Quantum Observables and Recollapsing Dynamics

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Abstract

Within a simple quantization scheme, observables for a large class of finite dimensional time reparametrization invariant systems may be constructed by integration over the manifold of time labels. This procedure is shown to produce a complete set of densely defined operators on a physical Hilbert space for which an inner product is identified and to provide reasonable results for simple test cases. Furthermore, many of these observables have a clear interpretation in the classical limit and we use this to demonstrate that, for a class of minisuperspace models including LRS Bianchi IX and the Kantowski-Sachs model this quantization agrees with classical physics in predicting that such spacetimes recollapse.
I. INTRODUCTION

A generalization of Kuchař’s “Hilbert space problem” [1] provides one of the greatest obstructions to developing a quantum theory of gravity. At issue are the questions “What are the physical (quantum) observables?” and “On what Hilbert space (if any) do they act?” This includes the familiar question “What is the inner product on the space of physical states?” Here, we combine the idea emphasized by DeWitt [2] of constructing “local” diffeomorphism invariants by integrating singular densities over a manifold with the quantization of constrained systems described by Dirac [3] and find that we are able to construct gauge invariant operators which (at least in the classical limit) have a clear interpretation and which are densely defined on a Hilbert space of physical states with a known inner product. This approach has the advantage that it is not necessary to identify an “internal time function” [1], that it may be applied to a large class of minisuperspace models – which includes the LRS Bianchi IX and Kantowski-Sachs cosmologies – and that for the models just mentioned it predicts that the corresponding spacetimes recollapse, in accord with the classical result. Note that it is highly nontrivial for a quantization scheme to satisfy this last condition and, in particular, that procedures based on a Klein-Gordon type inner product instead describe the universe as expanding “forever” [1].

Let us consider for a moment the more general situation of a diffeomorphism invariant system on a spacetime manifold $M$. Some interesting common examples are general relativity, topological field theories, parametrized Newtonian systems, and homogeneous cosmological models (such as the Bianchi models) for which $M$ is just the manifold $\mathbb{R}$ of time labels. Solving the equations of motion for such systems introduces a number of arbitrary functions corresponding to the freedom to choose coordinates on $M$. Physical information is contained in gauge invariant quantities constructed from such solutions (that is, quantities which do not depend on these arbitrary functions) so that, classically, we face the issue of constructing such objects and extracting useful information. We will refer to such gauge invariants as observables.
As has been pointed out a number of times (see, e.g. [2]), we do in fact know how to construct a great number of observables for classical diffeomorphism invariant theories. Given any density $\omega$ on an n-manifold $M$, $\int_M \omega$ is such an observable. Of course, these observables are not of the type with which we are familiar from, say, scalar field theory and they may be highly non-local. This is the case for simple examples such as $\int_M \sqrt{-g}R$ in Einstein gravity. Also, if the density $\omega$ is not chosen carefully, such an integral may converge only when evaluated for very special solutions of the dynamics.

However, as described in [2], some observables of this type can be easily interpreted. If the density $\omega$ is distributional, the resulting gauge invariant may be effectively local on $M$. A simple example of such an observable is the value of some scalar quantity at a point specified by an “intrinsic coordinate system.” For gravity coupled to a set of scalar fields $\phi^k$, $k \in \{0, 1, 2, 3\}$, the corresponding integral might be

$$\int_M R \prod_{i=0}^3 \delta(\phi^j) \left| \frac{\partial \phi^k}{\partial x^\mu} \right| d^4 x$$

(1.1)

where $R$ is the curvature scalar and $\left| \frac{\partial \phi^k}{\partial x^\mu} \right|$ is a Jacobian. This object defines a well-behaved function on any part of the classical space of solutions for which the fields $\phi^k$ vanish simultaneously only at a finite number of spacetime points and for which the metric is smooth whenever $\phi^k = 0$.

We would like to use similar ideas to define and discuss observables of this type for quantum theories with reparametrization or diffeomorphism invariance. Two standard criticisms of observables of this type in the classical setting are 1) that they will in general be well-defined (and finite) only on a part of the classical solution space and 2) that, as they involve integration over time, they are likely to be of little use unless the theory can be solved completely (so that the integrand may be written explicitly). Nevertheless, we will see that quantum analogues of these observables exist as densely defined operators on a space of physical states for interesting models and that certain properties of the resulting operators can be studied even though the models may not be exactly solvable. In particular, such observables can be used to show that, in correspondence with the classical
result, our quantization of appropriate minisuperspace models describes spacetimes whose homogeneous slices expand to some maximal size and then recollapse.

