic to the algebra of quantum Dirac observables (4.20).

In the configuration representation, states are functions $\psi = \psi(p^+, p^-)$ on Σ_R . A representation of the reduced space observable algebra is

$$\hat{p}^\pm \circ \psi = p^\pm \psi$$

$$\text{and } \widehat{B}_\pm \circ \psi = i\hbar(\mathcal{L}_{v_\pm}\psi + \frac{1}{2}\xi(v))\psi \quad (4.30)$$

where $\xi(v)$ satisfies the same properties as in (4.15). A natural ansatz for the inner product is

$$\langle \psi | \phi \rangle = \int_{\Sigma_R} \epsilon \bar{\psi} \phi \quad (4.31)$$

where ϵ is some two-form on Σ_R . We see immediately that the momentum observables (4.28) are Hermitian with respect to the inner product if and only if $\xi(v) = \text{Div}_\epsilon v$. Different choices of ϵ give rise to unitarily equivalent quantum theories.

As in the Dirac theory, a simplifying choice for the inner product can be made by requiring that the vector fields (4.27) corresponding to the momentum observables (4.28) be divergence free with respect to ϵ . The resulting set of differential equations on ϵ can be solved to yield

$$\epsilon = \frac{1}{p^+} dp^+ \wedge dp^- \quad (4.32)$$

which is unique up to the usual scale factor. The momentum operators (4.28) are now represented in (4.30) by just the Lie derivative terms.

To explicitly see the equivalence between the reduced and the Dirac quantum theories, note that there is a natural isomorphism, a projection mapping along the orbits of the vector field $(\partial/\partial\tilde{\pi}_0)^A$, between \mathcal{L}_R^- (defined in section (3.1)) and Σ_R (coordinatized by $\tilde{\pi}_\pm$). This induces a unitary mapping between \mathcal{V}_{phy} , the space of functions ψ on \mathcal{L}_R^- , and \mathcal{V}_{red} , the space of functions on Σ_R :

$$\psi(\tilde{\pi}_+, \tilde{\pi}_-) \longleftrightarrow \psi(p^+, p^-) \quad (4.33)$$

Note that the inner product is the same, since $\mu = \epsilon$. Since the configuration observables \widehat{p}^\pm and $\widehat{\mathbb{P}}^\pm$ are obviously transformed into each other, we only need to check the momentum operators. The above diffeomorphism between Σ_R and \mathcal{L}_R^- induces the following transformation between vector fields V tangential to \mathcal{L}_R^- and vector fields v tangential to Σ_R :

$$\begin{aligned} V^A(\tilde{\pi}_\pm) &= V^+(\tilde{\pi}_\pm) \left(\frac{\partial}{\partial\tilde{\pi}_+} \right)^A + V^-(\tilde{\pi}_\pm) \left(\frac{\partial}{\partial\tilde{\pi}_-} \right) + \frac{(\tilde{\pi}_+ V^+(\tilde{\pi}_\pm) + \tilde{\pi}_- V^-(\tilde{\pi}_\pm))}{\tilde{\pi}_0} \left(\frac{\partial}{\partial\tilde{\pi}_0} \right)^A \\ \longleftrightarrow \quad v^A(p^\pm) &= V^+(p^\pm) \left(\frac{\partial}{\partial p^+} \right)^A + V^-(p^\pm) \left(\frac{\partial}{\partial p^-} \right)^A. \end{aligned} \quad (4.34)$$

The vector fields V_\pm^A (4.18) are just the ‘‘lifts’’ of the vector fields (4.27). Since both sets of vector fields are also divergence free with the respective inner products, we see that the corresponding momentum operators are unitarily transformed into each other. Thus, the Dirac and reduced quantum theories are manifestly equivalent to each other: the physical states carry unitarily equivalent representations of the isomorphic observable algebras \mathcal{A}_{phy} and \mathcal{A}_{red} .

3.5 Remarks

Each of the models quantized in this chapter has clarified the role of some essential aspect of algebraic quantization. In this section I will summarize the lessons one has learnt from these examples.

Remark 1

The quantization of the particle on S^1 illustrates the importance of the ACRs. Before we imposed the ACR (2.2), there were ambiguities in the theory, which corresponded to a large number of spurious sectors. In this example, since the single ACR is a Casimir invariant of the algebra \mathcal{A} , each eigenspace carries an irreducible representation of \mathcal{A} . Only one of these spaces, in which the Casimir invariant has value 1, corresponds to the correct physical quantum theory. The ACR identifies the ambiguities, and imposing (2.2) on the quantum theory got rid of the spurious sectors. Of course in this model it is trivial to “see” the ambiguities and resolve them; the point however was not just to solve the quantum theory of the particle on S^1 , but rather to understand the role of the ACRs in a more general context.

Further, as I already mentioned at the end of section 2, in order to be able to find a good inner product, it is important to impose the ACRs and eliminate the spurious sectors *before* the \star -relations are imposed.

A key feature of algebraic quantization is the fact that it frees up the choice of representation from ties to the phase space. As we saw in subsection 2.1, this allows us to consider representations which are unusual but physically significant; and which could not have been obtained in other quantization schemes where the representation of \mathcal{A} is constructed on functions on the phase space.

Remark 2

From the construction of the quantum theory for the harmonic oscillator in the (q, z) variables we see that it is consistent to use a hybrid set of functions (one real, one complex) on a real phase space as the elementary variables for quantization. On the face of it, it appears counter-intuitive that a real momentum, represented by a holomorphic derivative operator d/dz , can be canonically conjugate to a complex variable. However, there is an inner product, selected uniquely by implementing the \star -relations on these variables, with respect to which d/dz is in fact Hermitian. This indicates that the hybrid connection-dynamical variables are a consistent choice for quantum gravity.

Remark 3

The homogeneous cosmological model Bianchi type II is the only constrained system quantized in this chapter. In the algebraic approach, real physical observables should be represented by operators which are Hermitian with respect to the physical inner product. This model demonstrates that the above criterion can be used to explicitly construct an inner product on physical states.

In the $\bar{\beta}$ variables, the constraint (4.3) is separable. The quantum constraint equation has been previously “solved”: the solutions are sinister looking Bessel functions in $\bar{\beta}^0$ [2, Table III.3, pp. 91], and it is not at all obvious what if anything one can learn from them. The set of solutions was in some ways considered complete. However, the Hilbert space structure necessary in quantum theory, and a physical interpretation, were absent. Until recently [12], there was no known inner product on these states. The algebraic framework provides a powerful tool to find the physical inner product; and it clarifies and emphasizes the role of physical operators. Since the problem is after all separable, once the importance of the observables was understood, it was relatively straightforward to construct them, and then to use the Hermiticity relations on them to find the physical inner product. As we will see in chapter 6, the existence of a kinematically complete quantum theory does open up some possibilities to extract a physical interpretation.

This model serves a few other purposes.

- It illustrates the importance of making good choices, for the algebra of elementary variables and its representation. As I already mentioned, the solutions in the $\bar{\beta}$ -representation are of a horrendous form. More importantly, it is difficult to see how the the physical operators $\tilde{\pi}_+$ (4.4) and $\widehat{\mathbb{B}}_+$ (4.19) could even have been found, let alone factor ordered and represented explicitly.
- We began with a fairly general representation of the algebra \mathcal{A} . Recall that in (4.14) $\xi(V)$ is an undetermined function in the representation of the momentum variables. It is necessary to include this term in order to satisfy some of the ACRs. Later, we make an ansatz for the physical inner product (4.21), and find that the physical operators are Hermitian if and only if $\xi(V)$ is the divergence of the vector field with respect to the measure μ . However, neither $\xi(V)$ nor the measure is determined. Different choices of the measure μ change the explicit representation of the momentum observables, but yield unitarily equivalent quantum theories. Thus the Hermiticity conditions determine the *relation* between the representation and the inner product, leaving us with the freedom to make unitarily equivalent choices, which can simplify the expressions of some of the interesting physical operators.
- In this model, Dirac and reduced space quantization can be explicitly compared. I showed in this case that the two quantum theories are unitarily equivalent, verifying the general claim (made in section 2.6) that this would be so for constraints independent of momenta.

Bibliography

- [1] Ashtekar A 1991 Lectures on *Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore).
- [2] Ryan M P 1972 *Hamiltonian Cosmology: Lecture notes in Physics* **13** Ehlers J *et al* (eds) (Springer-Verlag New York)
- [3] Uggla C 1991 private communication (Syracuse)
- [4] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-6
- [5] Isham C J 1984 in *Relativity, Groups and Topology II, Les Houches 1983*, DeWitt B S and Stora R (eds) (North-Holland Amsterdam)
- [6] Wald R M 1984 *General Relativity* (University of Chicago Press Chicago)
- [7] Misner C W 1972 in *Magic Without Magic* Klauder J (ed) (Freeman San Francisco)
- [8] Ryan M P and Shepley L C 1975 *Homogeneous Relativistic Cosmology* (Princeton University Press Princeton)
- [9] Arnowit R, Deser S and Misner C W 1962 in *Gravitation: An Introduction to Current Research* Witten L (ed) (Wiley New York)
- [10] Rosquist K, Uggla C and Jantzen R T 1990 *Class. Quantum Grav.* **7** 611
- [11] Taub A H 1951 *Ann. Math.* **53** 472
- [12] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-5
- [13] Ashtekar A 1980 *Comm. Math. Phys.* **71** 59
- [14] Ashtekar A and Geroch R 1974 *Rep. Prog. Phys.* **37** 1211-56

Chapter 4

ASHTEKAR-HOROWITZ MODEL

4.1 Introduction

In this chapter I will quantize a model, considered by Ashtekar and Horowitz [1], that mimics some of the features of general relativity. It was previously believed to display certain unexpected behaviour in quantum theory. Since this behaviour arose from precisely those features of this model that it possesses in common with general relativity, the authors speculated that similar surprises might occur in a quantum theory of gravity. In this chapter I will re-analyse this problem in the context of the algebraic quantization program.

Let us recall certain features of general relativity in the geometrodynamical variables. In the ADM formulation, the basic phase space variables are the 3-metric q_{ab} and its canonically conjugate momentum. The constraint surface¹ 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 structure of the constraint surface, $\bar{\Gamma}$, and the dynamical structure of general relativity are 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 allowed” region in the configuration space. More precisely, the image in the configuration space of the constraint surface $\bar{\Gamma}$ (under the natural projection map) is a *proper subset* of the configuration space \mathcal{C} .
- Second, in the asymptotically flat case, the Hamiltonian is not constrained to vanish. On $\bar{\Gamma}$, 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

¹For the purposes of this chapter, the diffeomorphism constraint can be ignored.

spatial derivatives².

- Finally, the positive energy theorems of classical general relativity state that on the allowed regions of \mathcal{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 shares the above features of general relativity (I will henceforth refer to this model as the A-H model.): Consider a particle in 3-dimensional Euclidean space, subject to the constraint

$$C \equiv p_{\phi}^2 - R(\phi) = 0. \quad (1.1)$$

The “potential”, $R(\phi)$, is a smooth function, which is not everywhere positive. As in general relativity, the constraint surface $\bar{\Gamma}$ projects down to a proper subset of the configuration space \mathcal{C} . The *classically allowed region* $\bar{\mathcal{C}}$ corresponds to those sectors where (1.1) has solutions, i.e., where $R(\phi) \geq 0$. Now introduce a Hamiltonian via

$$H = C + E(\phi), \quad \text{with} \quad E(\phi) \cdot R(\phi) \geq 0; \quad (1.2)$$

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 ϕ . Since $E(\phi)$ 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.

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 consider the situation if such states do exist. Now, physical states are solutions to the quantum constraint equation, on which the Hamiltonian acts via a multiplication by $E(\phi)$. Recall 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* $\tilde{\mathcal{C}} = \mathcal{C} - \bar{\mathcal{C}}$. Thus, on some physical states which penetrate into $\tilde{\mathcal{C}}$, the energy will be negative. Due to the close analogy with general relativity, such behaviour in this model might indicate similar tunnelling in quantum gravity.

The key result of the previous quantization was that in the Dirac quantum theory, there are indeed physical quantum states which tunnel into the forbidden region. Further, some states had support entirely in the forbidden region $\tilde{\mathcal{C}}$! Since the usual Euclidean measure on \mathbb{R}^3 was used, this led to the conclusion that a large number of physical quantum states in fact possessed negative energies: for this model the classical positive energy theorem was violated in quantum theory.

Ashtekar and Horowitz also compared the reduced space quantum theory with the Dirac quantum theory. They concluded that the former contained only some of the states

²I would like to point out, to readers who are somewhat familiar with the Hamiltonian formulation of general relativity and the specific form of the scalar constraint, that the surface integral is independent of the momenta since in the scalar constraint, all terms containing the momenta are ultralocal.

present in the Dirac theory and was thus incomplete. This comes about as follows: Recall that in the reduced space approach, one first solves the constraint classically. In the A-H model, clearly one can solve the constraint only in the region $R > 0$. The resulting reduced phase space does not contain any classically forbidden sectors, and the energy is positive everywhere on $\hat{\Gamma}$. The analogs of the Dirac states with negative energy are absent from the quantum theory on $\hat{\Gamma}$.

In the quantum theory constructed previously, the standard Euclidean measure on \mathbb{R}^3 was assumed to define the inner product on physical states. In terms of the present algebraic quantization program, the steps missing from the construction of this quantum theory are *precisely* the ones that require a physical inner product which realises the \star -relations on the Dirac observables as Hermiticity conditions. As we will see in detail, the Hermiticity conditions are satisfied only if the measure has support only on the classically allowed region $\bar{\mathcal{C}}$. Thus, while it is true that physical states can have support in the forbidden region, since this region is a set of measure zero in the physical inner product, they do not define unique states in the Hilbert space. States in the Hilbert space are specified completely by their support in the allowed region itself.

Thus, at least for this model, a complete and consistent quantum theory displays no extreme quantum tunnelling. A careful application of the \star -relations eliminates the pathological negative energy states. Further, as I will discuss in a later subsection, the Dirac and reduced quantum theories are (almost) equivalent.

4.2 Dirac quantization

Let $(\hat{r}, \hat{\theta}, \hat{\phi})$ denote the operators corresponding to the usual spherical polar coordinates in 3-dimensional Euclidean space, and let $(\hat{p}_r, \hat{p}_\theta, \hat{p}_\phi)$ be the canonically conjugate momenta. In the configuration representation, states are functions of the coordinates, $\Psi = \Psi(r, \theta, \phi)$, and the operators are represented by

$$\begin{aligned} \hat{r} \circ \Psi &= r\Psi, & \hat{\theta} \circ \Psi &= \theta\Psi & \text{and} & \hat{\phi} \circ \Psi &= \phi\Psi; \\ \hat{p}_r \circ \Psi &= \frac{\hbar}{i} \frac{\partial}{\partial r} \Psi, & \hat{p}_\theta \circ \Psi &= \frac{\hbar}{i} \frac{\partial}{\partial \theta} \Psi & \text{and} & \hat{p}_\phi \circ \Psi &= \frac{\hbar}{i} \frac{\partial}{\partial \phi} \Psi. \end{aligned} \quad (2.1)$$

These operators satisfy the usual CCRs. (Although (r, θ, ϕ) are not globally well-defined coordinates, this issue is not important here.) Since we have no inner product, the familiar divergence terms have been left out of the representations of the momentum operators³. In this representation, the constraint equation satisfied by physical states ψ is

$$\hbar^2 \frac{\partial^2}{\partial \theta^2} \psi + R(\phi)\psi = 0. \quad (2.2)$$

³The quantization of a classical system is not a linear or well-defined *process*, particularly when the system is constrained. One can only demand that the final theory constructed is internally consistent with its initial hypotheses. Hence I would urge readers to set aside their objections until after I have constructed the final quantum theory. In remarks at the end of this section, I will try and answer some objections that have been raised [2].

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

$$\psi_{\pm} = k_{\pm}(r, \phi) \exp(\pm \frac{i}{\hbar} \sqrt{R}\theta) \quad (2.3)$$

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 $k_{\pm}(r, \phi)$ are arbitrary. In particular, their support is, *not* restricted to the allowed region \mathcal{C} . and have support everywhere in configuration space, including the classically forbidden region $\tilde{\mathcal{C}}$. 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 state as

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}. \quad (2.4)$$

Note that since we have not yet defined an inner product, this is *not* an orthogonal decomposition of \mathcal{V} .

Let us construct the Dirac observables. Since the constraint is first class, there are two true degrees of freedom, and thus we expect four independent Dirac observables. From their representations, it is clear that $\hat{r}, \hat{p}_r, \hat{p}_{\theta}, \hat{\phi}$ 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 physical states $\hat{p}_{\theta} = \pm \sqrt{\widehat{R(\phi)}}$, and thus so far we only have three *independent* observables. In order for the set to be complete, we need another observable. In correspondence with the classical Dirac observable constructed by Ashtekar and Horowitz, consider the operator

$$\hat{P}_{\phi} = \begin{pmatrix} \hat{P}_{\phi}^+ & 0 \\ 0 & \hat{P}_{\phi}^- \end{pmatrix}, \quad \text{where} \quad \hat{P}_{\phi}^{\pm} = \hat{p}_{\phi} \mp \frac{1}{2} \left(\frac{R'}{\sqrt{R}} \theta \right). \quad (2.5)$$

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

$$\hat{P}_{\phi}^+ \circ \psi_+ = \frac{\hbar}{i} k'_+ \exp(+\frac{i}{\hbar} \sqrt{R}\theta) \in \mathcal{V}^+. \quad (2.6)$$

Similarly, $\hat{P}_{\phi}^- \circ \psi_- \in \mathcal{V}^-$. Hence \hat{P}_{ϕ} as defined above is a physical operator. We now have a ‘‘sufficient number’’, i.e. a locally complete set, of physical operators. For future reference, note that

$$\hat{P}_{\phi}^- \circ \psi_+ = \frac{\hbar}{i} k'_+ \exp(+\frac{i}{\hbar} \sqrt{R}\theta) + 2(\sqrt{R})' \theta k_+ \exp(+\frac{i}{\hbar} \sqrt{R}\theta) \notin \mathcal{V}, \quad (2.7)$$

is not a physical state, since the coefficient of the exponential in the second term is no longer a function only of (r, ϕ) .

We now have to find the \star -relations on the algebra of observables. Clearly, $\hat{r}^{\star} = \hat{r}$, $\hat{p}_r^{\star} = \hat{p}_r$, $\hat{p}_{\theta}^{\star} = \hat{p}_{\theta}$, $\hat{\phi}^{\star} = \hat{\phi}$ and are physical operators. In order to analyse the \star -relation on \hat{P}_{ϕ} , 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 $\tilde{\mathcal{V}}^+$ with support entirely in the classically forbidden region $\tilde{\mathcal{C}}$. Now, on the sector of states $\bar{\mathcal{V}}^+$, $(\sqrt{\widehat{R}})^* = \sqrt{\widehat{R}}$ and hence

$$(\widehat{\mathbb{P}}_\phi^+)^* = \left(\hat{p}_\phi - \frac{1}{2} \left(\frac{\widehat{R}'}{\sqrt{\widehat{R}}} \theta \right) \right)^* = \hat{p}_\phi - \frac{1}{2} \left(\frac{\widehat{R}'}{\sqrt{\widehat{R}}} \theta \right) = \widehat{\mathbb{P}}_\phi^+ \quad (2.8)$$

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

$$(\widehat{\mathbb{P}}_\phi^+)^* = \left(\hat{p}_\phi - \frac{1}{2} \left(\frac{\widehat{R}'}{\sqrt{\widehat{R}}} \theta \right) \right)^* = \hat{p}_\phi + \frac{1}{2} \left(\frac{\widehat{R}'}{\sqrt{\widehat{R}}} \theta \right) = \widehat{\mathbb{P}}_\phi^-, \quad (2.9)$$

which, as we see from (2.7), is *not* a physical operator. In terms of the matrix notation, on the sector of “allowed” states $\bar{\mathcal{V}}$, since $(\widehat{\mathbb{P}}_\phi^\pm)^* = \widehat{\mathbb{P}}_\phi^\pm$, $\widehat{\mathbb{P}}_\phi^* = \widehat{\mathbb{P}}_\phi$ is a physical operator; whereas on the sector of forbidden states $\tilde{\mathcal{V}}$,

$$(\widehat{\mathbb{P}}_\phi)^* = \begin{pmatrix} (\widehat{\mathbb{P}}_\phi^+)^* & 0 \\ 0 & (\widehat{\mathbb{P}}_\phi^-)^* \end{pmatrix} = \begin{pmatrix} \widehat{\mathbb{P}}_\phi^- & 0 \\ 0 & \widehat{\mathbb{P}}_\phi^+ \end{pmatrix} \quad (2.10)$$

does not leave the space of physical states invariant.

Clearly something peculiar is happening here. We have a complete set of physical states, and a complete algebra $\mathcal{A}_{phy} \subset \mathcal{A}$ of physical operators generated by $\{\hat{r}, \hat{p}_r, \hat{p}_\theta, \hat{\phi}, \widehat{\mathbb{P}}_\phi\}$. Further, the \star -involution on \mathcal{A} has a well-defined action on \mathcal{A}_{phy} and induces a map from \mathcal{A}_{phy} into \mathcal{A} . What fails however, is that the induced \star is *not an involution* on \mathcal{A}_{phy} ; its action on one of the generators of \mathcal{A}_{phy} , namely $\widehat{\mathbb{P}}_\phi$, takes it out of \mathcal{A}_{phy} . (This can be understood in terms of the Hamiltonian vector field of the observable, see Fig.4.2.) The algebra of physical observables, \mathcal{A}_{phy} , does not admit a \star -involution induced from $\mathcal{A}^{(\star)}$. Thus there is no sensible way to formulate the Hermiticity conditions on physical operators in terms of an inner product on physical states.

In remark 6, section 2.4, I noted that if the constraint is real and if the physical operators commute strongly with the constraint, then a \star -involution is induced on \mathcal{A}_{phy} . However, for the A-H model, as we have just seen, there is no \star -involution on \mathcal{A}_{phy} , inspite of the fact that it *appears* to satisfy the above sufficiency conditions. What goes wrong here? While it is true that the constraint is real, in the representation we have chosen the physical states are solutions not just of the constraint operator, but of one of its two square-roots. These square-root constraints are not necessarily real, thus violating the above-mentioned conditions which guarantee an induced \star -involution on \mathcal{A}_{phy} .

On the face of it, due to the above mathematical inconsistency, i.e. the lack of a \star -involution on \mathcal{A}_{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 that we were looking for.

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. Forward-flashing to the denouement, basically we will find that the measure on the forbidden region $\tilde{\mathcal{C}}$ is 0, and on the remaining states, \hat{P}_ϕ^* is an observable. I will now show this in detail.