The strategy is as follows. First, section II discusses the classical form of the observables of interest. This will provide insight into the definitions and arguments used in the quantum treatment. We then give the general quantum formalism for the operators and the physical Hilbert space in III and apply it to two test cases in IV. After verifying that appropriate results are produced for these simple cases, we turn to the cosmological models of interest in V. In each application, the integrals that define our observables will be shown to converge and we find a “complete set” of observables that are densely defined on the physical Hilbert space and symmetric with respect to a physical inner product. In addition, V shows that when applied to “separable semi-bound” cosmological models, this quantization describes spacetimes that recollapse. We conclude with a short discussion in section VI.

II. OBSERVABLES THROUGH INTEGRATION

Section II will address quantization of reparametrization invariant models and will focus on the properties of certain observables. In order to provide an intuitive understanding of the definition and use of these observables, we now discuss their classical counterparts. Thus, this section can be regarded as essentially heuristic background for the more rigorous results of III, IV, and V.

We are interested in systems that are time reparametrization invariant; that is, systems defined on some $d + 1$ dimensional spacetime $M$ for which there is a gauge symmetry that takes $f(t)$ to any $f(T(t))$ whenever $dT/dt > 0$ and $f$ is a scalar on $M$. We concentrate on the case $d = 0$ and on observables like [1.4]. However, because canonical techniques will be used, it is better to consider invariants of the form

\[ [a]_{q=\tau} = \int_{-\infty}^{\infty} dt \frac{dq}{dt} \delta(q(t) - \tau) a(t) \] (2.1)

which may be regarded (when the integral converges) as either functions on the space $S$ of classical solutions or, through the evolution map that constructs a solution from a piece of
initial data specified by a point on the constraint surface, on the part of the corresponding phase space in which any constraints are satisfied. When \( q(t) \) takes the value \( \tau \) once along a solution, this object gives the value of \( a(t) \) when \( q(t) = \tau \) up to a sign. Similar observables were used in [5–7].

The advantage of (2.1) is that it is invariant not just under reparametrizations \( (t \rightarrow T(t) \) with \( dT/dt > 0) \), but also under pull backs of the manifold of time labels through maps of degree 1 \( (t \rightarrow T(t) \) for any smooth \( T(t) \) of degree 1). This large class of transformations typically become gauge symmetries as well when a time reparametrization invariant system is written in Hamiltonian form.

In fact, if the canonical description is in terms of some phase space coordinates \( z_i(t) \) at each \( t \), a (constrained) Hamiltonian \( h \) and a lapse function \( N(t) \), it typically has

\[
\begin{align*}
\delta z_i(t) &= \epsilon(t) \{h, z_i\} = -\frac{\epsilon(t)}{N(t)} \frac{\partial z_i(t)}{\partial t} \\
\delta N(t) &= -\frac{\partial}{\partial t} \epsilon(t)
\end{align*}
\]

(2.2)
as a gauge symmetry. Here \( \{,\} \) is the canonical Poisson Bracket and \( \epsilon(t) \) is the gauge parameter.

Because canonical methods will be used, we invoke an abuse of language and refer to transformations of the form (2.2) as “reparametrizations” throughout this work. Reparametrizations of the first type (diffeomorphisms of the \( t \)-label set) will be referred to as “true reparametrizations.” Note that the infinitesimal form of a true reparametrization \( t \rightarrow t + \delta t \) is identical to that of a general reparametrization with parameter \( \epsilon = N \delta t \). Because its integrand is a one-form, expression (2.1) is in fact invariant under the more general reparametrizations (2.2).

Along a solution on which \( q = \tau \) more than once or not at all, the question “What is the value of \( a(t) \) when \( q(t) = \tau \)” may be ill-defined. However, expression (2.1) provides a natural generalization of the “answer.” It adds the values of \( a(t) \) at each \( t \) such that \( q(t) = \tau \) and \( dq/dt > 0 \) and subtracts those values of \( a(t) \) for which \( q(t) = \tau \) and \( dq/dt < 0 \). Of course, for some solutions \( s \) the integral in (2.1) may not converge, such as when \( q(t) \) takes the value \( \tau \)
an infinite number of times along \(s\), and on such solutions \([a]_{q=\tau}^{(2)}\) is undefined. However, this will not be a problem for the cases we consider.

Note that if \(q = \tau\) at several points along a solution, a calculation of \([a]_{q=\tau}\) involves cancellations between those points with \(q = \tau\) at which \(dq/dt > 0\) and \(dq/dt < 0\). To obtain an average without such cancellation while retaining invariance under \(2.2\), we might consider \([b]_{q=\tau}\) for \(b = a \, \text{sign}\left(\frac{1}{N} \frac{dq}{dt}\right)\) where \(\text{sign}(x) = \theta(x) - \theta(-x)\). In particular, \([\text{sign}\left(\frac{1}{N} \frac{dq}{dt}\right)]_{q=\tau}\) is the number of times for which \(q(t) = \tau\) and \(N(t) > 0\) minus the number of times for which \(q(t) = \tau\) and \(N(t) < 0\). In a “proper parametrization” for which \(N(t) > 0\) and proper time always flows forward, this is just the number of times for which \(q(t) = \tau\).

Thus, if we are considering a reparametrization invariant minisuperspace model and \(q\) is some measure of the size of the universe, the statement that

\[
\lim_{\tau \to \infty} \left[\text{sign}\left(\frac{1}{N} \frac{dq}{dt}\right)\right]_{q=\tau} = 0
\]

pointwise on \(\mathcal{S}\) (or the on the constraint surface) is equivalent to the statement that such models always recollapse; i.e., that any given solution \(s\) does not reach arbitrarily large values of \(q\). For such a model, we in fact have

\[
\lim_{\tau \to \infty} [a]_{q=\tau} = 0
\]

for any \(a = a(z_i)\). In \([\text{V}]\), we will deduce an analogous property of corresponding quantum operators for certain minisuperspace models. We interpret this as a demonstration that our quantization of these models describes recollapsing cosmologies.

III. GENERAL DIRAC METHODS

We now use the heuristic ideas embodied in \(2.1\) to quantize time reparametrization invariant systems. This section gives the general setting and formalism to be used while important examples are described in the next two sections. When the quantum version of the integral \(2.1\) converges, we will define the \([A]_{Q=\tau}\) through integration and show in
that they are observables in the canonical sense; that is, that they commute with the Hamiltonian. We introduce a space of physical states as in III and find a physical inner product in III with respect to which our operators are symmetric. The results of this section assume convergence of the integrals, which will be separately discussed for each of the examples of IV and V. However, results for systems outside the scope of IV and V should be considered as formal.

A. The Setting

Let us suppose that we wish to quantize a time reparametrization invariant system described by a phase space which is a cotangent bundle $T^*Q$ over a configuration space $Q$. We will also assume that the dynamics is expressed through a Hamiltonian $h$ and lapse function $N$. Because time reparametrization is to be a gauge symmetry of this system, the Hamiltonian is classically constrained to vanish: $h = 0$.

If we momentarily ignore the reparametrization invariance and the constraint, this system has a straightforward quantization. States of the system live in the Hilbert space $L^2(Q)$ and the Hamiltonian $h$ becomes a Hermitian operator $H$. In general, we will use capital letters for quantum operators and lower case letters for their eigenvalues and classical counterparts. $H$ generates a unitary (Newtonian) time evolution and may be used to define a set of Heisenberg picture operators corresponding to the functions and vector fields on $Q$ in the usual way. In order for $H$ to be self-adjoint, the $L^2(Q)$ functions may be required to satisfy additional boundary conditions.

Thus, our only tasks are to impose the constraint and to implement the time reparametrization invariance. For the second of these, we introduce a lapse operator $N(t)$ and an evolution in a parameter time $t$ instead of the Newtonian time evolution described above. We proceed with the following algebraic approach:

For each smooth function $q$ and each vector field $p$ on $Q$, introduce one parameter families $Q(t)$ and $P(t)$ of elements in a noncommutative algebra. Recall that such $q$ and $p$ form an
overcomplete set of functions on $T^*Q$ and that the classical Poisson Brackets are summarized by

$$\{q_1, q_2\} = 0$$
$$\{q_1, p_1\} = \mathcal{L}_{p_1} q_1 \equiv q'(q_1, p_1)$$
$$\{p_1, p_2\} = \{p_1, p_2\}_\mathcal{L} \equiv p'(p_1, p_2)$$  \hspace{1cm} (3.1)

where $q_1, q_2$ are smooth functions on $Q$, $p_1, p_2$ are smooth vector fields on $Q$, $\mathcal{L}_{p_1}$ denotes the Lie derivative along $p_1$, $\{,\}_\mathcal{L}$ is the Lie Bracket of vector fields, and the above expressions define the function $q'$ and the vector field $p'$ in terms of $q_1, p_1$, and $p_2$. We therefore impose the relations:

$$[Q_1(t), Q_2(t)] = 0$$
$$[Q_1(t), P_1(t)] = Q'(q_1, p_1)$$
$$[P_1(t), P_2(t)] = P'(p_1, p_2)$$  \hspace{1cm} (3.2)

on our algebra. We also introduce the family $N(t)$, each member of which commutes with every element in the algebra. Further, we require

$$-i\frac{\partial}{\partial t} Q(t) = N(t)[H(t), Q(t)]$$
$$-i\frac{\partial}{\partial t} P(t) = N(t)[H(t), P(t)]$$

where $H(t)$ is some symmetric factor ordering of the classical expression for $H$ in terms of the $q$'s and $p$'s with these objects replaced by the algebraic elements $Q(t)$ and $P(t)$. While this choice of algebra is not unique (see \[8,9\]) we will not consider other possibilities here.