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 we are 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. Thus, we are led to look for a physical operator which 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 $\hat{I}_z \circ \Psi(r, \theta, \phi) = \Psi(r, \pi - \theta, \phi)$. 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. Unfortunately, ψ_\pm are not eigenspaces. In fact, the even and odd physical eigenstates (with eigenvalues $+1$ and -1 respectively) are of the form

$$\psi_e = k_e(r, \phi) \cos\left[\frac{\sqrt{R}}{\hbar}(\theta - \pi/2)\right] = \begin{pmatrix} \frac{1}{2}k_e e^{-\frac{i\pi}{2\hbar}\sqrt{R}} \exp\left(+\frac{i}{\hbar}\sqrt{R}\theta\right) \\ \frac{1}{2}k_e e^{+\frac{i\pi}{2\hbar}\sqrt{R}} \exp\left(-\frac{i}{\hbar}\sqrt{R}\theta\right) \end{pmatrix} \quad (2.11)$$

$$\psi_o = ik_o(r, \phi) \sin\left[\frac{\sqrt{R}}{\hbar}(\theta - \pi/2)\right] = \begin{pmatrix} \frac{1}{2}k_o e^{-\frac{i\pi}{2\hbar}\sqrt{R}} \exp\left(+\frac{i}{\hbar}\sqrt{R}\theta\right) \\ -\frac{1}{2}k_o e^{+\frac{i\pi}{2\hbar}\sqrt{R}} \exp\left(-\frac{i}{\hbar}\sqrt{R}\theta\right) \end{pmatrix}. \quad (2.12)$$

Hence, $\mathcal{V} = \mathcal{V}_e \oplus \mathcal{V}_o$ should be an orthogonal decomposition in the desired inner product.

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 \mathcal{A}_{phy} of (continuous) Dirac operators. However, while it does commute with \hat{r} , \hat{p}_r , $\hat{\phi}$, \hat{P}_ϕ , it does not commute with \hat{p}_θ . In fact, they anticommute, $[\hat{p}_\theta, \hat{I}_z]_+ = 0$. Since \hat{p}_θ is not diagonal in the even/odd states, I will continue to use the $+/-$ decomposition, even though \mathcal{V}^+ and \mathcal{V}^- are not obviously orthogonal.

Let us consider as an ansatz, an inner product of the form

$$\begin{aligned} \langle \psi_1 | \psi_2 \rangle = & \int_{\tilde{\mathcal{C}}} (\mu_+ \overline{k_1^+} k_2^+ + \mu_- \overline{k_1^-} k_2^- + \mu_{+-} \overline{k_1^+} k_2^- + \overline{\mu_{+-}} \overline{k_1^-} k_2^+) \\ & + \int_{\tilde{\mathcal{C}}} (\tilde{\mu}_+ \overline{k_1^+} k_2^+ + \tilde{\mu}_- \overline{k_1^-} k_2^- + \tilde{\mu}_{+-} \overline{k_1^+} k_2^- + \tilde{\mu}_{+-} \overline{k_1^-} k_2^+) \end{aligned} \quad (2.13)$$

where the integration is with respect to $dr \wedge d\theta \wedge d\phi$; the $\mu = \mu(r, \theta, \phi)$ have arbitrary dependence on all three coordinates; and where factors of $\exp(-\frac{2i}{\hbar}\sqrt{R}\theta)$, $\exp(-\frac{2}{\hbar}\sqrt{|R|\theta})$, and $\exp(\frac{2}{\hbar}\sqrt{|R|\theta})$ have been absorbed into μ_{+-} , $\tilde{\mu}_+$ and $\tilde{\mu}_-$ respectively. The inner product can be positive definite if and only if the “diagonal” measures are positive and the “off-diagonal” measures satisfy

$$|\mu_{+-}| < \sqrt{\mu_+ \mu_-} \quad \text{and} \quad |\tilde{\mu}_{+-}| < \sqrt{\tilde{\mu}_+ \tilde{\mu}_-}. \quad (2.14)$$

(In terms of the matrix notation, the inner product corresponds to

$$\langle \psi_1 | \psi_2 \rangle = \begin{pmatrix} \overline{k_1^+} & \overline{k_1^-} \end{pmatrix} \begin{pmatrix} \mu_+ & \mu_{+-} \\ \overline{\mu_{+-}} & \mu_- \end{pmatrix} \begin{pmatrix} k_2^+ \\ k_2^- \end{pmatrix} \quad (2.15)$$

Suppose we write a general physical state as $\psi = \psi_+ + \psi_-$, and postulate the natural inner product $\langle \psi_1 | \psi_2 \rangle = \int_{\bar{C}} \mu \bar{\psi}_1 \psi_2 + \int_{\tilde{C}} \tilde{\mu} \bar{\psi}_1 \psi_2$. 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}_θ , shows that there is in fact no such inner product. Therefore one *has* to work with the general form (2.13).

Now let us impose the Hermiticity conditions on the observables. Clearly, \hat{r} and $\hat{\phi}$ are essentially self-adjoint. Requiring that \hat{p}_r is symmetric leads to the condition that $\partial\mu/\partial r = 0$ for all terms in the inner product. Next, let us consider in detail the Hermiticity of \hat{p}_θ . Since physical states are specified entirely by their coefficients k_\pm , we can represent operators entirely by their action on k_\pm :

$$\hat{r} \circ k_\pm = r k_\pm, \quad \hat{\phi} \circ k_\pm = \phi k_\pm; \quad (2.16)$$

$$\hat{p}_r \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial r} k_\pm, \quad \hat{P}_\phi \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial \phi} k_\pm; \quad (2.17)$$

and, in particular,

$$\begin{aligned} \hat{p}_\theta \circ \begin{pmatrix} k_+ \\ k_- \end{pmatrix} &= \begin{pmatrix} +\sqrt{R}k_+ \\ -\sqrt{R}k_- \end{pmatrix} && \text{on } \bar{C} \\ &= \begin{pmatrix} +i\sqrt{|R|}k_+ \\ -i\sqrt{|R|}k_- \end{pmatrix} && \text{on } \tilde{C}. \end{aligned} \quad (2.18)$$

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 ψ_1, ψ_2 . Consider states in \mathcal{V}_+ , i.e. $k_1^- = k_2^- = 0$. Then

$$\langle \psi_1 | \hat{p}_\theta | \psi_2 \rangle = \int_{\bar{C}} \mu_+ \bar{k}_1^+ \sqrt{R} k_2^+ + i \int_{\tilde{C}} \tilde{\mu}_+ \bar{k}_1^+ \sqrt{|R|} k_2^+. \quad (2.19)$$

On the other hand, by definition

$$\langle \psi_1 | \hat{p}_\theta^\dagger | \psi_2 \rangle := \overline{\langle \psi_2 | \hat{p}_\theta | \psi_1 \rangle} = \int_{\bar{C}} \mu_+ \bar{k}_1^+ \sqrt{R} k_2^+ - i \int_{\tilde{C}} \tilde{\mu}_+ \bar{k}_1^+ \sqrt{|R|} k_2^+. \quad (2.20)$$

Clearly, \hat{p}_θ can be Hermitian on \mathcal{V}_+ if and only if $\tilde{\mu}_+ = 0$. Similarly, one can conclude that $\tilde{\mu}_- = 0$. Thus, both the diagonal terms in the forbidden region vanish. But now, due to the condition (2.14), in the forbidden region the cross term also vanishes, $\tilde{\mu}_{+-} = 0$. *In the inner product (2.13), 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 \tilde{C} , this support is of measure zero in the physical inner product.

Let us return to the Hermiticity of \hat{p}_θ . Consider states $\psi_1 = \psi_{1+}$ and $\psi_2 = \psi_{2-}$, i.e. $k_1^- = k_2^+ = 0$. Then,

$$\langle \psi_1 | \hat{p}_\theta | \psi_2 \rangle = \int_{\bar{C}} \mu_{+-} \bar{k}_1^+ (-\sqrt{R}) k_2^-. \quad (2.21)$$

However,

$$\langle \psi_1 | \hat{p}_\theta^\dagger | \psi_2 \rangle := \overline{\langle \psi_2 | \hat{p}_\theta | \psi_1 \rangle} = \int_{\bar{C}} \mu_{+-} k_2^- (\sqrt{R}) \bar{k}_1^+. \quad (2.22)$$

Equating the two, we find that \hat{p}_θ is Hermitian if and only if $\mu_{+-} = 0$. Thus, it is the Hermiticity of a continuous operator which implies that the subspaces \mathcal{V}_+ and \mathcal{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 $\hat{r}, \hat{p}_r, \hat{p}_\theta, \hat{\phi}$ as Hermiticity conditions on the representation, we have reduced the form of the physical inner product (2.13) to

$$\langle \psi_1 | \psi_2 \rangle = \int_{\bar{\mathcal{C}}} (\mu_+ \overline{k_1^+} k_2^+ + \mu_- \overline{k_1^-} k_2^-), \quad (2.23)$$

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 $\bar{\mathcal{C}}$. In other words, by restricting the support of physical states to the classically allowed region, in this problem we do not lose any elements of the physical Hilbert space. Thus, as we saw earlier (2.6), on states with support only on $\bar{\mathcal{C}}$, \hat{P}_ϕ^\star is a physical operator, in fact $\hat{P}_\phi^\star = \hat{P}_\phi$. Since, in terms of k_\pm , the action of \hat{P}_ϕ is

$$\hat{P}_\phi \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial \phi} k_\pm. \quad (2.24)$$

it is now trivial to check that \hat{P}_ϕ is symmetric if and only if $\partial\mu_\pm/\partial\phi = 0$.

Thus, the measure depends only on θ , and furthermore, this dependence is undetermined by any Hermiticity conditions. How has this come about? In the quantization of ordinary unconstrained systems, the dependence of the measure on a coordinate θ is determined by requiring that the corresponding momentum operator \hat{p}_θ , which is represented by $\frac{\hbar}{i}\partial/\partial\theta$, should be Hermitian. In the quantum theory of constrained systems, one is finally only interested in the measure on physical states. In this example, the momentum operator \hat{p}_θ is represented *on physical states* by a multiplication (2.18). Hence there is no condition that determines the θ -dependence of the measure μ .

Now, since the coefficients k_\pm do not depend on θ either, we can choose $\mu_\pm(\theta)$ such that the integral over θ can be performed trivially, and the inner product is thus reduced to

$$\langle \psi_1 | \psi_2 \rangle = \mu_+ \int_{\bar{\phi}} dr \wedge d\phi \overline{k_1^+} k_2^+ + \mu_- \int_{\bar{\phi}} dr \wedge d\phi \overline{k_1^-} k_2^-, \quad (2.25)$$

where $\bar{\phi}$ indicates that the integral is performed only over classically allowed values of ϕ .

Is there a criterion that will fix the relative weights of the two terms? Note that we have not yet imposed the Hermiticity of the discrete symmetry \hat{I}_z . Since its eigenspaces must be orthogonal, we have

$$0 = \langle \psi_e | \psi_o \rangle = \frac{1}{4} [\mu_+ - \mu_-] \int_{\bar{\phi}} \overline{k_e} k_o. \quad (2.26)$$

Thus we can choose $\mu_+ = \mu_- = 1$, and the final form for the inner product is

$$\langle \psi_1 | \psi_2 \rangle = \int_{\bar{\phi}} dr \wedge d\phi [\overline{k_1^+} k_2^+ + \overline{k_1^-} k_2^-]. \quad (2.27)$$

4.2.1 Remarks

Let us first briefly review the process by which we have 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 forbidden region. Next, we constructed a set of generators of \mathcal{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 \mathcal{A}_{phy} , from \mathcal{A} . The \star s of most of the generators of \mathcal{A}_{phy} were also in \mathcal{A}_{phy} . However, the \star (evaluated in \mathcal{A}) of one of the physical operators was no longer a physical operator itself. Thus, we were unable to induce on \mathcal{A}_{phy} the structure of a \star -algebra. This appeared to be an impasse, in terms of constructing the physical inner product *à la* the prescription of the algebraic approach.

In desperation, 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 forced us to rule out the tunnelling solutions. The Hermiticity condition on one of the observables leads to the conclusion that *all solutions* to the constraint equation *cannot* be considered as *physical states*. Finally, the algebra of operators on the “smaller” space of physical states –which does not include the tunnelling solutions– *does* admit a \star -involution. Hence we were able to complete the quantization program.

Now, let us consider the Hamiltonian (1.2) in quantum theory. It is manifestly positive. On physical states the Hamiltonian operator is $\widehat{H} \circ \psi = E(\phi) \cdot \psi$. Since the states have (measurable) support only in \mathcal{C} , where $E(\phi) \geq 0$, $\langle \widehat{H} \rangle \geq 0$ for all physical states. As promised, a careful re-analysis of the problem has removed the peculiarities that were present in the previous quantization. While the final result seems somewhat disappointing (there are no extreme tunnelling states in the classically forbidden region, and the positivity theorem is not violated in quantum theory), this problem clearly demonstrates the power of the quantization program of chapter 2. While in retrospect our final result could have been obtained by a number of other quantization procedures, in other schemes the elimination of the spurious tunnelling states would almost certainly be 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 [3] proposes 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 much more general hypothesis: namely that real physical operators should be Hermitian in the physical inner product.

In another re-analysis of this model, Bouliware [4] assumes the usual Euclidean inner product on the representation space, and requires that p_θ be a Hermitian operator on the space of *all* $L^2(S^2)$ states⁴, *before* solving the constraint equation and isolating the physical states. Then, physical states have support only on the classically allowed region,

⁴ r and p_r can be safely ignored in this model, since they “just go along for the ride”. Thus the initial configuration space is S^2 .

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. A symmetric extension of \hat{p}_θ was chosen by defining its domain to consist of states which satisfy the following condition:

$$\left. \frac{\partial}{\partial \theta} \Psi(\theta, \phi) \right|_{\theta=0, \pi} = 0.$$

That is, the θ -derivative, of states in the domain of \hat{p}_θ , vanishes on the z -axis. \hat{p}_θ so-defined, clearly has discrete (integer) eigenvalues. Let us return to the constraint equation (1.1,2.2), $(\hat{p}_\theta^2 - R(\phi)) \circ \Psi = 0$. Due to the discrete spectrum of \hat{p}_θ , the support of physical states is further restricted to those regions where $R(\phi)$ is the square of an integer! However, these physical states, which have support only on a discrete set of longitudes on S^2 , are *not normalizable* with respect to the implicit measure on S^2 . Hence, this quantum theory is incomplete; a new inner product has to be introduced. Furthermore, since the θ dependence of the physical states is determined by the constraint, these states are labelled by functions of a *discrete set of points on S^1* (where $R(\phi) = n^2$) and, for generic choices of $R(\phi)$, the resulting Hilbert space is *finite dimensional*! However, as we will see, the reduced phase space is a perfectly well-defined co-tangent bundle over S^1 . Thus the above quantum theory does not appear to capture all the physics in the model.

In the quantum theory we constructed here, since p_θ is an observable (as much as ϕ is) we too required it to be Hermitian, *but only on physical states*. In the context of the algebraic approach, the most important facet of the Hermiticity of p_θ is the following: as we saw in (2.9), unless we impose the Hermiticity of p_θ , the rest of the formulation is *not mathematically well-defined*.

I will now address the question: "How well-defined is the constraint operator (2.2) in the representation (2.1)?" First of all, in ordinary quantum mechanics, there is an inner product available to make the "elementary" operators like (2.1) symmetric and to define their domains. However, in the quantum theory of a constrained system, we are eventually interested only in the physical operators. In general the elementary operators do not correspond to physical observables, and we may be able to ignore or postpone the issue of whether or not they are well-defined. At the very least though, to find physical states, we need a reasonably well-defined constraint operator, which –as is usually the case– may be quadratic in momenta and thus may pose even more difficulties. Recall that there are considerable ambiguities in constructing operators quadratic in momenta. Again, in ordinary quantum mechanics, one is able to eliminate these ambiguities, to a large degree, by using the inner product to define symmetric extensions or to specify the domains of the operators. However, in the quantum theory of a constrained system, one does not have an inner product on the representation space \mathcal{V} . One has considerable freedom, though, to define \mathcal{V} , and the operators thereon. Hence, one has to make choices, based on physical intuition for the system. Now one can proceed as follows: define a representation of the operators on a certain vector space, and if necessary enlarge the representation space to include the range of these operators. As far as the constraint operator is concerned, we are finally interested only in its kernel, and as long as this is large enough, the enlargement of \mathcal{V} is immaterial. As far as other physical operators

are concerned, since we are finally interested only in their actions on physical states, we need not define them too precisely until after the constraint has been solved.

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 A-H model in the following way: In the early part of section 2, I exploited the freedom to define the representation space and the operators, and was 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 Hermiticity conditions on these and found appropriate self-adjoint extensions of the physical observables.

The only remaining thing is to check the subsidiary result, whether Dirac quantization and reduced space quantization indeed yield inequivalent answers.

4.3 (†) Reduced space quantization

Recall from section 2.5 that in reduced space quantization, one solves the constraint classically and finds the reduced phase space $\hat{\Gamma}$, and then quantizes the resulting system, free of constraints. There are two steps involved in constructing the reduced phase space. First one has to find, i.e. construct an explicit parametrization of, the constraint surface $\bar{\Gamma}$. Then, one has to factor out $\bar{\Gamma}$ by the gauge orbits generated by the constraint. The space of orbits on the constraint surface is the reduced phase space. Let us use this approach to quantize the above model.

As has been mentioned before, the projection of the constraint surface to the configuration space is a proper subset of the configuration space. The constraint (1.1) can only be solved in the classically allowed regions where the “potential” $R(\phi)$ is positive. Let us focus on one such region. In this region, the constraint $C = p_\theta^2 - R(\phi) = 0$ can be solved for p_θ in terms of ϕ ,

$$p_\theta^\pm = \pm\sqrt{R(\phi)} \quad (3.1)$$

while the other phase space coordinates r, p_r, θ, p_ϕ are free. $\bar{\Gamma}$ appears to have two “sectors”, $\bar{\Gamma}_\pm$, corresponding to the choice of sign in (3.1). However, these two sectors are obviously connected at the points (denoted by ϕ_0) where $R(\phi) = 0$. The question then is whether or not the two halves of the constraint surface are *smoothly* joined at ϕ_0 . To answer this question, let us consider the intersection of the constraint surface with a (p_θ, ϕ) plane, and compare the slopes of the two halves of the constraint surface at ϕ_0 . We see that $(\partial p_\theta / \partial \phi)|_{\bar{\Gamma}_\pm} = (\sqrt{R})' = \pm R' / 2\sqrt{R}$. At ϕ_0 , both slopes are infinite. Since the $R > 0$ region is obviously bounded on both sides by ϕ_0 , and the two halves are ‘smoothly’ (at least C^1) joined there, there is in fact just one constraint surface. Thus, the topology of the constraint surface is non-trivial, it contains one S^1 component⁵ (see

⁵I am assuming that ϕ_0 is not a critical point, i.e. $R'(\phi_0) \neq 0$. If ϕ_0 is a first order critical point,

Figure 4.1: A-H model: Constraint surface

Fig.4.1). Clearly, this is a wholly different picture from the one we obtained in Dirac quantization.

Now let us analyse the gauge orbits. The Hamiltonian vector field of the constraint is

$$X_C = 2p_\theta \left(\frac{\partial}{\partial \theta} \right) + R' \left(\frac{\partial}{\partial p_\phi} \right). \quad (3.2)$$

Let t be an affine parameter along the Hamiltonian vector field. It is easy enough to find the gauge orbits, since r, p_r, p_θ, ϕ are constant. The orbits are then given by

$$\theta = 2p_\theta t + \Theta \quad (3.3)$$

$$p_\phi = R' t + P_\phi. \quad (3.4)$$

The orbits start on the positive z -axis and follow the lobes of the constraint surface down to the negative z -axis. Since the Hamiltonian vector field has no components in the p_θ or ϕ directions, it does not close on itself around the S^1 component of $\bar{\Gamma}$. Thus the reduced phase space (the space of orbits) also has nontrivial topology, with one S^1 component. (In fact, as we will see later, $\hat{\Gamma} = T^*(S^1 \times \mathbb{R}_+)$.) Our objective now is to find reduced space coordinates which make this structure manifest. In the absence of a specific form for $R(\phi)$, this is difficult to do. Let us then do the next best thing, which is to split $\bar{\Gamma}$ into the two “halves” $\bar{\Gamma}_\pm$, and concentrate henceforth on $\bar{\Gamma}_+$.

On the constraint surface $\bar{\Gamma}_+$, one can specify an orbit by the initial values of the *five* independent functions $r, p_r, \phi, p_\phi, \theta$. (The initial value of $p_\theta = +\sqrt{R(\phi)}$ is determined by that of ϕ .) However, the space of orbits is only four dimensional. Thus, of the five constants of motion corresponding to the initial values of the independent functions on

$R' = 0, R'' \neq 0$, the analysis becomes much more complicated. The constraint surface is no longer a (Hausdorff) manifold. In fact the corresponding cross-section is a “figure-eight”; or worse if ϕ_0 is a higher order critical point.

Figure 4.2: A-H model: Constraint surface and Hamiltonian vector field of P_ϕ^+ in $p_\theta - \phi$ space

$\bar{\Gamma}$, we have to choose the classical Dirac observables, i.e. four of these five constants which will coordinatize the reduced phase space. The function whose initial value is not included in the $\hat{\Gamma}$ coordinates will play the role of a parameter along the orbit, and should thus ideally be monotonic in the affine parameter t . For this model we have only two choices, θ or p_ϕ . Since the constraint is solved for p_θ , a natural choice would be to consider θ as an affine parameter and use (r, p_r, ϕ, P_ϕ) as the coordinates on (a half of) $\hat{\Gamma}$. Since in fact θ is monotonic in t almost everywhere on $\bar{\Gamma}$ (the exception is at the points ϕ_0), this is a reasonable choice. The value of the fifth constant of motion Θ then serves to fix the $t = 0$ cross-section of the gauge orbits. Setting $\Theta = 0$, we can solve the orbit equation (3.3) for t in terms of θ , $t = \theta/2p_\theta$. Substituting this expression in (3.4), we can solve for the only non-trivial Dirac observable,

$$P_\phi^+ = p_\phi - \frac{R'\theta}{2\sqrt{R}}. \quad (3.5)$$

(Now, I can explain classically why –in the Dirac approach– \hat{P}_ϕ^* is not an observable. Recall that physical observables are functions on $\bar{\Gamma}$ whose Hamiltonian vector fields are tangential to the constraint surface. Consider the Hamiltonian vector field of P_ϕ^+ :

$$X_{P_\phi^+} = \frac{\partial}{\partial \phi} + (\sqrt{R})' \frac{\partial}{\partial p_\theta} + (\sqrt{R})'' \theta \frac{\partial}{\partial p_\phi}, \quad (3.6)$$

and let us focus on its projection to the $p_\theta - \phi$ space (see Fig.4.2.) Note that in the $R > 0$ region, $X_{P_\phi^+}$ is real, and hence its complex conjugate is also tangential to $\bar{\Gamma}$. However, in the forbidden region $R < 0$, $X_{P_\phi^+}$ is *complex*, and as we can see from Fig.2, its complex conjugate is *not* tangential to $\bar{\Gamma}$. Hence, the corresponding generating function, and the operator \hat{P}_ϕ^* , are not observables.)

The reduced phase space $\hat{\Gamma}_+$ is coordinatized by (r, p_r, ϕ, P_ϕ^+) . The symplectic structure (or equivalently, the Poisson brackets) can be easily calculated, and we find that p_r, P_ϕ^+ are the momenta canonically conjugate to r, ϕ respectively.

Since the Dirac observables (both classical and quantum) are at most linear in momenta, there is no factor ordering ambiguity, and the reduced space quantum theory in the above coordinatization of $\hat{\Gamma}$ will be equivalent to the Dirac quantum theory. In the obvious configuration representation the states are represented by $k_\pm = k_\pm(r, \phi)$. Let us label the two sectors by \mathcal{V}_\pm respectively. On each sector the operators corresponding to the reduced space coordinates can be represented by

$$\hat{r} \circ k_\pm = r k_\pm, \quad \hat{\phi} \circ k_\pm = \phi k_\pm; \quad (3.7)$$

$$\hat{p}_r \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial r} k_\pm, \quad \hat{P}_\phi \circ k_\pm = \frac{\hbar}{i} \frac{\partial}{\partial \phi} k_\pm. \quad (3.8)$$

Note that the algebra of observables and the representation is equivalent to the quantum Dirac operator algebra (2.18).

Note that in the reduced space theory, there is no question of any cross terms (in the inner product) between the two sectors \mathcal{V}_\pm : the states simply live on different spaces. Thus, in the reduced space theory, \mathcal{V}_+ and \mathcal{V}_- are naturally mutually orthogonal. On the other hand, it is the symmetry I_z , which was so natural in the Dirac theory, that is “hidden” here. It shows up as the natural map between $\hat{\Gamma}_+$ and $\hat{\Gamma}_-$. The spaces \mathcal{V}_\pm each carry irreducible representations of the algebra of functions on one half of the reduced phase space, and the relative scale factor between the terms in the inner product is fixed by requiring that I_z is Hermitian. A brief calculation shows that the inner product is exactly that given by (2.27).

However, as I indicated above, this is an incomplete way to carry out reduced space quantization of this model. On each half of the constraint surface $\bar{\Gamma}_\pm$, the Hamiltonian vector field of the classical Dirac observable of P_ϕ is given respectively by

$$X_{P_\phi} = \frac{\partial}{\partial \phi} \pm \frac{R'}{2\sqrt{R}} \frac{\partial}{\partial p_\theta} + (\sqrt{R})'' \theta \frac{\partial}{\partial p_\phi}. \quad (3.9)$$

Its projection to the $\phi - p_\theta$ plane is then simply

$$X_{P_\phi} = \frac{\partial}{\partial \phi} \pm \frac{R'}{2\sqrt{R}} \frac{\partial}{\partial p_\theta}. \quad (3.10)$$

To see the incompleteness, consider the following quantization of a particle whose configuration space is the unit S^1 in the $x - y$ plane. (In terms of the variables we are using, the analogy is $\phi \leftrightarrow x, p_\theta \leftrightarrow y$.) Now, the analogous quantization of the particle on S^1 would be the following: First split S^1 into the top and bottom halves ($x > 0, x < 0$); and use in each half, x as the configuration variable and $\frac{\partial}{\partial x} \pm \frac{x}{y} \frac{\partial}{\partial y}$ as the vector field defining the momentum in each half (in analogy with the Hamiltonian vector field (3.10) of the observable P_ϕ). The correct matching boundary conditions at $x = \pm 1$ are difficult, if not impossible to state in terms of this chosen momentum. Even if one used the angular coordinate in the $x - y$ plane, and its conjugate momentum, a naive quantization would yield a spectrum for the momentum operator consisting of only the even eigenvalues;

because of the two sectors, this spectrum would also be doubly degenerate. However, as we well know, the spectrum for the angular momentum consists of all the integers, and is nondegenerate.

For definiteness, consider a model where, in a neighbourhood of the constraint surface, the “potential” is given by $R(\phi) = a^2 - (\phi - \pi)^2$, and $a < \pi$. (The specific form of $R(\phi)$, as long as it is smooth, will not change any of the topological considerations.) On the (p_θ, ϕ) cylinder, the projection of the constraint surface is a circle. In a neighbourhood of the constraint surface, introduce angular and radial coordinates

$$\rho = \sqrt{p_\theta^2 + (\phi - \pi)^2} \quad (3.11)$$

$$\alpha = \tan^{-1}(p_\theta/(\phi - \pi)) \quad (3.12)$$

and their corresponding conjugate momenta,

$$p_\rho = (-\theta p_\theta + (\phi - \pi)p_\phi)/\rho \quad (3.13)$$

$$p_\alpha = -\theta(\phi - \pi) - p_\theta p_\phi. \quad (3.14)$$

Then the constraint surface is specified by $\rho - a = 0$ and the Hamiltonian vector field of the constraint is $X_C = -(\partial/\partial p_\rho)$. The classical Dirac observables are r, p_r, α, p_α , and thus the reduced phase space is a cotangent bundle, over the configuration space $S^1 \times \mathbb{R}^+$. In the quantum theory, the eigenvalues of p_α are integer multiples of \hbar .

In the Dirac quantum theory, even if one is lucky enough to find the operators in the above form, or if one simply *uses* the above classical functions to motivate the corresponding operators, it is clear from the expressions (3.11-3.14) that in the representation of section 2 a good factor ordering would be extremely difficult to construct. In fact, the simplest or the only consistent representation and factor ordering may well be the one from the reduced quantum theory.

In conclusion, while the Dirac and reduced space quantum theories for this model are “locally” equivalent, in the sense that they are unitarily equivalent representations of the continuous physical operators, subtle differences arise due to the nature of the discrete symmetries. In addition, there are gross differences between the two since the topology of the reduced phase space is nontrivial.

Bibliography

- [1] Ashtekar A and Horowitz G T 1982 *Phys. Rev.* **D26** 3342-53
- [2] Louko J 1992 *private communication* Syracuse
- [3] Gotay M J 1986 *Class. Quantum Grav.* **3** 487-91
- [4] Boulware D G 1983 *Phys. Rev.* **D28** 414-16

Chapter 5

COUPLED OSCILLATORS: CONSTRAINED ENERGY DIFFERENCE

5.1 Introduction

In this chapter I will consider the system consisting of two harmonic oscillators with the same frequency, set to 1 for simplicity. In the main portion of this chapter (sections 2 to 5) I will consider the model in which the two oscillators are coupled to each other via a first class constraint on the energy difference. This model mimics some of the 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 is of indefinite sign. Due to these similarities, some of the results of the quantization of this model are of qualitative interest in quantum gravity or quantum cosmology.

As a matter of fact, this model arises when one conformally couples a massless scalar field to the Friedman-Robertson-Walker universe with S^3 spatial topology (section 4). Though for this cosmological model the energy difference –of the two “effective” oscillators– is fixed to be zero, we will consider generic (and possibly more interesting) models in which the constrained energy difference is *any* real number.

The phase space of the system is described by position and momentum coordinates $(x_I, p_I, I = 1, 2)$ and the first class constraint is

$$\frac{1}{4}(p_1^2 + x_1^2 - p_2^2 - x_2^2) = \delta, \quad (1.1)$$

where δ can be viewed as the (real) difference in energies of the two oscillators. This model has a number of interesting features:

1. This model is an example in which it is important to impose the Hermiticity conditions only on physical states. (The A-H model of the previous chapter is another such example.) If one imposes the Hermiticity conditions on the elementary operators, prior to solving the quantum constraint, then generically one does not obtain *any* physical states (see section 2).

2. Unlike in the constrained systems we have considered so far, the reduced phase space for this model is *not* a cotangent bundle. Another novel feature is that the algebra of observables is *overcomplete*, inspite of the trivial topology of the reduced phase space; 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,
3. In most of the models considered so far, \mathcal{A}_{phy} has comprised of operators which correspond to generators of *continuous* canonical transformations on the constraint surface. In this model, as in the A-H model, there is in addition a *discrete* classical symmetry of the constraint (call it “parity”), which maps entire gauge orbits to entire gauge orbits. A quantum operator corresponding to this symmetry must be included in the algebra of observables, inspite of the fact that the set of continuous physical observables is *locally* complete. The parity operator plays a role in obtaining an inner product on the physical states.
4. One can introduce a first class Hamiltonian which satisfies a classical positive energy theorem. In the canonical quantum theory (section 2), there exist representations of the physical operator algebra in which the above Hamiltonian acquires negative energy eigenvalues (section 3). However, going beyond the quantization program and using additional physical conditions, on semi-classical grounds one can rule out most –but not all– of these representations.
5. Classically, the parity transformation discussed above squares to unity. Also, in classical theory we can impose any real value for the energy difference δ . These two conditions are incompatible in the Dirac quantum theory (see section 3).
6. In section 4 I will construct the reduced space quantum theory. As we will then see, the two quantum theories are even *kinematically* inequivalent. This inequivalence arises from the specific form of the algebraic condition that the observables in the two theories satisfy.

In section 7, for the sake of completeness, I will quantize a related model, in which the sum of the energies is imposed as a constraint.

5.2 Dirac quantization

Choose as the set \mathcal{S} of elementary classical variables the standard ‘creation’ and ‘annihilation’ functions on Γ

$$z_I = \frac{1}{\sqrt{2}}(x_I - ip_I) \quad \text{and} \quad \bar{z}_I = \frac{1}{\sqrt{2}}(x_I + ip_I), \quad (2.1)$$

as well as the constant function. There are no ACRs on the elementary operators. In these variables, the constraint function is

$$C = \frac{1}{2}(z_1 \bar{z}_1 - z_2 \bar{z}_2) - \delta. \quad (2.2)$$

The quantum \star -algebra $\mathcal{A}^{(\star)}$ is straight forward 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 . $\mathcal{A}^{(\star)}$ is then generated by the set of elementary quantum operators $(1, \hat{a}_1, \hat{c}_1, \hat{a}_2, \hat{c}_2)$ satisfying the canonical commutation relations:

$$[\hat{a}_I, \hat{a}_J] = 0 = [\hat{c}_I, \hat{c}_J] \quad \text{and} \quad [\hat{a}_I, \hat{c}_J] = \delta_{IJ}, \quad I, J = 1, 2; \quad (2.3)$$

and subject to the \star -relation

$$\hat{a}_I^\star = \hat{c}_I. \quad (2.4)$$

In terms of these operators, the quantum constraint we wish to impose is

$$\hat{C}|\psi\rangle_{phy} := \left[\frac{1}{2}(\hat{c}_1\hat{a}_1 - \hat{c}_2\hat{a}_2) - \delta \right] |\psi\rangle_{phy} = 0, \quad (2.5)$$

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

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 \star -relations are ignored at this stage. Indeed, had we imposed them, i.e., had we introduced a \star -representation of $\mathcal{A}^{(\star)}$ by operators on a Hilbert space, we would have run into the following difficulty: The number operators $\hat{N}_1 := \hat{c}_1\hat{a}_1$ and $\hat{N}_2 := \hat{c}_2\hat{a}_2$ would have taken on only integral values, and if δ were *not* an integer or half-integer, the only state in the kernel of the constraint operator would have been the zero state. Thus, we would have been led to the conclusion that \mathcal{V}_{phy} is zero dimensional. This quantum theory is clearly incomplete, 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 \star -relations until after the physical states are isolated is *essential* in this example to obtain an acceptable quantum theory.

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 as V the complex vector space spanned by states of the form $|j, m\rangle$, where (to begin with) j and m are any *complex* numbers, and represent the elementary quantum operators as follows:

$$\begin{aligned} \hat{a}_1|j, m\rangle &= \alpha_1(j+m)|j - \frac{1}{2}, m - \frac{1}{2}\rangle, \\ \hat{c}_1|j, m\rangle &= \gamma_1(j+m+1)|j + \frac{1}{2}, m + \frac{1}{2}\rangle, \\ \hat{a}_2|j, m\rangle &= \alpha_2(m-j)|j + \frac{1}{2}, m - \frac{1}{2}\rangle \\ \text{and } \hat{c}_2|j, m\rangle &= \gamma_2(m-j+1)|j - \frac{1}{2}, m + \frac{1}{2}\rangle; \end{aligned} \quad (2.6)$$

where the coefficients, $\alpha_I(k)$ and $\gamma_I(k)$, functions only of their argument k , are subject to the conditions

$$\alpha_1(k)\gamma_1(k) = k \quad \text{and} \quad \alpha_2(k)\gamma_2(k) = k \quad (2.7)$$

It is straightforward to check that the commutation relations (2.3) are satisfied by this choice of representation. The notation $|j, m\rangle$ to represent the kets may seem strange at

first. Note, however, that $\hat{N}_1|j, m\rangle = (m+j)|j, m\rangle$ and $\hat{N}_2|j, m\rangle = (m-j)|j, m\rangle$. 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 $2m$, as well as of the constraint operator \hat{C} with eigenvalue $j - \delta$. (Thus, had we represented states as Bargmann type wave functions, we would have $\psi(z_1, z_2) := \langle z_1, z_2 | j, m \rangle \equiv z_1^{m+j} z_2^{m-j}$.) These angular momentum like states arise naturally because the constraint surface $\bar{\Gamma}$ is the group manifold of $SO(2, 1)$ and the Poisson bracket algebra of physical observables is the Lie algebra of $SO(2, 1)$ (see section 5). This is the reason I chose the angular momentum like $|j, m\rangle$ representation instead of the perhaps more familiar $|n_1, n_2\rangle$ representation.

Since \hat{C} is diagonal in this representation, with eigenvalues $j - \delta$, the quantum constraint is easy to solve. A basis for the *physical* subspace \mathcal{V}_{phy} is given simply by the kets $\{|\delta, m\rangle\}$. Physical operators are the elements of \mathcal{A} that map \mathcal{V}_{phy} 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 $\{1, \hat{J}_+, \hat{J}_-, \hat{J}_z\}$; 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 non-vanishing commutation relations between these operators are

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm \quad \text{and} \quad [\hat{J}_+, \hat{J}_-] = -2\hat{J}_z, \quad (2.8)$$

from which it is clear that they generate the Lie algebra of $SO(2, 1)$. \hat{J}_+ and \hat{J}_- are the (angular momentum) raising and lowering operators, respectively. Note further that it is in order to obtain the $SO(2, 1)$ commutation relations in (2.8) that I have chosen the definition $\hat{J}_z := \frac{1}{2}(\hat{N} + 1)$, as opposed to $\hat{J}_z = \frac{1}{2}\hat{N}$.

The classical analogs of $\{\hat{J}_z, \hat{J}_\pm\}$ are the functions

$$J_z = \frac{1}{2}(z_1\bar{z}_1 + z_2\bar{z}_2), \quad J_+ = z_1z_2, \quad J_- = \bar{z}_1\bar{z}_2 \quad (2.9)$$

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 $SO(2, 1)$.) One can easily check, using (2.4.5), that the set (J_+, J_-) is by itself *complete*, the set coordinatizes the reduced phase space. It is in order to ensure that the algebra of observables is *closed* that one has to include J_z in the set of generators of \mathcal{A}_{phy} , and thus make it *overcomplete*. As in some of the previous examples, the algebraic relation satisfied by this overcomplete set fixes a value of the Casimir invariant of \mathcal{A}_{phy} :

$$\hat{J}^2 := -\hat{J}_z^2 + \frac{1}{2}[\hat{J}_+, \hat{J}_-]_+ . \quad (2.10)$$

Using the definitions of \hat{J}_\pm and the commutation relations (2.3), one finds that

$$[\hat{J}_+, \hat{J}_-]_+ = \hat{1} + \hat{N}_1 + \hat{N}_2 + 2\hat{N}_1\hat{N}_2 . \quad (2.11)$$

Thus, $\hat{J}^2 = \frac{1}{4}[1 - (\hat{N}_1 - \hat{N}_2)^2]$. On physical states, therefore,

$$\hat{J}^2 = \frac{1}{4} - \delta^2. \quad (2.12)$$

Equivalently, the algebraic identity can be expressed as

$$\hat{J}_+ \hat{J}_- = (\hat{J}_z - \frac{1}{2})^2 - \delta^2, \quad (3.12')$$

which is a useful form for future calculations.

The \star -relation induced on \mathcal{A}_{phy} is given by:

$$\hat{J}_+^* = \hat{J}_- \quad \text{and} \quad \hat{J}_z^* = \hat{J}_z. \quad (2.13)$$

Using (2.6,2.7), we can evaluate the action of the physical operators on the physical states. Doing so, we get

$$\begin{aligned} \hat{J}_z |\delta, m\rangle &= (m + \frac{1}{2}) |\delta, m\rangle, \\ \hat{J}_+ |\delta, m\rangle &= \lambda_+(m+1) |\delta, m+1\rangle \\ \text{and } \hat{J}_- |\delta, m\rangle &= \lambda_-(m) |\delta, m-1\rangle, \end{aligned} \quad (2.14)$$

where λ_{\pm} are functions of their arguments only. The algebraic identity (2.12') is satisfied if and only if

$$\lambda_+(m)\lambda_-(m) = m^2 - \delta^2. \quad (2.15)$$

With this condition, the CCRs are also identically satisfied. Note that λ_{\pm} are just combinations of the coefficients α_I, γ_I in (2.6), so if one uses (2.7), (2.15) is trivially satisfied. However, as we will see, it is simpler to work with the λ_{\pm} . This notation is suggestive and also useful later for comparison to the reduced space quantization and the related model in section 6.

The last step in the program is to select an inner product by requiring that the \star -relations (2.13) become Hermitian adjointness relations on the resulting Hilbert space. The Hermiticity condition on \hat{J}_z requires that its eigenvalues m must be real, and its eigenkets orthogonal to each other. Before we proceed any further, let us recall from representation theory that the Hermiticity conditions should be implemented only on *ir-reducible* representations of the algebra. The representation (2.14), however, is reducible: Note that 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 the \hat{J}_z, \hat{J}_{\pm} . Consider $\mathcal{V}_{phy}^{\epsilon}$, the vector space of states with the same fixed value of ϵ . Each $\mathcal{V}_{phy}^{\epsilon}$ carries an irreducible representation of the $SO(2,1)$ Lie algebra (2.8).

Naturally, one is lead to ask whether there is some “hidden” symmetry in this problem, and whether the eigenvalues of the corresponding operator label the irreducible sectors $\mathcal{V}_{phy}^{\epsilon}$. In the classical theory, one notices that the function (2.2) $\frac{1}{2}(z_1 \bar{z}_1 - z_2 \bar{z}_2) - \delta$ corresponding to the constraint and the functions (2.9) $\{1, \frac{1}{2}(z_1 \bar{z}_1 + z_2 \bar{z}_2), z_1 z_2, \bar{z}_1 \bar{z}_2\}$ corresponding to the set of observables, are all invariant under the *parity* map $(z_I) \mapsto \mathbf{P}(z_I) := (-z_I)$. In quantum theory, this discrete symmetry should correspond to a *super-selected* physical operator, i.e. one which commutes with all other operators in \mathcal{A}_{phy} . In spite of the fact that the functions (2.9) are a locally (over)complete set on $\bar{\Gamma}$, the set of operators $\{1, \hat{J}_z, \hat{J}_{\pm}\}$ does *not* generate the full physical algebra; \mathcal{A}_{phy} is in fact generated by the set $\{1, \hat{J}_z, \hat{J}_{\pm}, \hat{\mathbf{P}}\}$. In the representation we have chosen, from

the action of the operators \hat{J}_z, \hat{J}_\pm (2.14), it is clear that on physical states the Parity operator must be diagonal, and its eigenvalues must depend only on ϵ . From the Bargmann-type representation, in which this discrete symmetry corresponds to the operation $\psi(z_I) \mapsto \psi(-z_I)$, we see that in the $|j, m\rangle$ representation (2.6) the action of the parity operator is given by

$$|j, m\rangle \mapsto \hat{\mathbf{P}}|j, m\rangle := (-1)^{2m}|j, m\rangle, \quad (2.16)$$

where, to evaluate the right hand side we will take the principal value, namely, $(-1)^{2m} = \exp(i2\pi\epsilon)$, and as before $\epsilon = \text{frac}(m)$ is the fractional part of m .

Let us now return to the question of the reducibility of the representation on \mathcal{V}_{phy} . Let $m = n + \epsilon$, $n = \dots - 2, -1, 0, 1, 2 \dots$. Recall that the physical operators change m in integral steps only and do not affect the fractional part ϵ . Consequently, \mathcal{V}_{phy} is reducible, and each eigenspace $\mathcal{V}_{phy}^\epsilon$ of the parity operator provides an irreducible representation of the algebra \mathcal{A}_{phy} . Each $\mathcal{V}_{phy}^\epsilon$ has a countable basis, labelled by n , the integer part of m , and it is on these irreducible representations that one implements the Hermiticity conditions on \mathcal{A}_{phy} . 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, consider a representation with a fixed value of ϵ . The Hermiticity of \hat{J}_z implies that on $\mathcal{V}_{phy}^\epsilon$ 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:

$$\langle \delta, m' = n' + \epsilon | \delta, m = n + \epsilon \rangle = \delta_{n', n}, \quad (2.17)$$

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 δ inner product on $\mathcal{V}_{phy}^\epsilon$ as opposed to a Dirac δ on \mathcal{V}_{phy} .

Now, the first of the \star -relations (2.13) implies that $\lambda_+(m) = \overline{\lambda_-(m)}$. Substituting this in (2.15), the condition on the undetermined coefficients, yields

$$|\lambda_+(m)|^2 = m^2 - \delta^2. \quad (2.18)$$

For solutions to exist, we require that physical states satisfy

$$m^2 \geq \delta^2. \quad (2.19)$$

Without loss of generality, we can choose the phase of $\lambda_+(m)$ to be zero, and solve (2.18). Then we have

$$\begin{aligned} \hat{J}_z |\delta, m\rangle &= (m + \frac{1}{2}) |\delta, m\rangle, \\ \hat{J}_+ |\delta, m\rangle &= \sqrt{(m+1)^2 - \delta^2} |\delta, m+1\rangle \\ \text{and } \hat{J}_- |\delta, m\rangle &= \sqrt{m^2 - \delta^2} |\delta, m-1\rangle. \end{aligned} \quad (2.20)$$

Under what conditions do states with $m^2 \geq \delta^2$ form an invariant subspace? Consider for example a state satisfying (2.19) with arbitrary $m \geq |\delta|$. Using \hat{J}_- repeatedly, one can

lower m until condition (2.19) is violated, unless there exists a state $|\delta, m_0\rangle$ annihilated by \hat{J}_- . From (2.20), we see that this will occur iff $m_0 = \pm|\delta|$. Acting with \hat{J}_+ repeatedly on the “ground” state $m_0 = +|\delta|$, we see that an allowed representation consists of states labelled by

$$m = |\delta| + n, \quad n = 0, 1, 2, \dots \quad (2.21)$$

This corresponds to a representation with a fixed eigenvalue of $\hat{\mathbf{P}}$, $\epsilon = \text{frac}(|\delta|)$.

Similarly, starting with arbitrary $m \leq |\delta|$ one can use \hat{J}_+ repeatedly to raise m until (2.19) is violated, unless there exists a “top” state, $m_0 = \pm\delta - 1$ annihilated by \hat{J}_+ . Thus, one obtains the inequivalent representation

$$m = -|\delta| - 1 - n, \quad n = 0, 1, 2, \dots, \quad (2.22)$$

with $\epsilon = 1 - \text{frac}(|\delta|)$. Thus for each value of δ one obtains the two representations (2.21, 2.22).

If $0 < |\delta| < \frac{1}{2}$ we have the additional representations

$$m = -|\delta| + n, \quad n = 0, 1, 2, \dots \quad 0 < |\delta| < \frac{1}{2}, \quad (2.23)$$

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

$$m = |\delta| - 1 - n, \quad n = 0, 1, 2, \dots \quad 0 < |\delta| < \frac{1}{2}, \quad (2.24)$$

with $\epsilon = \text{frac}(|\delta|)$. In fact, as Louko pointed out [1], for $|\delta| \in [0, \frac{1}{2})$, the above representations are only special cases. There is a whole slew of representations, one for each $\epsilon \in [|\delta|, \frac{1}{2})$ or $\epsilon \in (-\frac{1}{2}, -|\delta|]$. However, not that in all but the representation (2.23), which corresponds to $\epsilon = |\delta|$, m is unbounded below.

Note that the coefficients α_I, γ_I in (2.6) are left undetermined, and we have *not* obtained an inner product on the original representation space. However, (2.17) provides us with an inner product on \mathcal{V}_{phy} . Unexpectedly, we have two representations of the physical observable algebra, labelled by the eigenvalue of $\hat{\mathbf{P}}$.

This completes the quantization of the coupled oscillator, and I would like to discuss a number of interesting features.

5.3 Classical expectations and quantum theory

Remark 1: Positivity of energy

In the classical theory, the function $H(x_I, p_I) := \frac{1}{2}(x_1^2 + p_1^2 + x_2^2 + p_2^2)$, corresponding to $\hat{H} = 2\hat{J}_z^1$, is non-negative, i.e. $H \geq 0$. In the quantum theory however, we have obtained representations (2.22, 2.24) of \mathcal{A}_{phy} in which the corresponding operator \hat{H} is *unbounded below* (its eigenvalues are $\pm 2|\delta| - 2n - 1$, $n = 0, 1, 2, \dots$). Since \hat{H} is an *elementary physical observable*, it is not of the form $\hat{O}^*\hat{O}$ for any $\hat{O} \in \mathcal{A}_{phy}$, and we cannot impose positivity. Thus mathematically, one is stuck with the above representation.

¹In the case of two oscillators this corresponds to the total energy, and thus I will henceforth refer to $2\hat{J}_z$ as the Hamiltonian, though it may have nothing to do with dynamics.

However, in the representations corresponding to (2.22) and (2.24), there are *no* states with positive energy eigenvalues. Therefore, on *physical* grounds, in order to obtain a good classical limit of the theory, one may have to rule out the representations corresponding to $m < 0$. One cannot use the above argument to rule out a representation in which the Hamiltonian, though non-positive, is bounded below. For such a case, one could construct semi-classical states with the right behaviour. This occurs for the representations (2.23), in which there is only one negative-energy eigenstate.

Remark 2: Implications for quantum gravity?

Let us return to the general case. Quantum mechanically, as we have seen, for any value of δ there exist representations in which the Hamiltonian operator $\hat{H} = \hbar(\hat{c}_1\hat{a}_1 + \hat{c}_2\hat{a}_2 + 1)$ is *unbounded from below*! It thus appears that in the presence of non-trivial constraints, extreme quantum tunneling can occur in which “half” the (reducible) physical Hilbert space corresponds to states that are classically forbidden. In addition, when δ is less than half, we are allowed the representations (2.23) in which the energy has one negative eigenvalue, but is *bounded* below. In the context of quantum geometrodynamics it is extremely important to find out if the scalar constraint of non-perturbative canonical gravity allows such a phenomenon to occur. If it does, should one rule out the negative energy states on classical grounds, or will there in fact be some physical interpretation for them?

Remark 3: Inner product on \mathcal{V}

Suppose we restrict ourselves to positive energies, and fix for definiteness, the representation (2.21). Note that the total energy of the system ($2n + 2|\delta| + 1$) is allowed to be *any* positive real value, bounded below by $2|\delta| + 1$. This is a somewhat surprising result in light of the quantization we would have obtained had we chosen to implement the \star -relations on the entire quantum algebra \mathcal{A} . In that case the energies of each individual oscillator, $H_I = N_I + \frac{1}{2}$, which are physical observables, would have been positive half integers only, and the total energy a positive *integer*. Here on the other hand, from the definitions of the number operators we have:

$$\begin{aligned} \hat{N}_U|\delta, m\rangle &= (m + |\delta|) \cdot |\delta, m\rangle = (2|\delta| + n)|\delta, m\rangle \\ \text{and } \hat{N}_L|\delta, m\rangle &= (m - |\delta|) \cdot |\delta, m\rangle = n|\delta, m\rangle, \end{aligned} \quad (3.1)$$

where we have used (2.21), and U and L refer to the oscillators in the “upper” and “lower” states respectively. One can see that only the energy of the oscillator in the lower energy state is positive half integer, the oscillator in the higher state can have any energy! How does this come about? If one imposes reality conditions before solving the constraints, it is the requirement that the energy of each oscillator be positive definite and the fact that there exists a lowering operator that necessitates the half-integer energy eigenvalues. Here, on the other hand, since we impose \star -relations only on the space of physical states, once the energy of the ‘lower’ oscillator is positive definite (and thus half integer), the constraint *guarantees* that the energy of the ‘higher’ oscillator is positive definite too. This is no longer an independent requirement.

Remark 4: Classical conditions incompatible in quantum theory

Consider the following two features of the classical theory. First, classically, the parity transformation $\mathbf{P}(z_I) = (-z_I)$ satisfies

$$(I) \quad \mathbf{P}^2 = 1. \quad (3.2)$$

Second, since for any value of δ the reduced phase space (see section 5) is a non-compact two dimensional manifold (in fact topologically \mathbb{R}^2), the classical theory is well-defined for *any* real δ ,

$$(II) \quad \delta \in \mathbb{R}. \quad (3.3)$$

However, the eigenvalues of $\hat{\mathbf{P}}$ are given by $\exp(i2\pi\epsilon)$ (see (2.16)), where in the physical representation, $\epsilon = \text{frac}(|\delta|)$. If we require $\hat{\mathbf{P}}^2 = 1$ in the quantum theory, there are non-trivial representations only for $\frac{1}{2}$ -integer or integer values of δ .

Thus, *there are two conditions (I) and (II), satisfied in the classical theory, which cannot be satisfied simultaneously in quantum theory.*

Within quantum mechanics, there seems to be *no* compelling reason to restrict ourselves to states with eigenvalues ± 1 of $\hat{\mathbf{P}}$. However, to allow other eigenvalues seems to violate classical intuition. This is, however, not entirely unfamiliar. Indeed, a similar situation occurs in systems of identical particles in 2-spatial dimensions where the use of eigenvalues other than ± 1 for the parity or the permutation operators leads to the interesting quantum phenomena of fractional statistics.

5.4 FRW universe with conformally coupled scalar field

The Ricci scalar for the closed ($k = +1$) Friedman-Robertson-Walker universe is

$$R = \frac{6}{a^2} \left(a \frac{\partial^2 a}{\partial \tau^2} + \left(\frac{\partial a}{\partial \tau} \right)^2 + 1 \right), \quad (4.1)$$

where a is the scale-factor of the universe and τ 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:

$$\mathcal{L}_G = \frac{6}{G} \left(-a \left(\frac{\partial a}{\partial \tau} \right)^2 + a \right), \quad (4.2)$$

where G is the gravitational constant, and the action is $S = \int d\tau \mathcal{L}$. The Lagrangian for the homogeneous, conformally coupled ($\xi = \frac{1}{6}$, massless) scalar field is

$$\mathcal{L}_{KG} = 8\pi \left(a^3 \left(\frac{\partial \phi}{\partial \tau} \right)^2 + a \left(\frac{\partial a}{\partial \tau} \right)^2 \phi^2 + 2a^2 \phi \frac{\partial a}{\partial \tau} \cdot \frac{\partial \phi}{\partial \tau} - a\phi^2 \right). \quad (4.3)$$

Introduce a reparametrization of the time, $\partial t = \partial\tau/N$, where N is the lapse. Let $\dot{} \equiv (\partial/\partial t)$. Then the total Lagrangian is

$$\mathcal{L} = -\frac{6}{GN}a\dot{a}^2 + \frac{6Na}{G} + \frac{8\pi a}{N}(\dot{a}\phi)^2 - \frac{8\pi N}{a}(a\phi)^2. \quad (4.4)$$

Define the variables

$$x_1 := \sqrt{\frac{12}{G}}a \quad (4.5)$$

$$x_2 := \sqrt{\frac{16\pi}{G}}a\phi. \quad (4.6)$$

Now the Lagrangian takes the form

$$\mathcal{L} = -\frac{1}{2N}a\dot{X}_1^2 + \frac{1}{2N}a\dot{X}_2^2 + \frac{6Na}{G} - \frac{N}{2a}x_2^2. \quad (4.7)$$

Performing the Legendre transform, we find the canonical momenta:

$$p_1 := -\sqrt{\frac{12}{G}}\frac{a\dot{a}}{N} \quad (4.8)$$

$$\text{and } p_2 := \frac{4}{\sqrt{\pi N}}a(\dot{a}\phi). \quad (4.9)$$

The Hamiltonian for the system is $H = \frac{2N}{x_1}C$, where the scalar constraint is given by

$$C = \frac{1}{4}(p_1^2 + x_1^2 - p_2^2 - x_2^2) \approx 0. \quad (4.10)$$

We see that it is exactly of the form of (1.1), with $\delta = 0$. Note that there is a nonholonomic constraint, $a \geq 0$. A consistent approach to 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_I, p_I) . The solutions then describe a periodic, bouncing universe. Finally, since $\delta = 0$ in this case, we obtain only one physical representation ((2.23) and (2.21) are the same), which does not display any of the counter-intuitive behaviour discussed in the previous section. For the mathematically allowed representations in which the energy is unbounded below, no physical interpretation is immediately forthcoming.

5.5 (†) Reduced space quantization

As has been mentioned before, the constraint surface for the general problem is the group manifold of $SO(2, 1)$, which is topologically $\mathbb{R}^2 \times S^1$. The orbits of the canonical transformations generated by the constraint are closed curves in $\bar{\Gamma}$, and there are *no fixed points*. The space of orbits $\hat{\Gamma}$ is just the mass shell in 3-dimensional Minkowski space. The functions $\{J_z, J_+, J_-\}$ (see (2.9)) are good coordinates on M^3 , and the “radius” of the mass shell is given by the identity

$$J^2 := -J_z^2 + J_+J_- = -\delta^2. \quad (5.1)$$

(Since the classical function J_z is positive, the reduced phase space is in fact the *future* mass shell, $J_z \geq 0$.) One can easily compute the Poisson brackets between these elementary variables: $\{J_+, J_-\} = 2iJ_z$ and $\{J_\pm, J_z\} = \pm iJ_\pm$.

We choose as our set of elementary functions $\mathcal{S} = \{1, J_z, J_\pm\}$, and construct our algebra accordingly. The commutation relations in the reduced space observable algebra \mathcal{A}_{red} are given by: $[\hat{J}_+, \hat{J}_-] = -2\hat{J}_z$ and $[\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm$, which are exactly the same as in \mathcal{A}_{phy} (2.8). Not surprisingly the commutator algebra is again a representation of $SO(2, 1)$. Note however that the quantum *algebraic relation* (obtained from (5.1) via the rule (2.2.3)),

$$\begin{aligned} \hat{J}^2 &:= -\hat{J}_z^2 + \frac{1}{2}[\hat{J}_+, \hat{J}_-]_+ = -\delta^2 \\ \text{or, } \hat{J}_+ \hat{J}_- &= (\hat{J}_z - \frac{1}{2})^2 - \frac{1}{4} - \delta^2, \end{aligned} \quad (5.2)$$

is *different!* (Compare to (2.12): both \mathcal{A}_{phy} and \mathcal{A}_{red} are representations of the $SO(2, 1)$ algebra, but for different values of the Casimir invariant \hat{J}^2 !) Therefore the two operator algebras, \mathcal{A}_{phy} , the physical operator algebra constructed previously for constrained quantization, and \mathcal{A}_{red} , the reduced space algebra, are *not identical*. Obviously, the quantum theories will also be different.

In fact, carrying out the quantization, one finds the following (the representation of the CCRs in \mathcal{A}_{red} is chosen as in (2.14): Corresponding to (2.19) here one obtains the condition

$$m^2 \geq \delta^2 + \frac{1}{4}. \quad (5.3)$$

(The reduced space quantum theory can be obtained from the Dirac theory by making the substitution $\delta^2 \mapsto \delta^2 + \frac{1}{4}$.) However, since we have to impose the non-holonomic constraint $\hat{J}_z \geq 0$, for each value of $|\delta|$ one obtains a single representation consisting of states with

$$m = \sqrt{\delta^2 + \frac{1}{4}} + n, \quad n = 0, 1, 2, \dots \quad (5.4)$$

The representation of the elementary operators in \mathcal{A}_{red} is then given by

$$\begin{aligned} \hat{J}_z |m\rangle &= (m + \frac{1}{2}) |m\rangle \\ \hat{J}_+ |m\rangle &= \sqrt{(m+1)^2 - \frac{1}{4} - \delta^2} |m+1\rangle \\ \hat{J}_- |m\rangle &= \sqrt{m^2 - \frac{1}{4} - \delta^2} |m-1\rangle \\ \text{and } \hat{\mathbf{P}}^2 |m\rangle &= \exp i2\pi\epsilon |m\rangle. \end{aligned} \quad (5.5)$$

Note that the quantum theory is well-defined for *all* real δ , not just integers.

Comparing this representation to (2.20), one can see that the quantum theories cannot be made equivalent. (The particular representation of \hat{J}_z has been chosen to facilitate the comparison with the Dirac theory. This leads to just an overall shift in the spectrum of \hat{J}_z . Now, construct e.g. the Hermitian operators $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$, $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$, and compare spectra in the two quantum theories. These are not related to each other by just a shift.) This was not unexpected: due to the ACRs, the algebras \mathcal{A}_{red} and \mathcal{A}_{phy} are different. This arises because of the different stages at which consistent factor-ordering is carried out in the two programs. To construct \mathcal{A}_{phy} one factor-orders in \mathcal{A} *first* and then looks for operators that commute with the constraints. Since the

algebraic relation is calculated at the operator level (2.11 – 2.12), and is not derived as the “quantization” of some classical identity, there is no ambiguity of the kind in (2.4.3). On the other hand, to construct \mathcal{A}_{red} one first finds functions which have vanishing Poisson brackets with the constraints (on $\bar{\Gamma}$), and then uses these as *elementary* variables. Now, when one constructs the abstract algebra \mathcal{A}_{red} , the elementary classical Dirac observables are to have unambiguous quantum analogs, and there is no factor-ordering ambiguity at this stage. However, the classical identity (5.1) has to be incorporated in quantum theory, and we have chosen to do so by imposing the ACR (5.2).

As in the Dirac quantum theory, there is a superselected operator $\hat{\mathbf{P}}$ which is unitary. However, since the classical parity operator on Γ , $\hat{\mathbf{P}}(z_I) = -z_I$, leaves the gauge orbits invariant (it maps a point on a gauge orbit to a diametrically opposite point on the *same* gauge orbit), it has no action on $\hat{\Gamma}$ *whatsoever*. Thus in the reduced space quantization of this problem, the operator $\hat{\mathbf{P}}$ is introduced as a mathematical device to allow us to first decompose the representation space into orthogonal subspaces labelled by the eigenvalues of $\hat{\mathbf{P}}$, and then proceed to find an inner product. In the context of the reduced space quantum theory, there can be no physical interpretation attached to \mathbf{P} ; in particular, there is no justification even classically to require that $\mathbf{P}^2 = 1$.

5.6 (†) Coupled oscillators: constrained energy sum

I will briefly discuss the quantization of a model that has proven useful in the past as a testing ground for various ideas (e.g. the issue of time [2]) and has been studied extensively (see also [3]). Consider two harmonic oscillators as in section 2, but unlike the previous model impose the *total energy* as a first class constraint:

$$C := \frac{1}{2}(p_1^2 + x_1^2 + p_2^2 + x_2^2) - E \approx 0, \quad (6.1)$$

where $E \geq 0$ in order for the classical system to be well-defined. (Note that since the geometrodynamical scalar constraint is not of this form (see the remarks in the introduction to this chapter), the constrained energy sum model we consider here is *not* a model of general relativity.)

We will use the notation of section 2. In terms of the quantum operators defined in section 2, the constraint equation is given by:

$$\hat{C}|\psi\rangle_{phy} \equiv (\hat{c}_1\hat{a}_1 + \hat{c}_2\hat{a}_2 + 1 - E)|\psi\rangle_{phy} = 0. \quad (6.2)$$

Consider the algebra generated by the set of operators $\{1, \hat{L}_z, \hat{L}_\pm\}$, 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, given by $[\hat{L}_+, \hat{L}_-] = 2\hat{L}_z$ and $[\hat{L}_z, \hat{L}_\pm] = \pm\hat{L}_\pm$, provides a representation of the $SO(3)$ Lie algebra. The algebraic relation is $\hat{L}_+\hat{L}_- = \frac{1}{4}E^2 - (\hat{L}_z - \frac{1}{2})^2$, or equivalently in terms of the Casimir invariant, $\hat{L}^2 := \hat{L}_z^2 + \frac{1}{2}[\hat{L}_+, \hat{L}_-]_+ = l(l+1)$ where $l = \frac{E-1}{2}$.

The quantization of this algebra is straightforward, and though this model is not as rich as the previous one, it does have a few interesting features, most of which are familiar from the quantization of the standard angular momentum algebra.

1. Consider the parity operator corresponding to the discrete canonical transformation $\mathbf{P}(z_I) = -z_I$. It is certainly superselected, but in this case it does not serve to further reduce the physical representation. On states in the kernel of the constraint, its action is given by

$$\hat{\mathbf{P}}|m\rangle = (-1)^{E-1}|m\rangle, \quad (6.3)$$

it has the same eigenvalue on the full physical subspace. The parity operator satisfies $\hat{\mathbf{P}}^2 = 1$ only for integer E .

2. Quantum mechanically, there is however another superselected discrete operator that one can construct, the eigenvalues of which characterize the irreducible representations:

$$\hat{\mathbf{T}}|m\rangle = (-1)^{2m}|m\rangle \quad (6.4)$$

On each eigenspace of $\hat{\mathbf{T}}$ one can introduce a discrete, countable basis, and this allows us to choose an inner product of the form $\langle m|m'\rangle = \delta_{m,m'}$, rather than $\langle m|m'\rangle = \delta(m-m')$. Unfortunately, this operator does not correspond to any known classical canonical transformation on the phase space, thus it has *no interpretation in classical terms*.

3. One finds that there exist non-trivial representations only when E is integer (l is half integer or integer). The representation is unique, and not surprisingly (since the reduced phase space is compact), it is finite-dimensional, of dimension $2l+1$. A basis is provided by states with $m = -l, -l+1, \dots, l-1, l$. The representation of the other generators of \mathcal{A}_{phy} is

$$\begin{aligned} \hat{L}_z|m\rangle &= m|m\rangle, \\ \hat{L}_+|m\rangle &= \sqrt{(l-m)(l+m+1)}|m+1\rangle \\ \text{and } \hat{L}_-|m\rangle &= \sqrt{(l+m)(l-m+1)}|m-1\rangle, \end{aligned} \quad (6.5)$$

where as before $l = \frac{(E-1)}{2}$.

4. For general, non-integral E , there is *no quantum theory*. (However, see [4].) There are many levels at which this can be understood, or at least seen to be not unfamiliar. From the point of view of geometric quantization, this is not a surprise since the reduced phase space is a compact manifold, S^2 , and it admits a Kähler structure only for integer values of the radius [5]. Related to this, obviously, is the fact that \mathcal{A}_{red} is just the Lie algebra of $SO(3)$. From ordinary quantum mechanics, we are familiar with the fact that this has only the integer and half-integer spin representations.
5. For this model, *in this representation* the reduced space quantum theory is not obviously unitarily equivalent to the Dirac theory. However, with a suitable choice of factor-ordering of the quantum constraint, the Dirac theory can be made equivalent to the reduced space theory, see [4]. (See also [2].)

Bibliography

- [1] Louko J 1992 *private communication* Syracuse
- [2] Rovelli C 1991 *Phys. Rev.* **D43** 442-56
- [3] Hajicek P 1990 *Class. Quantum Grav.* **7** 871
- [4] Tate R S 1993 *private communication* Santa Barbara
- [5] Stillerman M 1985 *Ph.D. thesis* Syracuse University

Chapter 6

PHYSICAL INTERPRETATION FOR SYSTEMS WITH A CONSTRAINED HAMILTONIAN

6.1 Introduction

In classical mechanics, interpretational issues are well understood: the physical questions one is interested in are mostly related to predictions about the values of various phase space functions. The issues of interest in a quantum theory, however, are generally very different from those in a classical theory. In classical mechanics, e.g. in the Kepler problem, one is interested in questions about the orbits of the particle and in predicting future positions and momenta of the particle from initial data. In the quantum theory of the Hydrogen atom, on the other hand, one is more interested in questions about the spectra of operators corresponding to various phase space functions –e.g. the energy and angular momentum operators– and the transition amplitudes between their eigenstates. To a certain extent, we know that these are the right questions to ask because the full quantum theory is available to us. In general, until one has at least the rudiments of a quantum theory, one cannot be certain that the questions one asks will remain meaningful in the full quantum theory.

In the quantum theory of constrained systems the interpretational problems are further complicated since not all operators can be considered physically interesting. Recall that the allowed quantum states of the system are represented by the solutions to the quantum constraint equations. Hence, we are allowed to consider as physical only those operators which leave the space of physical states invariant.

Now, given a vector space of physical states, it is trivial to construct linear operators on it, say by selecting a basis and then writing down arbitrary matrices in this basis. In the loop representation for general relativity, for example, one can easily construct such operators on the known physical states: they simply break and join loops in appropriate ways. However –and I want to emphasize this point– this construction is not sufficient for the purposes of quantum theory. It is true that these are physical operators, since by construction they leave the space of physical states invariant. However, unless one knows

which functions on phase space they correspond to, one cannot relate mathematical properties of these operators to, e.g., the results of measurements. The main difficulty is to obtain the correct Hermiticity conditions on these operators, and their interpretation¹.

The above discussion shows, that in contrast to ordinary quantum mechanics, in the quantum theory of constrained systems, one is interested in the explicit representations on physical states of operators corresponding to a *restricted* class of functions on phase space, namely the gauge invariant functions on the constraint surface.

Among constrained systems themselves there is a further distinction. For *ordinary* constrained systems, like gauge theories, the Hamiltonian –which generates dynamics– is distinct from the constraint functions and 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. I will refer to such theories as *dynamically constrained systems* since the dynamical trajectories are generated by a Hamiltonian which is constrained to vanish. General relativity, in the spatially compact case, is an important example.

In order to understand some of the difficulties endemic to dynamically constrained systems, 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. This construction is completely independent (at least conceptually) from the dynamical structure of the theory: one does not need the Hamiltonian to carry out the above construction. After this kinematical construction, one can consider the issue of dynamics. Since the (non-vanishing) Hamiltonian is first-class, it projects unambiguously to the reduced phase space, and all physically interesting dynamics can be considered to occur on the reduced phase space itself. In 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. Since in such systems “time” is not an external parameter, but one of the canonical variables, the question of the identification of the true degrees of freedom and the physical Hilbert space takes on dynamical overtones. For example, can one in fact complete the kinematical construction of the Hilbert space of physical states *without* explicitly isolating a “time” variable? An equally important issue is that of observables. The dynamical trajectories are “gauge” orbits. Hence, a set of Dirac observables (or “gauge invariants”) is the set of initial data. Using these observables, or even the constants of motion, it is difficult to see the evolution explicitly. How do we recover a dynamical picture for such theories? Where, e.g., is a time variable hidden, and how does one construct *time*

¹On the other hand, the corresponding classical observables do not have to be simple functions of some particular choice of the elementary variables. Also, the representation *itself* does not have to be tied directly to the phase space. For example, unlike in the configuration representations, in the $|n, l, m\rangle$ representation for the H-atom or the Fock representation for the free Maxwell theory, the states are *not* functions on phase space. However, the states themselves can be identified as eigenstates of operators corresponding to functions on phase space; and the interesting operators on these states do correspond to known functions on the phase space.

dependent states or operators? Or, are constants of motion the only operators about which we can or would want to formulate well-defined questions in quantum theory?

Clearly, the dynamical treatment and physical interpretation of the two types of constrained systems (distinguished, recall, by the vanishing or non-vanishing of the Hamiltonian on the constraint surface) will perforce be different. In this chapter, I will concentrate on some interpretational issues in the quantum theory of dynamically constrained systems.

In order to focus on these issues, consider, as a specific example of a dynamically constrained system, the *nonrelativistic parametrized particle*. As I will discuss in detail in section 2, the classical theory for the ordinary nonrelativistic particle can be written as a constrained system, by including “time” and its conjugate momentum as (extended) phase space variables and imposing as a first class constraint the condition that the momentum conjugate to time equal the “true” Hamiltonian. (See ADM [1], Kuchař [2] and references therein.) Now, in the usual, unparametrized version of the theory, time is an *external* parameter, evolution along which is determined by the Hamiltonian. In the process of constructing a Hilbert space of states, one need not make any reference to the Hamiltonian or the time. In subsection 2.1, we will see that for the parametrized theory too, the construction of the kinematical quantum theory –i.e. a Hilbert space of physical states– can be accomplished without isolating a time variable. As far as the second issue –that of the observables– is concerned, recall first that in the unparametrized theory one has no trouble posing questions about the action of *instantaneous* position and momentum operators on the quantum states; hence one expects that in the parametrized theory too one should be able to pose such questions. Now, in the parametrized theory, it turns out that the algebra of physical observables is generated by the constants of motion, e.g. the *initial* positions and momenta. However, in the quantum theory one is not interested in questions only about the constants of motion. As an example, consider the quantum theory of the Hydrogen atom. One *is* interested in the expectation values of the instantaneous position operator \hat{x} , say to calculate the effect of a uniform electric field as a perturbation. As we will see, in the parametrized theory, since \hat{x} does not commute with the constraint, it is not a Dirac observable, and one cannot calculate its expectation value on physical states. How can one resolve this conflict –in the ability to pose certain questions– between the parametrized and unparametrized theories?

To begin with, let us consider a related question in the context of ordinary gauge theories, ones in which the constraints do not generate dynamics. Can one only formulate questions about the gauge-invariant observables? In a certain sense, the answer is “yes”. However, since a gauge fixing –or a cross-section of the gauge orbits– is related to the space of orbits (the reduced phase space $\hat{\Gamma}$) by a symplectic diffeomorphism, the pull-back of an arbitrary function to this cross-section naturally defines a function on $\hat{\Gamma}$ and is thus manifestly gauge-invariant. Therefore, corresponding to *any* function on the phase space one can *construct* a gauge-invariant observable.

The details of the construction are useful to keep in mind during the rest of this chapter: Let λ be an affine parameter along the gauge orbits, and fix a cross-section $\lambda = \lambda_0$. Now, consider an arbitrary function f on $\bar{\Gamma}$, and assume to begin with that its Lie derivative along the gauge orbits does *not* vanish (if it does, f , being constant along the gauge orbits, is already a Dirac observable and we are done). We can construct a

gauge invariant observable corresponding to f in the following way: First, evaluate f on the cross-section. Now construct a new function f_{λ_0} by Lie transporting this “data” on the cross-section along the gauge orbits, i.e. $\frac{\partial}{\partial \lambda} f_{\lambda_0} = 0$, $f_{\lambda_0}|_{\lambda=\lambda_0} = f|_{\lambda=\lambda_0}$. Thus, e.g., if $f = 2$ at the point of intersection of a gauge orbit with the cross-section, then $f_{\lambda_0} = 2$ *everywhere* on that orbit. Thus, *in this gauge*, we have obtained a classical observable corresponding to the function f . In quantum theory, one would try to construct the corresponding physical operator \hat{f}_{λ_0} , and formulate questions in this gauge. This is the sense in which the connection in the Coulomb or transverse gauge is a gauge invariant observable². Note that the specific form of these operators will in general depend on the value of the gauge parameter chosen to fix the cross-section. The freedom is quite large, since we can not only choose a different value for the parameter λ , but we can also choose entirely different foliations of the constraint surface, instead of $\lambda = \text{const.}$ cross-sections.

This is the approach in gauge theories, such as QED. In these theories, gauge fixing is usually not considered to be of tremendous *conceptual* importance. In principle, one could work with gauge invariant observables, i.e. on the reduced phase space itself. It is not conceptually necessary to work with gauge-fixed observables: it is only a matter of practical and technical comfort that we choose to work with a cross-section of the gauge orbits.

However, dynamically constrained systems are different from ordinary gauge theories in certain conceptually important ways. First, recall that since the dynamical trajectories are gauge orbits *i)* there is no natural notion of dynamics on the reduced phase space itself, and *ii)* gauge-invariant observables are constants of motion. For dynamically constrained systems, one does not have the luxury of working on the reduced phase space. It is in order to see the explicit unfolding of dynamical evolution that one is forced to work on the constraint surface, scored by the congruence of “gauge” orbits. Second, since a gauge parameter is identified as a time variable, then unlike in ordinary gauge theories, one is *not* free to gauge-fix it. Hence, on the constraint surface, one is interested not just in one cross-section of the gauge orbits, but a 1-parameter family of cross-sections. Now, given a preferred foliation of the constraint surface by such “constant time” slices, for each function on $\bar{\Gamma}$ one obtains a *1-parameter family of observables*, not just a single gauge-fixed observable. Each observable in this 1-parameter family commutes (or has vanishing Poisson bracket) with the constraint and is therefore a Dirac observable.

Up to now, in order to convey some of the conceptual ideas, the discussion has been mostly classical. The above general procedure can be attempted in both the Dirac and the reduced space quantum theories. Since both methods involve solving the (classical or quantum) Heisenberg equations of motion in order to obtain the 1-parameter family of observables corresponding to the particular function on the constraint surface in which we happen to be interested, I will refer to such observables as *Heisenberg observables*. Note that there may not always be a clear distinction between “ordinary” Dirac observables and these Heisenberg observables.

²I am not suggesting that questions about the connection are important in QED. However, *some* questions of this nature may be important: since we do not know in advance which ones, we need a device to formulate them in the quantum theory.

So far, in the Dirac quantum theory, the above approach to physical and dynamical interpretation is (even formally) well-defined only for systems which can be deparametrized³, i.e. where the constraint can be written as a Schrödinger equation, in a form linear in a variable which can be identified as the momentum conjugate to some time parameter. Such systems are formally similar to the nonrelativistic parametrized particle, which I will discuss in section 2. On the other hand, one can construct the reduced space quantum theory only for systems which have been completely solved classically, but then for such systems the interpretational problem is well under control, even if the constraint has not been written explicitly in the Schrödinger form. In section 3, I will construct an interpretational framework for the reduced space quantum theory of dynamically constrained systems, along the lines of the approach discussed above for ordinary gauge theories. This closely follows the approach discussed by Rovelli [3, 4]. In section 4 I will apply this approach to the Bianchi I cosmology, and consider the issue of the initial singularity in quantum theory. In section 5 I will draw conclusions and outline some ideas to extend the above interpretational framework to either Dirac quantum theories which are not in deparametrized form, or reduced space quantum theories of classical systems which have not been exactly solved.

6.2 Non-relativistic parametrized particle

Consider a non-relativistic particle moving in (3-dimensional) Euclidean space. Dynamics is specified by a “true” Hamiltonian $H(q^i, p_i)$, where p_i are the momenta conjugate to the coordinates q^i . (For simplicity, I will consider the Hamiltonian to be the sum of two terms: a kinetic term quadratic in momenta, and a potential term V independent of momenta.) This simple system can be “parametrized” by adding to the 3-dimensional configuration space the time variable q^0 . Thus, the (enlarged) configuration space, \mathcal{C} , is now *4-dimensional*, coordinatized by (q^0, q^i) ; and the phase space is 8-dimensional. There is one (first class) constraint:

$$C(q, p) := p_0 + H(q^i, p_i) = 0, \quad (2.1)$$

where q and p stand for (q_0, q_i) and (p_0, p_j) 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 $H(q^i, p_i)$.

6.2.1 Kinematical quantum theory

Let us now carry out the quantization program. (In this section, the details of the calculation follow Ashtekar [6, 7]. Kuchař [9] and Rovelli [3] have similar if not identical approaches to the physical interpretation of such systems, and the roots probably go further back.) Let the space \mathcal{S} of elementary observables be the complex vector space

³In this chapter, I will use the term “deparametrized” to mean that not only has a “time” variable q_0 been identified, but also, the constraint is linear in the conjugate momentum p_0 and of the form $C = p_0 + H(q_0, q_i, p_i)$.

spanned by the 9 functions $(1, q, p)$ on the phase space Γ , with the usual commutation relations. Choose for the representation space \mathcal{V} the space of smooth functions on the *4-dimensional* configuration space \mathcal{C} , and represent the operators by the usual multiplication and partial derivative operators⁴. The quantum constraint is now given by:

$$\hat{C} \circ \Psi(q) \equiv \frac{\hbar}{i} \frac{\partial \Psi(q)}{\partial q^0} + \hat{H} \circ \Psi(q) = 0, \quad (2.2)$$

which, when we identify q^0 with time, is nothing but the time-dependent Schrödinger equation, in a parametrized guise. The space of physical states, \mathcal{V}_{phy} , now consists of solutions of this equation, given *formally* by:

$$\Psi(q) = e^{-\frac{i}{\hbar} \hat{H} q^0} \circ \psi(q^i), \quad (2.3)$$

where the $\psi(q^i)$ are arbitrary functions which depend only on the “true degrees of freedom”. Note that the solutions $\Psi(q)$ to the quantum constraint are complex valued functions on the 4-dimensional configuration space \mathcal{C} ; they are *not* functions of q_i alone; 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 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 (2.2). Clearly, none of the elementary quantum operators, \hat{q}^0 , \hat{q}^i or \hat{p}_i , corresponding to the set \mathcal{S} , is a physical operator. Therefore, the \star -relations between the elementary operators cannot be directly used to single out an inner-product on \mathcal{V}_{phy} .

Our task now is to find a complete set of physical operators. Fortunately, this is not difficult to accomplish, at least formally. The Dirac operators are given by:

$$\begin{aligned} \hat{Q}^i(0) \circ \Psi &:= \hat{U}(0) \hat{q}^i \hat{U}^{-1}(0) \circ \Psi = e^{-\frac{i}{\hbar} \hat{H} q^0} \hat{q}^i \circ \psi \equiv e^{-\frac{i}{\hbar} \hat{H} q^0} \circ \hat{q}^i \psi(q^i), \\ \text{and } \hat{P}_i(0) \circ \Psi &:= \hat{U}(0) \hat{p}_i \hat{U}^{-1}(0) \circ \Psi = e^{-\frac{i}{\hbar} \hat{H} q^0} \hat{p}_i \circ \psi \equiv e^{-\frac{i}{\hbar} \hat{H} q^0} \circ \frac{\hbar}{i} \frac{\partial}{\partial q^i} \psi(q^i), \end{aligned} \quad (2.4)$$

where

$$\hat{U}(0) := e^{-\frac{i}{\hbar} \hat{H} q^0}; \quad (2.5)$$

\hat{q}^0 acts by multiplication and has been replaced by q^0 ; and the Hamiltonian operator $\hat{H} = H(\hat{q}^i, \hat{p}_i)$. (The reason for the notation $\hat{U}(0)$ will become clear later.) In (2.4), the states in the last step are manifestly solutions of (2.2), of the form (2.3). In fact, 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 \star 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:

$$\langle \Psi(q) | \Phi(q) \rangle = \int_{\mathcal{C}} d^4 q \mu(q) \bar{\Psi}(q) \Phi(q), \quad (2.6)$$

⁴Note 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.

for all physical states $\Psi(q)$ and $\Phi(q)$. To determine the measure, we impose the Hermiticity requirements. The condition that \hat{Q}^i 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 μ on q^i . The important point is that the dependence of μ on q^0 is left undetermined.) Thus, the inner-product can now be calculated:

$$\begin{aligned}
\langle \Psi(q) | \Phi(q) \rangle &= \int d^4q \mu(q^0) \bar{\Psi}(q) \Phi(q) \\
&= \int dq^0 \mu(q^0) \int d^3q^i \bar{\Psi}(q^0, q^i) \Phi(q^0, q^i) \\
&= \int dq^0 \mu(q^0) \int d^3q^i \bar{\psi}(q^i) \phi(q^i) \\
&= K \int d^3q^i \bar{\psi}(q^i) \phi(q^i) \equiv K \int d^3q^i \bar{\Psi}(q^0, q^i) \Phi(q^0, q^i) \quad (2.7)
\end{aligned}$$

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 (2.2). 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 kinematical picture is the following: the physical Hilbert space consists of solutions to the constraint equation (2.2), with the Hermitian inner product given by (2.7). The Hamiltonian \hat{H} is a symmetric operator on this Hilbert space. Up to this point, the physical operators (2.4) were formal constructs, used to find an inner product. Now, however, we can use the the physical inner product to *rigorously* define the unitary operator (2.5), and hence the physical operators.

So far, 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 (2.3), 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:

$$\psi_0(q^i) := e^{\frac{i}{\hbar} \hat{H} q^0} \circ \Psi(q) \equiv \Psi(q)|_{q^0=0}. \quad (2.8)$$

With $K = 1$, the inner product on these states is simply (2.7). 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 (2.4) is simply

$$\hat{Z}(0) \circ \psi_0(q^i) = \hat{z} \circ \psi_0(q^i). \quad (2.9)$$

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 Ψ back to $q^0 = 0$ ” (or, via (2.8), 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 (2.4).

6.2.2 Dynamics and interpretation

Are these the only operators or the only states that one can define? Recall, from the introduction, that in the classical picture, on the constraint surface (the space of allowed classical states), any cross-section of the gauge orbits (say $q^0 = 0$, where for the relativistic parametrized particle we have identified the “gauge” parameter λ with q^0) is isomorphic to the reduced phase space. There is a 1 – 1 correspondence between the classical states (points) on this cross-section, and the gauge orbits. Hence, the pull-back of a function to this cross-section naturally defines a classical observable. There is analogous structure on the space of allowed quantum states $\Psi(q)$. Since they are solutions to the quantum constraint equation, they are in 1 – 1 correspondence with the initial states $\psi_0(q^i)$ satisfying $q^0 = 0$. Extending the analogy, we see that quantum observables can be (and as I emphasized in the discussion above, have been) obtained by evaluating their action on the states $\psi_0(q^i)$ in the “cross-section” $q^0 = 0$.

However, recall also, that for dynamically constrained systems, in order to recover a notion of evolution it is necessary to consider not just one particular cross-section (which would be adequate for an ordinary gauge theory), but a *foliation* of the constraint surface by a 1-parameter family of cross-sections of the gauge orbits (corresponding say to successive values of λ , or in this case, q^0). By analogy, since the covariant configuration space can be foliated by $q^0 = \text{constant}$ surfaces, each covariant state $\Psi(q)$ defines a 1-parameter family of Schrödinger states $\psi_\tau(q^i)$:

$$\psi_\tau(q^i) := e^{\frac{i}{\hbar}\hat{H}(q^0-\tau)} \circ \Psi(q) \equiv \Psi(q)|_{q^0=\tau}. \quad (2.10)$$

Note that this correspondence exists *only* because the states $\Psi(q)$ satisfy the constraint equation.

To construct dynamical observables, recall that in the classical theory, given any function on the constraint surface, we evaluate its pull-backs to successive cross-sections, and obtain a 1-parameter family of classical observables. Analogously, the physical operators corresponding to a particular foliation $q^0 = \tau$ are simply given by

$$\hat{Z}(\tau) \circ \psi_\tau(q^i) = \hat{z} \circ \psi_\tau(q^i). \quad (2.11)$$

In order to see clearly the corresponding 1-parameter family of physical operators, let us use (the inverse of) the unitary transformation (2.10) to obtain the action of the τ -dependent operators on the covariant states. Doing so, we find

$$\hat{Z}(\tau) \circ \Psi(q) = \hat{U}(\tau)\hat{z}\hat{U}^{-1}(\tau) \circ \Psi(q) = e^{-\frac{i}{\hbar}\hat{H}(q^0-\tau)}\hat{z} \circ \psi_\tau(q^i), \quad (2.12)$$

where

$$\hat{U}(\tau) = e^{-\frac{i}{\hbar}\hat{H}(q^0-\tau)} \quad (2.13)$$

is the unitary transformation defined in (2.10). It is now manifest from this analogy that we can identify q^0 with the time even in quantum theory, and that the $\hat{Z}(\tau)$ are the “evolving” Heisenberg operators.

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 $q^0 = \tau_0$:

$$\hat{Z}(\tau) \circ \psi_{\tau_0}(q^i) = \left[e^{\frac{i}{\hbar}\hat{H}(\tau-\tau_0)} \hat{z} e^{-\frac{i}{\hbar}\hat{H}(z)(\tau-\tau_0)} \right] \circ \psi_{\tau_0}(q^i). \quad (2.14)$$

As expected, we have lost all reference to q^0 , and have obtained the complete deparametrization of the theory to the usual Heisenberg/Schrödinger picture.

In retrospect we see that we could have worked always in the covariant picture, with the τ -dependent Heisenberg operators defined in (2.12). However, we would then have lost the analogy with the classical picture, and hence, 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 “hidden” dynamics 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.

To conclude this section, note 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 and without integrating over only the true degrees of freedom q^i ; the reality conditions on \mathcal{V}_{phy} suffice to give us the inner product. This is an important point, since it illustrates that it is not necessary to isolate time in order to construct the kinematical quantum theory and a Hilbert space of physical states. (For an original and more complete discussion of this aspect of the issue of time in quantum gravity, see [5, 7, 8].) Note however, that 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 H . In addition to the states, one will also have to construct explicit expressions for a complete set of interesting operators.

Another important lesson that we have learnt is the following: *if* the constraint for any system can be deparametrized and expressed in the form of a Schrödinger equation, *then* the problem of constructing a *kinematical* quantum theory (by which I mean the identification of a complete set of observables, and a unitary representation on a Hilbert space) and a dynamical interpretation is formally completely solved!

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 normal ordering the $U(\tau)$) or to replace the Euclidean space by a 3-manifold.

6.3 Reduced space quantization and interpretation

In the previous section we saw that if a dynamically constrained system could be deparametrized and a time-like variable identified, then one could formally construct the

Hilbert space of physical states. Furthermore, there is well-defined framework in which to tackle the physical interpretation of the theory. However, there are two obvious disadvantages to the above framework. In the first place it is absolutely essential that the constraint is deparametrized and expressed as a Schrödinger equation. Secondly, even when this can be done, the solutions (2.3) one obtains are only formal expressions, and in general the observables (2.12) pose formidable factor-ordering problems. In fact, as in ordinary Schrödinger quantum mechanics, the only known way to obtain explicit expressions for (2.12) begins with diagonalizing the Hamiltonian [9].

However, there are many systems in which, though a time variable can be identified, the constraint equation does not simplify to the Schrödinger equation. For example, consider the two coupled oscillator system quantized in chapter 5. For this model, the natural time variable is angular. The momentum conjugate to the time is then a “radius-squared” variable. (Roughly, $dp_1 \wedge dx^1 = d(\frac{r^2}{2}) \wedge d\theta$ is the symplectic structure.) The constraint is linear in this new momentum variable, however, there is a *non-holonomic* constraint that the new momentum should be positive. Due to this, nontrivial subtleties arise in the quantum theory.

Similarly, there are systems for which the constraint equation is in a second order, Klein-Gordon form. For example, consider (super-)stationary Bianchi cosmologies, i.e. ones which admit a causal KVF on minisuperspace. In such cases a positive/negative-frequency decomposition of the constraint has to be carried out to identify a “true” Hamiltonian [10]. Due to the “square-root” nature of the Hamiltonian, for such systems the approach of section 2 may be too cumbersome or difficult to implement. If on the other hand such systems are classically exactly solvable, then we can construct the reduced space quantum theory. In this section I will discuss how a physical interpretation of such systems can be obtained, without a Schrödinger like constraint equation. Admittedly, the examples I have given above *can* be treated in the Dirac framework. However, there are some difficulties, as I have mentioned, and therefore it seems worthwhile to elucidate the classical, reduced space approach. In this approach I have taken after Rovelli [3].

Consider a $2n + 2$ dimensional phase space with a single constraint C , with a specific choice of lapse. As in spatially compact general relativity, the constraint is also the generator of dynamics. Let z^μ , $\mu = 1 \dots 2n + 1$ be a set of independent functions on the constraint surface⁵. Our aim is find the observables of the theory, which correspond to functions on the reduced phase space. Denote these by Z^i , $i = 1 \dots 2n$.

The constraint generates canonical transformations whose orbits lie in the constraint surface itself. (The reduced phase space, as we know, is the space of orbits.) The infinitesimal canonical transformation is given by the Hamiltonian vector field X_C of the constraint. Let τ be an affine parameter along these orbits. (Note that τ is really the same as the λ used in section 1; however, we use τ here to emphasize that this is a dynamically constrained system.) Now, the observables Z^i pull-back from the reduced

⁵For the sake of simplicity, I will assume that the set is complete but not overcomplete, so that there are no algebraic identities amongst them. In the more general case, the range of μ will be greater, and there will be the appropriate number of algebraic identities, so that there are again only $2n + 1$ independent functions, even though one may not be able to solve for them explicitly. In the following discussion, the counting will then change in only a trivial manner.

phase space to functions on the constrained surface which are *constant* on the gauge orbits. At this point, a very useful choice can be made: choose τ such that (Z^i, τ) is a new set of coordinates on the constraint surface. (Note that nothing we have said so far prevents us from making this choice, in fact this can always be done.) This choice fixes the direction of the coordinate vector field of τ : it has to be parallel to the Hamiltonian vector field of the constraint. Further, since by definition τ is an affine parameter along the gauge orbits, we know in fact that $(\frac{\partial}{\partial \tau}) = X_C!$

So, we have *two* sets of coordinates on the constraint surface $\bar{\Gamma}$: the “old” coordinates (z^μ) induced from Γ , and the new coordinates (Z^i, τ) “induced” from the reduced phase space $\hat{\Gamma}$. Our problem is to relate these two sets of coordinates: To do this we have to integrate the gauge orbits.

Let us return therefore to the transformation generated by the constraint. This canonical transformation induces a 1-parameter family of transformations on the algebra of functions. The infinitesimal transformation on a function f is the Lie derivative, $\mathcal{L}_{X_C} f$. Now, since $(\frac{\partial}{\partial \tau}) = X_C$, we can identify the infinitesimal canonical transformation with the τ derivative of f : $\dot{f} := \frac{\partial f}{\partial \tau} = \{f, C\}$! This identification helps us to determine the relation between the two sets of coordinates.

On the constraint surface, the canonical transformation is completely specified by

$$\dot{z}^\mu = \frac{d}{d\tau} z^\mu = \{z^\mu, C\}. \quad (3.1)$$

Note that this is a set of coupled, but *ordinary* differential equations for the z^μ as functions of τ . The algebra of observables is generated by the initial data for the above equations, which we can identify with the Z^i . Since the space of orbits is $2n$ dimensional, the initial values of $2n$ of the $2n+1$ z^μ specify the orbit. The initial value of the remaining one, say $z^{(2n+1)}$, serves to fix the initial slice ($\tau = 0$) itself; assume for simplicity that $z^{(2n+1)}(0) = 0$. For later use, note that the formal solution to the above Hamiltonian equation of motion is given by the Taylor series

$$z^\mu(\tau) = \sum_N \frac{\tau^N}{N!} \left(\frac{d^N z^\mu}{d\tau^N} \right) \Big|_{\tau=0} \equiv \sum_N \frac{\tau^N}{N!} \left(\mathcal{L}_{X_C}^N z^\mu \right) \Big|_{\tau=0}, \quad (3.2)$$

where the coefficients of τ^N on the RHS are functions of Z^i . If it can be found, the solution of (3.1) is in the form

$$z^\mu = z^\mu(Z^i, \tau), \quad (3.3)$$

which is the coordinate transformation we were looking for on the constraint surface between the set of coordinates (z^μ) on the one hand and the set (Z^i, τ) on the other. This coordinate transformation can be inverted, to yield the time and the constants of motion explicitly as functions on the constraint surface

$$\begin{aligned} \tau &= \tau(z^\mu) \\ Z^i &= Z^i(z^\mu). \end{aligned} \quad (3.4)$$

The Z^i are classical Dirac observables. They parametrize the reduced phase space $\hat{\Gamma}$, and the Poisson bracket on $\hat{\Gamma}$ can be derived from (3.4) (equivalently, the symplectic

structure on $\hat{\Gamma}$ can be obtained from (3.3). Now, for each value of τ , one obtains a cross-section of the orbits. Evaluating (3.3) at a fixed value of τ , the RHS is a function on the reduced phase space, and hence an observable. Thus, (3.3) defines a 1-parameter family of observables corresponding to each z^μ . These are the Heisenberg observables. Note that as Heisenberg observables, the Poisson brackets between z^μ are to be evaluated on $\hat{\Gamma}$, and can be evaluated at different times τ .

To construct the reduced space quantum theory, one has to represent the classical Dirac observables Z^i as (Hermitian) operators \hat{Z}^i on some Hilbert space of physical states. Physical interpretations and dynamical information about any function on $\bar{\Gamma}$ can be obtained from the operator analog of (3.3):

$$\hat{z}^\mu(\tau) = :z^\mu(\hat{Z}^i, \tau):, \quad (3.5)$$

where $:z^\mu:$ indicates that difficult factor ordering problems may have to be resolved in order to make the RHS a well-defined operator. For each value of the parameter τ , (3.5) defines an operator on physical states corresponding to the classical function z^μ . We can easily generalize this to arbitrary functions $f(z^\mu)$ on the constraint surface. Corresponding to f we have the 1-parameter family of physical operators

$$\hat{f}(\tau) = :f(z^\mu(\hat{Z}^i, \tau)): . \quad (3.6)$$

As always with the reduced space approach to quantum theory, the complete classical solution is necessary before one can even begin to quantize. In the absence of the classical solution, one can not even “get off the ground”.

On another note, an important conceptual difference between this approach and that of the previous section is that here the full constraint is thought of as the generator of dynamical evolution, whereas in the Schrödinger approach, a piece of the constraint is considered as the true Hamiltonian. Correspondingly, while the time variable one obtains in the Schrödinger approach is an “internal” time, obtained explicitly right from the start as a specific function of the elementary operators, the time variable in the reduced space approach is an “external” time, only implicitly defined by the solutions (3.3). Since the time is an external variable (it belongs to a different set of coordinates on $\bar{\Gamma}$) the z^μ are treated democratically in the sense that not one of them is singled out beforehand as a time variable.

6.4 Bianchi I model

In this section I will illustrate the above approach to the physical interpretation of constrained dynamical systems by studying Bianchi I model in some detail. As a practical application I will analyze the issue of singularities in quantum cosmology. As we saw in section 3.4 (see also [11]), the reduced space and Dirac quantum theories of the solvable models are kinematically equivalent. Since the issues will be conceptually easier to grasp, I will take the reduced space approach to the canonical quantization of Bianchi I.

On the spatially homogeneous (SH) slices introduce a SH co-basis, ω^i (see [13, 14, 12]). For Bianchi I this basis of 1-forms satisfies $d\omega^i = 0$. In this basis, the components

of the 3-metric on the SH slices are constants. Further, there is a spacetime symmetry [15] which allows one to eliminate the off-diagonal components of the 3-metric q_{ij} and its conjugate momentum p^{ij} . In this gauge, the diffeomorphism constraint of general relativity vanishes identically. The gravitational phase space Γ is thus the cotangent bundle over the configuration space \mathcal{C} parametrized by the 3 diagonal components q_i of the metric. Define new coordinates on \mathcal{C} by

$$\begin{pmatrix} \beta^0 \\ \beta^+ \\ \beta^- \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/6 & 1/6 & -1/3 \\ 1/2\sqrt{3} & -1/2\sqrt{3} & 0 \end{pmatrix} \begin{pmatrix} \ln q_1 \\ \ln q_2 \\ \ln q_3 \end{pmatrix}. \quad (4.1)$$

The canonically conjugate momenta are

$$\begin{pmatrix} \pi_0 \\ \pi_+ \\ \pi_- \end{pmatrix} = 2 \begin{pmatrix} q_1 & q_2 & q_3 \\ q_1 & q_2 & -2q_3 \\ \sqrt{3}q_1 & -\sqrt{3}q_2 & 0 \end{pmatrix} \begin{pmatrix} p^1 \\ p^2 \\ p^3 \end{pmatrix}, \quad (4.2)$$

so that the symplectic structure is $\Omega = d\pi_A \wedge d\beta^A$, $A = 0, \pm$. In terms of the momenta, the diagonal components of the extrinsic curvature can be obtained via $K_i = \frac{1}{V} (p^j q_i^2 - \frac{1}{2}(\sum_j p^j q_j) q_i)$, where $V = (q_1 q_2 q_3)^{1/2}$ is the spatial volume element.

In cosmological models, in the gauge $N = \text{const.}$, the supertime (the affine parameter along the dynamical trajectories in phase space) can be identified with the proper time of an unaccelerated observer whose world line is orthogonal to the SH slices. In this physical time gauge, the initial singularity in classical theory occurs at a finite time in the past.

Choosing $N = 4$, the scalar constraint for Bianchi type I is

$$C = \frac{1}{6} e^{-3\beta^0} \eta^{AB} \pi_A \pi_B = \frac{1}{6} e^{-3\beta^0} (-\pi_0^2 + \pi_+^2 + \pi_-^2). \quad (4.3)$$

For an expanding universe, there is an additional nonholonomic constraint $\pi_0 < 0$. (See subsection 4.2 for a complete discussion of this choice.)

Let τ be an affine parameter along the ‘‘gauge’’ orbits generated by the constraint, chosen as in the previous section such that $\dot{f} \equiv \frac{\partial f}{\partial \tau}$. Then the Heisenberg equations of motion are $\dot{f} = \{f, C\}$. For Bianchi type I these can be easily solved on the constraint surface, to yield

$$\begin{aligned} \pi_{\pm} &= p^{\pm}, \\ -\pi_0 &= p^0 := \sqrt{(p^+)^2 + (p^-)^2}, \\ \beta^0(\tau) &= \frac{1}{3} \ln(p^0 \tau), \\ \beta^{\pm} &= b_{\pm} + \frac{p^{\pm}}{3p^0} \ln \tau, \end{aligned} \quad (4.4)$$

where $\tau \geq 0$, the initial value of β^0 has been chosen to simplify the solutions, and the initial data (b_{\pm}, p^{\pm}) are canonical coordinates on the reduced phase space $\hat{\Gamma}$. The reduced symplectic structure (which can be obtained by pulling back the symplectic structure on Γ to the constraint surface, and then evaluating at some fixed value of τ ,

say $\tau = 1$) is $\hat{\Omega} = dp^{\hat{A}} \wedge db_{\hat{A}}$, $\hat{A} = \pm$. Thus $\hat{\Gamma}$ is the cotangent bundle over the reduced configuration space $\hat{\mathcal{C}} = (\mathbf{p}^+, \mathbf{p}^-)$.

The algebra of elementary, reduced space observables is given by the commutation relations

$$[\hat{b}_{\hat{A}}, \hat{p}^{\hat{B}}] = i\hbar \delta_{\hat{A}}^{\hat{B}}. \quad (4.5)$$

From the point of view of later calculations, it is convenient to choose the (p)-representation for quantum theory. The states $\psi = \psi(\mathbf{p}^+, \mathbf{p}^-)$ are C_0^∞ functions on $\hat{\mathcal{C}}$, and the operators are represented by

$$\begin{aligned} \hat{p}^\pm \circ \psi(\mathbf{p}^+, \mathbf{p}^-) &= \mathbf{p}^\pm \cdot \psi(\mathbf{p}^+, \mathbf{p}^-) \\ \hat{b}_\pm \circ \psi(\mathbf{p}^+, \mathbf{p}^-) &= i\hbar \frac{\partial}{\partial \mathbf{p}^\pm} \psi(\mathbf{p}^+, \mathbf{p}^-). \end{aligned} \quad (4.6)$$

One can immediately see that the operators are symmetric with respect to the inner product

$$\langle \psi | \phi \rangle = \int_{\hat{\mathcal{C}}} d^2\mathbf{p} \bar{\psi} \phi. \quad (4.7)$$

6.4.1 Physical interpretation

To extract a physical interpretation, we have to “quantize” the classical solutions (4.4). The 1-parameter families of quantum “Heisenberg observables” are

$$\begin{aligned} \hat{\pi}_\pm &= \hat{p}^\pm, & -\hat{\pi}_0 &= \hat{p}^0 = \sqrt{(\hat{p}^+)^2 + (\hat{p}^-)^2}, \\ \hat{\beta}^0(\tau) &= \frac{1}{3} \ln(\hat{p}^0 \tau), & \hat{\beta}^\pm(\tau) &= \hat{b}_\pm + \frac{\hat{p}^\pm}{3\hat{p}^0} \ln \tau. \end{aligned} \quad (4.8)$$

Note that while the β^A are not by themselves Dirac observables, and are thus not well defined operators on the space of physical states, when they are expressed as Heisenberg operators (4.8) then (up to factor-ordering) they do have a well-defined action on the physical states. We can represent the Heisenberg observables on physical states by

$$\begin{aligned} \hat{\pi}_\pm \circ \psi &= \mathbf{p}^\pm \psi, \\ \hat{\pi}_0 \circ \psi &= \mathbf{p}^0 \psi, \\ \hat{\beta}^0(\tau) \circ \psi &= \frac{1}{3} \ln(\mathbf{p}^0 \tau) \psi, \\ \hat{\beta}^\pm(\tau) \circ \psi &= i\hbar \frac{\partial}{\partial \mathbf{p}^\pm} \psi + \frac{\mathbf{p}^\pm}{3\mathbf{p}^0} (\ln \tau) \psi. \end{aligned} \quad (4.9)$$

For Bianchi I we have the good fortune that there is a representation in which there are no (insurmountable) factor-ordering problems, at least for the elementary Heisenberg observables.

Note that the above procedure allows one to represent *any* phase space function as a 1-parameter family of Heisenberg operators on physical states. Corresponding to any classical phase space function $f(\beta^A, \pi_A)$, by substituting (4.9) we have the Heisenberg operator

$$\hat{f}(\tau) = :f(\beta^A(\hat{b}_{\hat{A}}, \hat{p}^{\hat{A}}, \tau), \pi_A(\hat{b}_{\hat{A}}, \hat{p}^{\hat{A}}, \tau)): \quad (4.10)$$

where $:f$: indicates an appropriate factor-ordering.

Some observables of particular interest are the 3-volume $V = \exp(3\beta^0)$ and the trace of the extrinsic curvature $\text{tr}K = -\frac{1}{4}\pi_0 \exp(-3\beta^0)$. The Heisenberg operators are

$$\widehat{V}(\tau) \circ \psi = \widehat{p}^0 \tau \circ \psi = \tau p^0 \psi, \quad \widehat{\text{tr}K}(\tau) \circ \psi = \frac{1}{\tau} \psi. \quad (4.11)$$

We see from the above expression that the quantum operator corresponding to the spatial volume vanishes as $\tau \rightarrow 0$; and that the operator corresponding to the trace of the extrinsic curvature becomes unbounded. This gives us a hint of things to come in the next section.

Ideally, one would like to eliminate the τ entirely from the above equations, since in general relativity we do not have an external time. (For a recent review of the issue of time in quantum gravity, see [16].) Rovelli's suggestion for the general case [3] is that this can be done by substituting the quantum version of the solution $\tau = -\frac{4}{\pi_0} \exp(3\beta^0)$ back into the rest of the Heisenberg observables (4.9). However, in general, this is an ill-defined procedure, since it is the quantum analog of substituting part of a coordinate transformation back into itself.

In this framework, there is an alternate viewpoint one can take on the issue of time, which is to *eliminate the time τ interpretationally*, by asking only *relational* questions. Consider Bianchi I. As an Heisenberg operator, $\widehat{\text{tr}K}$ commutes with all other operators. Conceivably, we can measure $\text{tr}K$, and this provides us with a “time”. Now we can simultaneously measure any other phase space function of interest, say the volume. As a result of such an experiment (which involves 2 measurements) one would make a physically meaningful statement of the form: “At the time $\text{tr}K = 3$, the universe was found to be half full.”

6.4.2 The initial singularity in quantum cosmology

Classically, for generic solutions, the initial singularity is a curvature singularity in Bianchi type I: the Weyl curvature squared scalar $W^2 := C_{abcd}C^{abcd}$ blows up at a finite time in the past. What happens to this behaviour in the quantum theory?

The operator we would like to analyse is the Heisenberg observable corresponding to W^2 . Thus we want to express W^2 in terms of the Cauchy data: either the 3-metric and extrinsic curvature or, equivalently, the pair (β^A, π_A) . By a *P2C2E*⁶ it follows that [18]

$$W^2 = \frac{1}{216} e^{-12\beta^0} \pi_0^4 (1 + \cos 3\theta), \quad (4.12)$$

where $\theta = \tan^{-1}(\pi_-/\pi_+)$ is an angular coordinate on the π_{\pm} plane. (Note that here as in full general relativity, the Weyl scalar is independent of the lapse (and shift) [18, 19].)

Substituting the classical solutions (4.4), the classical Heisenberg observable, in terms of the reduced space observables is

$$W^2(\tau) = \frac{32}{27\tau^4} (1 + \cos 3\Theta) \quad (4.13)$$

⁶“Process Too Complicated To Explain” [17].

where $\Theta = \tan^{-1}(p^-/p^+)$ is an angular coordinate on the reduced configuration space. Fortunately, in the (p) -representation the factor ordering of (4.13) is trivial. The action of the Heisenberg operator corresponding to the Weyl scalar on physical states is

$$\widehat{W}^2 \circ \psi(p^+, p^-) = \frac{32}{27\tau^4} (1 + \cos 3\Theta) \cdot \psi(p^+, p^-) . \quad (4.14)$$

As $\tau \rightarrow 0$, the whole spectrum of W^2 blows up. Clearly, the classical spacetime singularity persists in quantum theory. Similar results have been obtained previously by Gotay and Demaret [21]; and for Gowdy models by Husain [22]. Such results for Bianchi models have also been hinted at in [12, pp. 198].

Remarks:

Remark 1

Since τ is thought of as a fiducial parameter, one is perhaps more interested in relating W^2 to some other physical quantity, say $\frac{1}{\text{tr}K}$. (As Gotay and Demaret have pointed out [21], since this is a relativistic model, one is free to rescale the parameter time so that the singularity does not occur at a finite parameter time. When one does this in the classical theory, though, certainly no one claims that the singularity has been eliminated.) Then, the relational statement is that W^2 blows up when $\frac{1}{\text{tr}K}$ vanishes. However, there is no guarantee that $\frac{1}{\text{tr}K}$ itself vanishes at some finite time as measured by a physical clock. I have chosen a time parameter τ for the quantum theory which appears to be closest to a classical time in which the Universe has existed for a finite time only, and corresponds to the proper time for an unaccelerated observer.

Remark 2

Functions with support only on the regions $\Theta = \pi, \pm\frac{\pi}{3}$ are indeed annihilated by the Weyl scalar operator (4.14), for all times τ . However, these functions are not normalizable states in the Hilbert space. Furthermore, the classical spacetime constructed from initial data which lies in this region is just locally flat space⁷. So, for this region of the reduced phase space, there is no curvature singularity classically either.

Remark 3

Note that the same result can be obtained even if one quantized the theory using the operator constraint method of Dirac, since in the β^A representation the observables (4.8) and the Weyl scalar (4.13) are at most linear in momenta and do not pose any factor-ordering problem. Alternately, since the constraint (4.3) can be written in the form of

⁷Louko [20] has pointed out that while the origin (in the (p^+, p^-) plane) corresponds to Minkowski space, the other points on $\Theta = \pi, \pm\frac{\pi}{3}$ correspond to spacetimes with conical singularities. To study the behaviour in quantum theory of these solutions, one could, for example, express the deficit angle as a function on the phase space and then use (4.10) to construct the corresponding quantum operator on physical states.

a nonrelativistic free particle (2.1)

$$C \equiv p_0 + H = 0, \quad \text{where} \quad H = \sqrt{(p_+)^2 + (p_-)^2}, \quad (4.15)$$

we can carry out the analysis using the formalism of section 2. Though this corresponds to a different time parametrization, the qualitative results will be the same. The persistence of the singularity in quantum theory is independent of whether or not one “quantizes” the constraint, and the singularity can not be avoided by exploiting any factor ordering ambiguity.

Remark 4

At least some of the potential ambiguities and inconsistencies in a quantum theory of gravity arise from a choice of a time variable which corresponds to *3-dimensional, spatial* scalars (like the volume V or $\text{tr}K$). In order to eliminate some of these inconsistencies, and possibly even for aesthetic reasons, one may require the time variable to be *4-dimensional, spacetime* scalar. One such choice would be to use the Weyl scalar itself (or some other curvature scalar) as a time variable. One obvious disadvantage, indicated by (4.14), is that with this requirement we may have to give up a state-independent notion of time. However, this appears to be a promising avenue for exploration.

Remark 5

This way of formulating the problem relies heavily on the solvability of the model. Over and above the solvability, though, it was essential that the final expression for the Weyl scalar as a Heisenberg observable was relatively simple. Consider what happens in the next simplest homogeneous cosmology. Bianchi type II, as we saw in section 3.4, is kinematically completely solved. One can even find an explicit expression for the classical Heisenberg observable corresponding to the Weyl scalar. However, this expression is horrendous, involving products of exponentials and quartics in the elementary reduced space operators, and I have been unable so far to construct a good quantum operator.

In spite of the factor-ordering difficulties one can make some qualitative claims: There is again a pre-factor $1/\tau^4$ in the classical expression of the Heisenberg observable corresponding to the Weyl scalar. Thus if there is *any* factor-ordering which makes the operator well-defined and non-trivial at some non-zero time, it is sure to blow up at $\tau \rightarrow 0$. This is likely to be a fairly generic feature of all the solvable cosmological models (see [11]).

6.4.3 (†) Expanding or contracting Universe, or both?

I will now discuss the choice of sign of π_0 . When solving the constraint, I assumed a specific choice, $\pi_0 < 0$, corresponding to an expanding universe. Suppose that one does not make this choice. Then, the projection of the constraint surface into the configuration space is the entire null cone, $-\pi_0^2 + \pi_+^2 + \pi_-^2 = 0$. However, the future (contracting Universe) and past (expanding Universe) null cones are “dynamically disconnected” from each other (and in fact from the origin): in the sense that there are no (continuous)

observables which will map a point in the future null cone to a point in the past null cone, since all vector fields on the cone have to vanish at the origin. There is of course a discrete transformation, $T : \pi_0 \mapsto -\pi_0$, corresponding to time reversal. The corresponding operator is superselected, it commutes with all the rest of the elementary Dirac observables (b_{\pm}, p^{\pm}) . Thus the reduced phase space consists of two disconnected sectors, namely the cotangent bundles over the past and future null cones. The Hilbert space of states on any one half carries a faithful unitary representation of the algebra of (continuous) Dirac observables (b_{\pm}, p^{\pm}) . The Dirac operators \hat{b}_A, \hat{p}^B are block diagonal and are represented on each half of the Hilbert space by (4.6). The two halves are distinguished by the sign of π_0 , $\pi_0 = \pm p^0 = \pm \sqrt{(p^+)^2 + (p^-)^2}$ on the future and past halves respectively.

However, the Heisenberg observables *do* have different representations on each half. (4.9) represents the Heisenberg observables (4.8) on the past half of the Hilbert space. On the future half, the representation can be obtained simply by replacing $p^0 \mapsto -p^0$. Hence we see that on the future (contracting) half, due to our choice of the initial value of β^0 , $\tau \leq 0$, and the singularity occurs at a finite time in the future.

Since there is no tunneling between states in either half of the Hilbert space, if the universe is in an expanding state, it is consistent to do quantum theory entirely in this half. Else, one has to contend with the following scenario: one can find appropriate choices of the initial values for β^0 such that the ranges of τ in each half overlap. Now consider “mixed” states, say eigenstates of \hat{T} . In such a state, the Weyl scalar operator blows up at both a finite time in the past and a finite time in the future. Clearly, it is only sensible to restrict oneself to one half of the Hilbert space, say the expanding half.

6.5 Discussion

Both the Schrödinger and the reduced space approach have noteworthy features:

1. In the Schrödinger approach of section 2, it is absolutely essential that the constraint be deparametrized and written in the form $C = p_0 + H$, where the true Hamiltonian H is its own \star -adjoint, so that it is represented on physical states by a Hermitian operator. Furthermore, as I have emphasized before, the solutions are only formal, and a substantial amount of work is still required in order to obtain physical predictions. However, there is at least a kinematical framework within which various issues can be addressed.
2. On the other hand, the reduced space approach works for any form of the constraint, as long as it is classically solvable. When the complete classical solution is known, one can again construct the kinematical quantum theory. The difficulties have to do with factor-ordering *known* classical expressions for the Heisenberg observables.
3. Time plays a slightly different role in the two approaches. In the Schrödinger approach, it is essential to single out a time variable before one can proceed further. This time is an *internal time* in the sense that this variable and its conjugate

momentum are part of the set of elementary variables. Dynamics, or evolution in this internal time, is generated not by the constraint, but by the true Hamiltonian, via $\hat{f} = \frac{1}{i\hbar}[\hat{f}, \hat{H}]$.

This is in contrast to the reduced space approach (which is more closely related to ordinary gauge theories), in which to begin with time is just an affine parameter along the gauge orbits, *undetermined* as a function on $\bar{\Gamma}$ until *after* the classical equations of motion have been solved. Then, it is part of a new set of coordinates on $\bar{\Gamma}$, related to the elementary variables by a canonical transformation generated by the constraint. In this picture, time evolution is generated by the constraint itself, via $\dot{f} = \{f, C\}$. This approach is more democratic, since *a priori* all the elementary variables are treated on an equal footing. Further, since only relational questions are asked, this is a more relativistic approach. If at all, a particular phase space function is identified with time only after the complete solutions are obtained, and then, this is done only interpretationally.

4. Of course, in the Schrödinger approach one can attempt standard perturbation techniques. In addition, both approaches lend themselves to another approximation technique. The idea here is to truncate the equations of motion in “time”. In the Schrödinger approach, this amounts to expanding either (2.12) or (2.14) using the Baker-Hausdorff lemma and retaining only a finite number of terms. On Schrödinger states, the approximate Heisenberg observables are then given by:

$$\hat{Z}_{(k)}(\tau) = \hat{z} + \frac{\tau}{i\hbar} [\hat{z}, \hat{H}] \Big|_{\tau=0} + \dots + \left(\frac{\tau}{i\hbar}\right)^k [..[[\hat{z}, \hat{H}], \hat{H}].., \hat{H}]^k \Big|_{\tau=0} \quad (5.1)$$

where it is understood that the terms on the RHS, since they are evaluated at $\tau = 0$, are functions of \hat{Z} . The Hilbert space structure can be used to make various truncated operators well defined. The constraint is obviously exactly satisfied. Such an approach can be used on certain Bianchi models [10] which are not exactly soluble, but where the existence of a causal supersymmetry permits one to do a \pm frequency decomposition of the constraint, identify the true Hamiltonian and construct a physical Hilbert space.

In the reduced space approach an approximation is needed before one can even construct a Hilbert space, but the approximation itself is done classically, so perhaps it has some advantages. The idea here is to truncate the Taylor series for the observables (3.2) at finite order in τ :

$$z_{(k)}^{\mu}(\tau) = \sum_N^k \frac{\tau^N}{N!} \left(\frac{\partial^N z^{\mu}}{\partial \tau^N} \right) \Big|_{\tau=0}, \quad (5.2)$$

where $\frac{\partial f}{\partial \tau} = \{f, C\}$ and the RHS is in terms of Z . Pictorially, one identifies a particular cross-section of the gauge orbits with $\hat{\Gamma}$ and then, to extract dynamical information one approximates the gauge orbits by higher and higher order polynomials in τ . The constraint can either be solved exactly, or to a particular order only.

Clearly, such approximation techniques will *not* provide answers about the existence or structure of singularities, the issue of chaos in Bianchi IX etc. It is not immediately obvious which interesting issues in quantum gravity can be addressed by applying *such* approximations.

5. Yet another possibility is a hybrid approach. The major flaw of the Schrödinger approach is that the constraint has to be deparametrized, while in the reduced space approach one has to find the full classical solutions. In a hybrid approach, one might try to repeat the construction of section 3, but quantum mechanically. One might look for quantum versions of the solutions (3.2), or undeparametrized versions of (2.12):

$$\hat{Z}(\tau) = e^{\frac{i}{\hbar}\hat{C}\tau}\hat{z}e^{-\frac{i}{\hbar}\hat{C}\tau}. \quad (5.3)$$

Unfortunately, this naive extension of the approach of section 3 to Dirac quantization is inconsistent, for a multitude of reasons. However, some possibilities appear worth investigating.

I do not want to give the impression that the approaches described in sections 2 and 3 are the only way to obtain physical interpretations of a theory. Quantum gravity will certainly have many inter-related “phases”: isolated, asymptotically flat systems in which one may be interested in quantum effects on the spectrum of gravitational radiation from binary stars; strong curvature/black hole regimes with particle production; microstructure of spacetime, wherein will lie the justification for and understanding of quantum field theory; cosmology and large scale structure. These phases may or may not all be described by the “same” quantum theory, and certainly the questions one asks will be very different. The above approach to physical interpretations is clearly not applicable in all the regimes. Also, many classically important, Kepler-like questions, e.g. the deflection of light, the Shapiro time delay, the precession of the perihelion, decay of the orbital frequency of binaries, etc. may not be relevant questions in quantum gravity.

However, one question we do know will be important is whether a quantum theory of gravity is free of curvature and other singularities (which we know are generic in classical theory) or renders them irrelevant, or leads to a better picture of their “internal structure”. The above framework for physical interpretation is applicable to this question, at least in the context of quantum cosmology. The result, that the classical singularity persists in quantum cosmology, leads one to the conclusion that homogeneous cosmologies as models of full general relativity are far too simplistic and fail to share some of its essential features. For example, due to the imposition of spatial homogeneity, the behaviour of the geometry of spacetime on the micro-scale is frozen out. The possible discrete nature of the spatial geometry on the small scale, which would be one avenue to avoid singularities and infinities in quantum theory obviously never plays a role in the quantum theory. In this light the above result is not surprising.

On the other hand, the result agrees with the “rule of unanimity”. Wheeler’s conjecture [23] was that in cosmological models, if *generic* initial data evolved classically to a singularity in finite time, then generic physical states would have support on such data and the singularity would still be present in the quantum theory. Where classically there are powerful theorems that fairly generic initial data evolve in finite time to a

singularity, is it too speculative to wonder if such a rule of unanimity applies to full quantum gravity as well?

Bibliography

- [1] Arnowitt R, Deser S and Misner C W 1962 in *Gravitation: An Introduction to Current Research* Witten L (ed) (John Wiley New York)
- [2] Kuchař K 1981 in *Quantum Gravity 2: A Second Oxford Symposium* Isham C J, Penrose R and Sciama D W (eds) (Clarendon Press Oxford)
- [3] Rovelli C 1991 *Phys. Rev.* **D43** 442
_____ 1992 *private communication* Pittsburgh January 1992
- [4] Rovelli C 1990 *Phys. Rev.* **D42** 2638
- [5] Ashtekar A 1989 in *Conceptual Problems in Quantum Gravity* Ashtekar A and Stachel J (eds) (Birkhäuser Boston)
- [6] Ashtekar A 1992 *private communication* Syracuse
- [7] Ashtekar A and Tate R S Syracuse University pre-print in preparation
- [8] Ashtekar A 1991 Lectures on *Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore), see chapter 10
- [9] Kuchař K 1992 *private communication* Cincinnati March 1992
- [10] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-5
- [11] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-6
- [12] Ryan M P and Shepley L C 1975 *Homogeneous Relativistic Cosmologies*, (Princeton University Press Princeton)
- [13] MacCallum M A H 1979 in *Physics of the Expanding Universe* Demianski M (ed) (Springer-Verlag Berlin)
- [14] Misner C W 1972 in *Magic Without Magic* Klauder J (ed) (Freeman San Francisco)
- [15] Ashtekar A and Samuel J 1991 *Class. Quantum Grav.* **8** 2191

- [16] Kuchař K 1992 *Time and interpretations of Quantum Gravity* in *Proceedings of the 4th Canadian Conference on General Relativity and Relativistic Astrophysics* Kunstaatter G, Vincent D and Williams J (eds) (World Scientific Singapore)
- [17] Rushdie S 1990 *Haroun and the Sea of Stories* (Viking Penguin New York)
- [18] Pullin J and Uggla C 1991 *private communication* Syracuse
- [19] Torre C G 1992 *private communication* Cincinnatti March 1992
- [20] Louko J 1992 *private communication* Syracuse April 1992
- [21] Gotay M J and Demaret J 1983 *Phys. Rev.* **D28** 2402
- [22] Husain V 1987 *Class. Quantum Grav.* **4** 1587
- [23] Wheeler J 1977 *Gen. Rel. & Grav.* **8** 713

Chapter 7

DIALOGUE

(This concluding chapter is in the form of a conversation, mostly between two characters: Achilles and the Tortoise. I have borrowed this format from Hofstadter [1]. Other characters put in cameo appearances, the resemblance of any of these characters to real persons is coincidental.)

Achilles: Doubtless, Mr. T, this thesis has presented a reformulation, in an algebraic framework, of the Dirac approach to the quantization of constrained systems. Some rather simple illustrative examples have also been worked out. But what are really the new elements in algebraic quantization? After all, consider the issue of finding the inner product using the Hermiticity conditions on certain operators. Isn't this exactly what we do in ordinary quantum mechanics?

Tortoise: I would object that this not quite so. In ordinary quantum mechanics, Achilles, one has a metric on the configuration space and its volume element defines an inner product on quantum states. One then *checks* that various interesting operators are actually Hermitian in this inner product; if they are not, one symmetrizes them. This leads e.g. to the addition of a $\frac{1}{r}$ term in the representation of the radial momentum operator. Here on the other hand, one stands this procedure on its head. We work with a *fixed* representation of the operators on a complex vector space, and *use* the Hermiticity conditions on them to *find* an inner product. As we saw in various examples ($q-z$ variables for the oscillator and the Bianchi II model), in the configuration representation this process yields differential equations for the measure, which can usually be solved. In some cases of course, no solution may exist. Then one has to start all over again by choosing another linear representation of the algebra of operators.

Achilles: Radical! But what about constrained systems?

Tortoise: As discussed in chapter 1, for constrained systems there really weren't any criteria established for introducing the physical inner product. Typically one could use available background structure (e.g. the metric) to construct the inner product. Or, as in quantum cosmology, this issue was considered of secondary importance and often left unresolved. Consider, e.g., the Bianchi II models. Previously, in the

$\bar{\beta}$ -representation a large number of solutions to the scalar constraint were known. However, it was not at all clear in what sense this set of solutions is complete, or what inner product one could use on these states.

The algebraic framework provides criteria which resolve both these issues: The space of physical states should be large enough to carry a faithful representation of the physical operator algebra; and, the physical inner product on these states should be such that physical operators corresponding to real functions on phase space are Hermitian. Obviously, in order to implement the criteria we need a complete set of physical operators. However, once these criteria were established, we were able to apply them, e.g. to the Bianchi II model, and construct the complete kinematical quantum theory. In this case a clever choice of elementary variables gave us a complete set of physical observables and we then used the Hermiticity relations amongst these to construct an inner product on physical states.

Achilles: Consider that in Bianchi models –and indeed in full general relativity– the scalar constraint contains a term quadratic in momenta whose coefficient defines a (super)metric on the configuration space. Couldn't we have used the volume element of this metric to introduce the inner product?

Tortoise: I don't think so. This volume element does define an inner product on \mathcal{V} , the vector space which carries a representation of the elementary operators themselves. One can certainly use this inner product as a technical device for various intermediate calculations. However, in general physical states are not normalizable with respect to it (as happens in Bianchi II models), and a new inner product has to be introduced. There is another potential problem, illustrated by the coupled oscillators and the A-H model. In these cases, one *can* introduce an inner product on the representation space \mathcal{V} , make the constraint a Hermitian operator on the resulting Hilbert space and then solve the constraint equation. There are normalizable solutions. However, if one does this, the space of physical states may be just too small to capture all the physics.

Consider also the quantum theory of chaotic systems. Perturbation calculations for some systems indicate that the spectrum of the (Hermitian) Hamiltonian becomes non-degenerate as one enters the chaotic regime. Now, certain relativistic cosmologies may well be classically chaotic. For these models, the Hamiltonian is constrained to vanish. If one introduces an inner product on \mathcal{V} itself, and if the spectrum of the Hamiltonian constraint is non-degenerate, we would find at most *one* physical state. Thus this quantum description would again be highly incomplete.

Achilles: I see now that one should first solve the quantum constraints for the physical states, find physical observables and only then construct an inner product, on the space of physical states, that makes the observables Hermitian. But, in previous versions of Dirac quantization most of the emphasis was placed on the solutions to the quantum constraint. Why do we need an inner product on these states? Don't they already contain all physical information?

Tortoise: To extract any physical interpretation one needs a *Hilbert* space of physical states, and a set of operators corresponding to first class functions on the phase space. One needs an inner product on physical states for the same reason as in ordinary quantum mechanics. One is not interested in just the wavefunctions and their support, but in probability *densities*. A particular physical state might be found to have large support in some interesting area of the configuration space, but if the measure itself is very small in that region, then the state will not contribute much in quantum theory.

Achilles: Aha! the A-H model of chapter 4 provides an extreme example of this. There we found *solutions* to the quantum constraint equations which actually had support *entirely* in the classically forbidden, negative energy regions. Since they were normalizable in the fiducial (Euclidean) metric inner product, one was tempted to conclude all sorts of interesting things in the quantum theory. However, since the *physical* inner product *vanishes* in that region, as elements of the Hilbert space, these solutions are identified with the zero state.

Tortoise: Glory be, Achilles! What a good example of the pitfalls associated with jumping to conclusions about the quantum solutions themselves.

Achilles: Another issue that has me confused is the following: In the language of chapter 6, general relativity is a “dynamically constrained system”, in which the generator of dynamics is constrained to vanish. Time is considered to reside in one of the canonical variables. For the sake of discussion, choose a polarization in which the time parameter is a configuration variable. In the Dirac theory, in the configuration representation, wavefunctions –and in particular the physical states– will depend on this time variable. So, any inner product would appear to necessarily involve an integral over the time variable too. Now, if one repeats this in Schrödinger quantum mechanics (where too the states depend on time) –i.e., if one integrates the usual inner product over time to define a *new* inner product– the states will not be normalizable in the new inner product. Doesn’t this indicate that in dynamically constrained systems too, one should first isolate time from the “true” degrees of freedom, and *then* look for an inner product, involving, say, an integral over only the true degrees of freedom? We did this, e.g., in the reduced space quantization of the Bianchi type I and type II models.

Tortoise: True enough, but one is not *forced* to take this approach. Let us consider what happens in the non-relativistic parametrized particle model, which is a paradigm for some dynamically constrained systems. There, as far as the inner product is concerned, we did *not* isolate a time variable. In fact, at the level of the kinematical quantum theory, we did not even *explicitly identify* a time variable. Now, returning to the inner product, this is a 4-dimensional integral over *all* the configuration variables (q^0, q^i). We followed the algebraic program “blindly”, and imposed the Hermiticity conditions on the observables. Lo and behold, we *did* find the inner product on physical states.

Similarly, in the Dirac quantum theory of the Bianchi II models, we did not identify any time variable. Yet, there too, the Hermiticity conditions on observables yield the physical inner product.

In sum, to find the physical inner product, it is *not* necessary to isolate or even identify a time variable. If we have a sufficient number of observables, we can follow the prescription of the algebraic program, and proceed to use the Hermiticity conditions on observables to find an inner product. Time itself could be an approximate or interpretational notion, identified *after* the kinematical quantum theory has been completed.

Achilles: I think I understand the separation of the interpretational or semi-classical role of time from its role in finding an inner product. But, if I recall correctly, something unexpected happened in the non-relativistic parametrized particle, as we proceeded to construct the inner product. Even after we imposed the Hermiticity conditions on all the observables, the dependence of the measure on one of the variables, q^0 , was left undetermined. Using the properties of physical states, this allowed us to choose the measure so that the integral over q_0 was finite; and thus reduce the inner product to a 3-dimensional integral over only the variables q^i .

Tortoise: If you think about it, we do not encounter this unexpected behaviour only in dynamically constrained systems. A similar thing happened in the A-H model, but we didn't pay much attention to it, since it was so incidental at the time. Recall that in the A-H model, the θ dependence of the measure on physical states was undetermined by the Hermiticity conditions on observables. Although one could have done so, *we* certainly did not consider θ to be a time-like variable.

What is common to both models is the following: Recall, that in each model, one of the momentum operators $-p_0$ and p_θ , respectively— is represented by a *multiplication* operator on *physical* states. Thus, we do not have to *require* that $i(\partial/\partial q^0)$ (or $i(\partial/\partial\theta)$) is a Hermitian operator, and the corresponding derivative of the measure is left undetermined.

So you see, this “unexpected” behaviour is quite common, and perfectly reasonable.

Achilles: If we do consider θ to be a timelike variable in the A-H model —i.e. if we consider the constraint itself as the generator of dynamics— then it is a *Euclidean* time, in the sense that if the overall sign for the constraint is chosen so that the potential is negative —and thus corresponds to bound states— then the kinetic energy is positive. In the Bianchi models, the natural time variable is Lorentzian, and in the non-relativistic parametrized particle, the time is Newtonian. Yet in all of these models, we were able to find an inner product.

Tortoise: Hmm..., yes. It certainly appears as if this issue —whether in a particular model the time is Euclidean, Newtonian or Lorentzian— does not play a terribly significant role as far as finding the inner product is concerned.

Achilles: Let me turn now to the second “new” feature: the algebraic relations and their role in quantum theory. Why are these rarely encountered, even in constrained systems like gauge theories?

Tortoise: Typically the configuration spaces one deals with are linear spaces; even for gauge field theories, the configuration space –the space of connections– is an affine space. Hence one has the luxury of introducing Cartesian coordinates and doing quantum theory. Or, as in problems with spherical symmetry, one is sloppy and uses spherical “coordinates”. As elementary variables for the quantum theory, such coordinates are complete but not overcomplete and there are no algebraic relations between them. In simple cases, one can get by because one has experience in handling pathologies that arise at points (such as the poles on the 2-sphere) where the “coordinate systems” fail. In general, however, one can simply get incorrect results.

Beaver: But Mr. T, why do you call this feature “new”? I think one does encounter algebraic relations in ordinary quantum mechanics. Consider something like $\widehat{x}\widehat{p} = \frac{1}{2}(\widehat{x}\widehat{p} + \widehat{p}\widehat{x})$, isn’t it an algebraic relation?

Tortoise: In the usual treatment of quantum mechanics, x , p and 1 are the elementary variables; xp is not. The relation you mentioned is actually a definition of the *new* operator $\widehat{x}\widehat{p}$ in terms of the known expressions for the operators \widehat{x} and \widehat{p} .

Achilles: I am still somewhat unfamiliar with this concept. Are there situations in which algebraic relations are unavoidable?

Tortoise: Yes. One situation occurs when one cannot find Cartesian coordinates. Consider the case when the configuration space is a non-trivial manifold (e.g. S^1), and does not admit a global coordinatization. Unfortunately, one does not know how to do quantum mechanics on (collections) of patches. One has two options: the first is to imbed the configuration space into some \mathbb{R}^n, \dots

Achilles: Which is usually how the configuration space is given to us in the first place.

Tortoise: ... then the finite number of imbedding functions are the algebraic relations on the elementary variables. For example, for T^*S^1 , we used the set $(1, q_1 = \sin \theta, q_2 = \cos \theta, p)$, and the imbedding function is $(q_1)^2 + (q_2)^2 - 1 = 0$.

The second option is to consider the space of a large class of –or indeed, all– functions on configuration space and a similar class of functions linear in momenta, as we did for the Bianchi II model. There are then infinitely many algebraic relations, which have to be represented in quantum theory.

Achilles: Could it happen that the phase space itself is a well-defined manifold, but for which there is no configuration space?

Tortoise: Yes, such situations arise when one constructs the reduced phase space for a classical constrained system. For example, for the model in section 5.7 (two oscillators with the energy sum as a constraint), the reduced phase space is S^2 .

There is another situation in which algebraic relations are unavoidable, in spite of the trivial topology of the phase space. This situation can arise because we are interested in the manifold as a *symplectic* space, not just as a topological or metric space. The Cartesian coordinates on the phase space may not be canonical, and in fact may not generate a vector space closed under Poisson brackets. Then one is forced to enlarge the set of operators, even though it is complete, and this leads to algebraic relations. For example, when the energy difference is imposed as a constraint on a system of two oscillators (chapter 5) the reduced phase space is topologically \mathbb{R}^2 , and Cartesian coordinates are J_{\pm} . However, $\{J_+, J_-\} = (J_+J_- + \delta^2)^{1/2}$; as a symplectic manifold, it is natural to consider the phase space to be the future mass shell in 3-dimensional Minkowski space. In order to do quantum theory, one has to introduce the additional function $J_z = (J_+J_- + \delta^2)^{1/2}$, and the appropriate algebraic relation.

So, algebraic relations on \mathcal{S} arise due to the twin requirements that \mathcal{S} should be (over)complete *and* closed under Poisson brackets. When there are algebraic relations, as we learned from the example of the particle on S^1 , the anticommutation relations have to be imposed in quantum theory to ensure that one stays on the correct, physical sector of the theory.

Achilles: Hmm... (*long pause as he digests all this*) now I am confused about something else. General relativity in the new variables was mentioned as part of the motivation for formulating an approach which encompasses such algebraic relations. But it is a theory of the dynamics of a connection and so the configuration space is an affine space. Why are there algebraic relations in the connection-dynamical formulation?

Tortoise: True, the algebraic relations are neither unavoidable nor necessary in the classical theory. However, it currently appears that *loops* play a fundamental role in quantum gravity. For example, the loop variables seem indispensable to express and regulate physically interesting operators without reference to background fields such as a metric or a connection. It is, in particular, natural to consider the holonomies of the connection around loops as the elementary configuration variables for quantum theory. These holonomies are genuinely *overcomplete*, and hence it is perhaps not surprising that there are algebraic identities between them. However,...

Achilles: However,...

Tortoise: ...since the loop variables are nonlocal quantities...

Achilles: ...since general relativity is a field theory...

Tortoise: ...the counting of the number of algebraic identities is quite non-trivial.

Achilles: ...the counting of the number of algebraic identities is quite non-trivial.

I see now that the algebraic approach provides a framework for *canonical* quantization which is general enough to apply to a large class of constrained systems,

including general relativity. Also, I think I understand the role of the two new ingredients in this approach, the use of the Hermiticity conditions on observables to fix the physical inner product, and the presence and incorporation of algebraic relations. However, I still have some questions about the general framework. In the first place, it is not really a constructive *procedure* for quantization. For example, one is instructed “to find a representation of \mathcal{A} ”, but *how* one should do this is left unspecified. On the other hand, in Schrödinger mechanics one is explicitly given a representation. Even in path integral quantization, fairly detailed instructions are issued, it is another matter that there are immense technical difficulties in carrying them out.

Giselle: In this sense perhaps geometric quantization is also “not constructive”; one is told to “find a polarization” on phase space, but one is not told how to explicitly construct it. However, I get your general drift, Achilles.

Tortoise: Yes, there is certainly much more freedom in the algebraic framework. There are specific steps at which crucial choices have to be made. The first is in the selection of the set of elementary functions and a linear representation of the resulting operator algebra. In general there will exist many overcomplete sets, and representations of the corresponding algebras may be equally easy (or difficult) to find. However, these choices will have ramifications later, in terms of the ability to complete the quantization. A poor choice for \mathcal{S} may make it difficult to solve the constraints or find physical operators.

Owl: **P**ardon me for interrupting, but a dramatic example is provided by the Bianchi II model. In the $\bar{\beta}$ variables, even though the constraint had been solved “explicitly” in terms of power series solutions, a complete set of physical operators was not known. In retrospect we can see why: in terms of the $\bar{\beta}, \bar{\pi}$ variables the classical expressions for the *physical observables* are ridiculously complicated. While apparently suitable in the sense that they satisfy the requirements of completeness and closure, the $\bar{\beta}, \bar{\pi}$ variables are not adapted to the symmetries of the constraint and the algebra of observables. In contrast, when we introduce the symmetry adapted variables $(\tilde{\beta}, \tilde{\pi})$, the construction of the complete quantum theory is almost trivial.

Tortoise: As another example of a poor choice of \mathcal{S} , consider the coupled oscillators, in real Cartesian coordinates and the Schrödinger representation. A few minutes of toying around will convince anyone that this choice of variables and representation is obviously ill-suited to construct solutions to the constraint equation, particularly for the generic case when the energy difference is non-integer. Solutions are products of generalized Hermite polynomials with non-integer indices, and things are a total mess.

van Gogh: Right, but considerable improvement is achieved by using a z_1, z_2 representation. However, a naive power series ansatz or the holomorphic representation does not yield all physical states, since solutions to the constraint contain real—rather than integral—powers of z_1, z_2 . In a more sophisticated representation,

physical states are Bessel functions, and while it is quite unobvious and somewhat technically difficult, a physical inner product can be found.

Tortoise: I have no objection in principle to technical difficulties. However in this case it seems that the technical difficulties may thwart one from considerable physical insight. Consider on the other hand the angular momentum like representation for the coupled oscillators. This is the ideal situation: the representation is well adapted to the algebra of observables and chosen such that the constraint is actually diagonal, solving it is then a piece of cake.

Achilles: That brings up another question. Is there freedom in the choice of the physical observables too?

Tortoise: Yes. A trivial source of freedom is just the re-coordinatization of the reduced phase space. Consider the coupled oscillators again. Since the reduced phase space is topologically \mathbb{R}^2 , one could introduce operators corresponding to radial/angular coordinates.

Achilles: Except that in quantum theory, there are obvious difficulties with this, since the radius (squared) and the angle are then conjugate to each other.

Tortoise: I agree. To continue my point, a choice with non-trivial implications presents itself in the quantization of the A-H model. There was an obvious choice of a set of physical operators which is locally overcomplete. However, as we saw, this set failed to capture some of the *global* structure of the reduced phase space, and led to results that are qualitatively different from the correct ones. In most other examples (recall e.g., the Bianchi I model) the choices were rather obvious, and so it is difficult to construct good examples of bad choices.

Achilles: Now, in the next step, we have to implement the \star -relations on \mathcal{A}_{phy} to find the physical inner product. If I recall correctly, in both the Bianchi II model and the coupled oscillator model, even after all the Hermiticity conditions are imposed there is freedom to choose the inner product. For, as we have seen, the \star -relations fix only the *relation* between the representation and the inner product. We are free to choose an inner product, as long as the representation is fixed appropriately, or vice versa.

Tortoise: Sure. But in the examples you mention, this freedom is rather trivial. It is easy to see that these choices yield the same, i.e. unitarily equivalent, quantum theories. It is still useful though, since we can use this freedom to simplify the representations of interesting observables.

Achilles: To summarize then, the power of this approach arises from a tension between two contrasting aspects: the tight set of criteria that various choices should satisfy, and the looseness in prescribing what those choices should be.

Tortoise: Exactly. When taking the algebraic approach to the quantization of a problem, one has to use one's physical intuition for the problem in making these choices.

One has to anticipate the structures (mainly \mathcal{A}_{phy}) that arise in later steps, and use this knowledge to guide the decision-making in the earlier steps, just as in a conversation one sometimes has to anticipate the other person's thoughts in order to decide what to say. For example, in many of the models we considered, we used detailed insight into the algebra of observables before finally selecting a representation of the elementary algebra \mathcal{A} itself.

Achilles: I was thinking ... (*Appears lost in thought.*) ... about the A-H model again. First, it clearly indicates that one cannot always *sequentially* follow the steps outlined in section 2.3. In this model, after step 5, we have a large set of solutions to the quantum constraint equation. However, the operators that leave this space invariant do not form a \star -algebra, and we seemed to be at an impasse. In spite of this we tried to implement step 7 partially: the \star -relations on part of \mathcal{A}_{phy} then forced us to go back to step 5 and discard many of the solutions from the space of physical states. The operators that leave this newly defined, smaller \mathcal{V}_{phy} invariant do form a \star -algebra and we are finally able to complete the quantization of this model.

Second, this model emphasizes the distinction between solutions to the constraint and physical states. All physical states are solutions to the constraints, but not vice versa.

I am sorry, I missed something you said a short while ago.

Tortoise: Not much. I was just saying that in carrying out the quantization program one has to go back and forth, correcting poor decisions taken in the early steps, as one's intuition for the problem develops. As was emphasized in the discussion of the A-H model, we can insist only that the final quantum theory is consistent and complete. We cannot quibble about the intermediate steps. Of course, a complete quantum theory is one in which we have obtained a (faithful) \star -representation of a complete algebra of physical observables. The step-by-step approach, and the conditions spelt out in chapter 2 are just guidelines to achieve this final result.

Achilles: Do we obtain an inner product or a quantum theory which is *unique* –up to unitary equivalence– if we satisfy all these conditions?

St. Joseph: Oh no, Achilles! Even for quantum mechanics on a finite dimensional *manifold* there are no such uniqueness theorems. The only known statement, the Stone-von Neumann theorem, states only that there is a unique, weakly continuous representation of the Weyl operator algebra constructed on $T^*\mathbb{R}^n$.

Tortoise: Right! In fact, as you know, there are inequivalent unitary representations of the Weyl algebra for the particle on the real line, in which the spectrum of the momentum operator includes all real numbers, but this spectrum is *discrete*! The only problem is that these representations are not weakly continuous. Since we did not introduce topological considerations, such discrete representations may well arise in the algebraic approach.

Furthermore, there are counter-examples, in this thesis itself, to a naive “uniqueness conjecture”. Recall the fractional spin representations for the particle on S^1 , and the interval’s worth of ambiguity in the representation of the coupled oscillator model when the energy difference is less than $\frac{1}{2}$.

Achilles: I would have intuitively expected to obtain a unique inner product by imposing the Hermiticity conditions on a complete set of generators of \mathcal{A}_{phy} .

Tortoise: Now you are jumping to conclusions again. The test to check that the set of physical observables is (over)complete on the reduced phase space guarantees only *local* completeness. The observables may not “know” enough about the global structure. We have already seen the importance of the role of additional, discrete physical operators (which arise from discrete symmetries of the constraint) in reducing the ambiguities in the inner product. Another source of ambiguity in the inner product arises if the physical operators are complete only *almost* everywhere on the constraint surface, i.e. if there are lower dimensional submanifolds on which the physical observables are not complete.

Achilles: Even so, this algebraic approach to the quantization of constrained systems is certainly very powerful. We have been able to use it to quantize numerous models of general relativity, some of which were previously only incompletely solved. However, all the difficulties and subtleties in the quantization of these relatively simple *finite dimensional* models, which you have so kindly commented on, make me wonder about the prospects for a quantum theory of gravity, which after all, is a *nonlinear field theory*. While a large (but certainly incomplete) set of solutions to the quantum scalar constraint is known in the new variables, there is still not a single known local observable. Perhaps you have sold the quantization program to me too strongly, but currently, it *appears* to me that physical observables are crucial even in quantum gravity; not just to construct the kinematical quantum theory, but perhaps also, as we saw in chapter 6, to understand dynamics and obtain a certain type of physical interpretation. Given all this, I wonder if I can ask you one last question. Do you expect to see a complete theory of quantum gravity in your lifetime, Mr. T?

Tortoise: ...possibly, Achilles, but then you know how long-lived tortoises are!

Bibliography

- [1] Hofstadter D.R. 1979 *Gödel, Escher, Bach: An Eternal Golden Braid* (Basic Books New York (Division of HarperCollins))

Appendix A

QUANTIZATION OF SECOND CLASS CONSTRAINTS

In the main part of my thesis, I have dealt only with first class constraints, since, as is well known, second class constraints have to be solved classically. If we were to represent the constraint functions as operators, then because they are second class, i.e. because they do not commute with each other weakly, there is no common kernel [1]. (Consider the action of the commutator on states annihilated by both constraint operators, clearly this vanishes. On the other hand, the commutator is proportional to the identity operator since the constraints are second class, and so we have an inconsistency.) More intuitively, if there is a Hermitian inner product on the representation space (so we can calculate expectation values), then we see that a state annihilated by both second class constraint operators violates the uncertainty principle.

In this appendix I will show that there is a mathematically well-defined sense in which one can “solve” second class constraints in quantum theory. Of course, since the argument in the preceding paragraph is a strict mathematical theorem, one of its hypotheses must be violated by our solution. We will construct quantum states which are “solutions” to the pair of second class constraints. These are not solutions in the standard sense: they are not annihilated by both constraint operators. The idea is to first write the second class pair as complex conjugate functions of each other. Then, solve *one* of the constraints using a *holomorphic* δ function, which I will describe in section A.1. Call these solutions the physical states. Now one can introduce an inner product such that the action of the second constraint on the above physical states results in states *orthogonal* to the space of physical states, thus, it sends physical states to the zero element of the physical Hilbert space. I will clarify this issue after I have presented the details of the solution in section A.2.

There are not yet any applications of this approach, in which we quantize and then solve second class constraints. However, there are situations in which this approach is potentially useful, and I will comment briefly on these at the end of the appendix.

A.1 Holomorphic δ function

Let us define a *holomorphic distribution* (or a generalized function) $\delta(z)$ as follows [2]: it is a complex linear mapping from the space of functions of the type $\sum f_i(z)g_i(\bar{z})$, where $f_i(z)$ are entire holomorphic functions and $g_i(\bar{z})$ are entire anti-holomorphic functions, to the space of entire anti-holomorphic functions:

$$\delta(z) \circ \sum_i f_i(z)g_i(\bar{z}) = \sum_i f_i(0)g_i(\bar{z}). \quad (1.1)$$

We can also define the anti-holomorphic distribution $\delta(\bar{z})$ simply by taking the complex conjugate of $\delta(z)$ and this new distribution has the action:

$$\delta(\bar{z}) \circ \sum_i f_i(z)g_i(\bar{z}) = \sum_i f_i(z)g_i(0) \quad (1.\bar{1})$$

We will also need the product of a polynomial $a(z, \bar{z})$ with a distribution $\mathcal{F}(z)$. This is a distribution defined by:

$$[a(z, \bar{z})\mathcal{F}(z)] \circ \sum_i f_i(z)g_i(\bar{z}) := \mathcal{F}(z) \circ a(z, \bar{z}) \sum_i f_i(z)g_i(\bar{z}) \quad (1.2)$$

Using, as usual, the Leibnitz rule as a motivation, one can define the derivative of a distribution $\mathcal{F}(z)$, as

$$\begin{aligned} \left[\frac{d}{dz} \mathcal{F}(z) \right] \circ \sum_i f_i(z)g_i(\bar{z}) \\ : = \frac{d}{dz} \left(\mathcal{F}(z) \circ \sum_i f_i(z)g_i(\bar{z}) \right) - \mathcal{F}(z) \circ \frac{d}{dz} \sum_i f_i(z)g_i(\bar{z}), \end{aligned} \quad (1.3)$$

and similarly for the derivative w.r.t. \bar{z} . Applying this to (1.1), for example, we find

$$\frac{d}{dz} \delta(z) = 0, \quad \text{and} \quad \left[\frac{d}{dz} \delta(z) \right] \circ \sum_i f_i(z)g_i(\bar{z}) = - \sum_i \left. \frac{df_i(z)}{dz} \right|_{z=0} g_i(\bar{z}). \quad (1.4)$$

Thus, *the δ -distribution is holomorphic and its derivative with respect to z is a distribution with the expected property*. Finally, we notice that the product of the two distributions (1.1) and (1.1') is well-defined:

$$[\delta(z)\delta(\bar{z})] \circ \sum_i f_i(z)g_i(\bar{z}) = \sum_i f_i(0)g_i(0). \quad (1.5)$$

Note that this is just the two dimensional δ -distribution and therefore admits the standard integral representation (which is useful as a mnemonic for the definitions (1.1-1.3)):

$$\begin{aligned} \int dq \wedge dp \delta^2(q, p; 0, 0) \sum_i f_i(z)g_i(\bar{z}) \\ := [\delta(z)\delta(\bar{z})] \circ \sum_i f_i(z)g_i(\bar{z}) = \sum_i f_i(0)g_i(0) \end{aligned} \quad (1.6)$$

where, we have used $z = q - ip$. Thus, one can regard $\delta(z)$ as the ‘‘holomorphic square-root’’ of the standard 2-dimensional δ -distribution on the 2-plane, (picked out by the complex structure).

A.2 Second class constraints in quantum theory

Consider the n dimensional system with real configuration coordinates q^i , $i = 1, \dots, n$ and the conjugate momenta p_i . The symplectic structure is $\Omega = dp_i \wedge dq^i$. The system is constrained by the two *second class* constraints $q^1 = 0$, $p_1 = 0$. The reduced phase space is coordinatized by the true degrees of freedom $(q^{i'}, p_{i'})$, $i' = 2, \dots, n$.

We want to solve the pair of second class constraints in quantum theory. Let us first introduce complex coordinates on (a portion of) the phase space, $z_1 := (p_1 - iq_1)/\sqrt{2}$, and $\bar{z}_1 := (p_1 + iq_1)/\sqrt{2}$. Hence, the algebra \mathcal{A} of elementary operators contains the pair $\hat{z}_1, \hat{\bar{z}}_1$, with the commutation relation $[\hat{z}_1, \hat{\bar{z}}_1] = -1$. The \star -relation between these operators is $\hat{z}_1^\star = \hat{\bar{z}}_1$. The pair of second class constraints can now be expressed as: $\hat{z}_1 = 0$, $\hat{\bar{z}}_1 = 0$.

Classically, we know that $z_1 = 0 \Rightarrow \bar{z}_1 = 0$. In the quantum theory, if there is an inner product that implements the \star -relations, then $\hat{z}_1 = 0 \Rightarrow \hat{z}_1^\star = 0 \Rightarrow \hat{\bar{z}}_1 = 0$. Therefore the strategy is to first find a representation of \mathcal{A} and impose the \star -relations to find an inner product such that $\hat{z}_1^\dagger = \hat{\bar{z}}_1$, and then solve only the constraint $\hat{z}_1 = 0$. The inner product will automatically implement $\hat{\bar{z}}_1 = 0$.

Let us choose as a representation space the vector space of holomorphic distributions $\Psi(z_i)$ of the kind introduced in section 1. The elementary operators are represented by:

$$\begin{aligned} \hat{z}_1 \circ \Psi &= z_1 \Psi \\ \text{and } \hat{\bar{z}}_1 \circ \Psi &= \frac{\partial}{\partial z_1} \Psi. \end{aligned} \quad (2.1)$$

Let

$$\langle \Psi | \Phi \rangle := \bar{\Psi} \Phi \circ \mu(z_1, \bar{z}_1) \quad (2.2)$$

be an ansatz for the inner product. A straightforward calculation –using the definitions from section A.1 and discarding the surface term, as usual– shows that the inner product is given by

$$\mu = e^{-z_1 \bar{z}_1}. \quad (2.3)$$

The constraint equation $\hat{z}_1 \circ \Psi = 0$ is solved by distributions of the form

$$\Psi(z_i) = \delta(z_1) \psi(z_{i'}). \quad (2.4)$$

Call these the physical states, and denote the vector space by \mathcal{V}_{phy} . Note that $\hat{z}_1 \circ \Psi$ vanishes as a *distribution*, as can be confirmed by using the definition (1.1) of the delta function; and also that one has no need of the inner product to do this calculation. However, physical states are normalizable with respect to this inner product.

Now, on solutions (2.4), it is not true that $\hat{\bar{z}}_1 \circ \Psi = 0$, in fact, as a distribution,

$$\hat{\bar{z}}_1 \Psi \circ f = -\Psi \circ \frac{\partial f}{\partial z_1} = - \left. \frac{\partial f}{\partial z_1} \right|_{z_1=0} \cdot \psi \neq 0, \quad (2.5)$$

where f is an arbitrary test function of the type used in section 1. However, $\hat{\bar{z}}_1 \circ \Psi$ is orthogonal to the physical states. Namely, for $\Psi, \Phi \in \mathcal{V}_{phy}$,

$$\langle \Psi | \hat{\bar{z}}_1 | \Phi \rangle = \bar{\Psi}(\bar{z}_i) \left(\frac{\partial}{\partial z_1} \Phi(z_i) \right) \circ \mu$$

$$\begin{aligned}
&= -\bar{\Psi}\Phi \circ \frac{\partial\mu}{\partial z_1} = \bar{\Psi}\Phi \circ \bar{z}_1\mu \\
&= \bar{\psi}\delta(\bar{z}_1)\phi\delta(z_1) \circ \bar{z}_1\mu = 0.
\end{aligned} \tag{2.6}$$

Hence, we have a representation in which both $\hat{z}_1 = 0$ and $\hat{\bar{z}}_1 = 0$. In this sense, the second class constraints have, apparently, been imposed as if they are first class.

How have we circumvented the argument, presented in the introduction, against solving second class constraints in the quantum theory? This question can be asked and analyzed at various levels. First, note that at the vector space level –i.e. prior to the introduction of an inner product– there is no contradiction since we have *not* solved for $\hat{\bar{z}}_1 = 0$: the space of physical states is defined simply by $\hat{z}_1 \circ \Psi = 0$. Second, when we do introduce an inner product, on physical states there is again no contradiction, since $\hat{\bar{z}}_1$ is not a physical operator. The inner product is defined not only on physical states, but on all distributions. Now, the action (2.5) of $\hat{\bar{z}}_1$ takes physical states *out* of \mathcal{V}_{phy} . The resulting state is still a distribution, and we can compute its inner product with a physical state. It is this *projection* that vanishes. Finally, using the inner product, we can define a projection to the physical states, and consequently a new operator $\hat{\bar{z}}_1|_{phy}$. On physical states, $\hat{\bar{z}}_1|_{phy} \circ \Psi = 0$. However, this new operator is (by construction) a physical operator: it is easy to see that $[\hat{z}_1, \hat{\bar{z}}_1|_{phy}] = 0$ on physical states. However, now \hat{z}_1 and $\hat{\bar{z}}_1|_{phy}$ do *not* satisfy the CCR. Thus, at this level, there is no contradiction with the theorem since the CCR is itself changed.

This seems like an awful lot of heavy artillery brought to bear on a simple problem that one knows how to deal with, and there are no obvious applications of this approach. However, if solving the second class constraints complicates the remaining first class constraints, or results in complicated algebraic relations on the variables, then “quantizing” second class constraints may be helpful. Perhaps a more useful application could be to the following situation: Suppose that factor ordering and/or regularizing constraints which are *classically first class* leads inevitably to second class constraints in the quantum theory (and assume that this can be done while keeping the true degrees of freedom the same). This presents us with a dilemma, since the second class constraints are *derived* and *defined* in the quantum theory itself. Our approach to solving second class constraints in quantum theory might provide a way out of this dilemma.

Bibliography

- [1] Dirac P A M 1964 *Lectures on Quantum Mechanics* (Yeshiva University New York)
- [2] Ashtekar A 1991 Lectures on *Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore); see section 11.4

Bibliography

- [1] Ashtekar A and Geroch R 1974 *Rep. Prog. Phys.* **37** 1211-56
- [2] Ashtekar A and Magnon A 1975 *Proc. R. Soc. (Lond.)* **A346** 375
- [3] Ashtekar A 1980 *Comm. Math. Phys.* **71** 59
- [4] Ashtekar A and Horowitz G H 1982 *Phys. Rev.* **D26** 3342-53
- [5] Ashtekar A and Magnon A 1982 *Comm. Math. Phys.* **86** 55-68
- [6] Ashtekar A and Stillerman M 1986 *J. Math. Phys.* **27** 1319
- [7] Ashtekar A 1986 *Phys. Rev. Lett.* **57** 2244
- [8] Ashtekar A 1987 *Phys. Rev.* **D36** 1587
- [9] Ashtekar A 1989 in *Conceptual Problems in Quantum Gravity* Ashtekar A and Stachel J (eds) (Birkhäuser Boston)
- [10] Ashtekar A 1991 *Lectures on Non-perturbative canonical gravity* Notes prepared in collaboration with Tate R S (World Scientific Singapore)
- [11] Ashtekar A and Samuel J 1991 *Class. Quantum Grav.* **8** 2191
- [12] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-5
- [13] Ashtekar A, Tate R S and Uggla C 1992 Syracuse University pre-print SU-GP-92/2-6
- [14] Ashtekar A and Tate R S 1992 Syracuse University pre-print in preparation
- [15] Arnowitt R, Deser S and Misner C W 1962 *Gravitation: An Introduction to Current Research* Witten L (ed) (Wiley New York)
- [16] Brüggman B, Gambini R and Pullin J 1992 *Phys. Rev. Lett.* **68** 431-4
- [17] Boulware D G 1983 *Phys. Rev.* **D28** 414-16
- [18] Dirac P A M 1964 *Lectures on Quantum mechanics, Belfer Graduate School Monograph Series No. 2* (Yeshiva University New York)

- [19] Feynmann R P and Hibbs A R 1965 *Path Integrals and Quantum Mechanics* (McGraw Hill, New York)
- [20] Gelfand I M and Naimark M A 1943 *Mat. Soberniki* **12** 197
- [21] Geroch R 1974 *University of Chicago Lecture Notes on Quantum Mechanics* unpublished
- [22] Gotay M J and Demaret J 1983 *Phys. Rev.* **D28** 2402
- [23] Gotay M J 1986 *Class. Quantum Grav.* **3** 487-91
- [24] Hajicek P 1990 *Class. Quantum Grav.* **7** 871
- [25] Husain V 1987 *Class. Quantum Grav.* **4** 1587
- [26] Isham C J, Penrose R and Sciama D W (eds) 1981 *Quantum Gravity 2: A Second Oxford Symposium* (Clarendon Press Oxford); see in particular the overview by Isham C J
- [27] Isham C J 1984 in *Relativity, Groups and Topology II, Les Houches 1983* DeWitt B S and Stora R (eds) (North-Holland Amsterdam)
- [28] Kuchař K 1981 in *Quantum Gravity 2: A Second Oxford Symposium* Isham C J, Penrose R and Sciama D W (eds) (Clarendon Press Oxford)
- [29] Kuchař K 1981 *J. Math. Phys.* **22** 2640-54
- [30] Kuchař K 1982 *J. Math. Phys.* **25** 1647-61
- [31] Kuchař K 1992 *Time and interpretations of Quantum Gravity* in *Proceedings of the 4th Canadian Conference on General Relativity and Relativistic Astrophysics* Kunstaatter G, Vincent D and Williams J (eds) (World Scientific Singapore)
- [32] Loll R 1990 *Phys. Rev.* **D41** 3785
- [33] MacCallum M A H 1979 in *Physics of the Expanding Universe* Demianski M (ed) (Springer-Verlag Berlin)
- [34] Misner C W 1972 in *Magic Without Magic* Klauder J (ed) (Freeman San Francisco)
- [35] Romano J D and Tate R S 1989 *Class. Quantum Grav.* **6** 1487-500
- [36] Rosquist K, Uggla C and Jantzen R T 1990 *Class. Quantum Grav.* **7** 611
- [37] Rovelli C 1990 *Phys. Rev.* **D42** 2638
- [38] Rovelli C 1991 *Phys. Rev.* **D43** 442-56
- [39] Rovelli C 1991 *Class. Quantum Grav.* **8** 1613-75

- [40] Ryan M P 1972 *Hamiltonian Cosmology: Lecture notes in Physics* **13** Ehlers J *et al* (eds) (Springer-Verlag New York)
- [41] Ryan M P and Shepley L C 1975 *Homogeneous Relativistic Cosmology* (Princeton University Press Princeton)
- [42] Segal I E 1947 *Bull. Amer. Math. Soc.* **53** 73
- [43] Smolin L 1992 in *Proc. XXII Gift Intl. Seminar on Theo. Phys., Quantum Gravity and Cosmology, June 1991 Catalonia Spain* (World Scientific, Singapore)
- [44] Sniatycki J 1980 *Geometric Quantization and Quantum mechanics* (Springer-Verlag, New York)
- [45] Stillerman M 1985 *Ph.D. thesis* Syracuse University
- [46] Tate R S 1992 *Constrained systems and Quantization, Lectures at the Advanced Institute for Gravitation Theory, Session: December 91 Cochin* Syracuse University pre-print No SU-GP-92/1-4
- [47] Taub A H 1951 *Ann. Math.* **53** 472
- [48] Wald R M 1984 *General Relativity* (University of Chicago Press, Chicago)
- [49] Woodhouse N J M 1981 *Geometric Quantization* (Oxford University Press, Oxford)
- [50] Wheeler J 1977 *Gen. Rel. & Grav.* **8** 713