The presence of the lapse makes the dynamics reparametrization invariant. That is, the above equations are unchanged by the transformations

$$\delta Q(t) = -ie(t) [H(t), Q(t)] = -\frac{e(t)}{N(t)} \frac{\partial Q(t)}{\partial t}$$
$$\delta P(t) = -ie(t) [H(t), P(t)] = -\frac{e(t)}{N(t)} \frac{\partial P(t)}{\partial t}$$
$$\delta N(t) = -\frac{\partial}{\partial t} e(t)$$  \hspace{1cm} (3.4)
We may thus consider \(3.3\) as simply a Heisenberg picture version of the Schrödinger equation imposed in \([3]\).

As in unconstrained quantum mechanics, we now search for irreducible Hilbert space representations \(\mathcal{H}\) of \(\mathcal{B}\). For fixed \(t\), they can be constructed in the usual way through “coordinate representations” carried by square integrable functions on \(Q\), on which the \(Q(t)\) act by multiplication by \(q\) and the \(P(t)\) generate diffeomorphisms along the integral curves of \(p\). Since we require \(H\) to be Hermitian, the dynamics \(3.3\) identifies representations of operators at the times \(t\) and \(t'\) through

\[
Q(t) = \exp \left( iH \int_t^{t'} dt N(t) \right) Q(t') \exp \left( -iH \int_t^{t'} dt N(t) \right)
\]
\[
P(t) = \exp \left( iH \int_t^{t'} dt N(t) \right) P(t') \exp \left( -iH \int_t^{t'} dt N(t) \right)
\]  

(3.5)

where, as usual \(H = H(t)\) is actually time independent. Since \(N(t)\) commutes with every operator, we have \(N(t) = n(t)\mathbb{I}\) for some real-valued \(n(t)\) in any irreducible representation for which \(N(t)\) is Hermitian. From now on, we will assume that \(n(t)\) satisfies

\[
\lim_{t' \to \pm \infty} \int_0^{t'} n(t) dt = \pm \infty.
\]

(3.6)

All such smooth choices of \(n(t)\) are equivalent and are related to each other by gauge transformations. Note that, given a choice of \(n(t)\), this representation is unique to the same extent as in usual quantum mechanics. In particular, if the phase space is \(T^*\mathbb{R}^n\) with the standard symplectic structure, it is unique by the Stone-von Neumann theorem if weak continuity is assumed.

In order to enforce the constraint in our quantum theory, we will say that “physical” states \(|\psi\rangle\) lie in the physical subspace \(\mathcal{H}_{\text{phys}}\) determined (as in \([3]\)) by

\[
H|\psi\rangle = 0
\]

(3.7)

In general, such states will only be delta-function normalizable. That is, such states will not lie in \(\mathcal{H}_{\text{aux}}\) at all, but in the dual to the nuclear space associated with the spectrum of \(H\). We will deal with this feature later.
B. The Quantum Observables

Our task will be to construct observables; that is, operators which are invariant under 3.4. We will again use operators that correspond to the classical objects \( [a]_q = \tau \) defined through:

\[
[A]_{Q=\tau} = \int_{-\infty}^{\infty} dt \frac{dQ}{dt} \delta(Q(t) - \tau) A(t)
\]  

(3.8)

where, for the moment, we will not worry too much about the factor ordering of the integrand or the definition of the delta-function. To show that \( [A]_{Q=\tau} \) commutes with \( H \), we will prove the more general result that time reparametrization invariant operators of the form

\[
\Omega = \int \omega(t) dt
\]  

(3.9)

for one-forms \( \omega dt \) commute with \( H \). We consider only those \( \omega(t) \) for which 3.9 converges when acting on the part of \( H \) corresponding to some spectral interval \([a, b]\) of \( H \) that contains the eigenvalue zero. Note that 3.3 does not depend on the choice of lapse function \( n(t) \).

Since \( \omega dt \) is a one-form, we assume that it satisfies the equation

\[
-i \frac{\partial}{\partial t} \left( \frac{\omega(t)}{N(t)} \right) = N(t) [H(t), \frac{\omega(t)}{N(t)}].
\]  

(3.10)

This is the case when \( \omega \) is a sum of terms of the form:

\[
N(t) \prod_{j=1}^{l} \left( \frac{1}{N(t)} \frac{\partial}{\partial t} \right)^{n_j} \omega^{(j)}(t)
\]  

(3.11)

and the \( \omega^{(i)}(t) \) are built from the \( Q(t) \)'s and the \( P(t) \)'s so that they satisfy

\[
-i \frac{\partial}{\partial t} \omega^{(i)}(t) = N(t) [H(t), \omega^{(i)}(t)].
\]  

(3.12)

To show that \( \Omega \) commutes with the constraint, we consider a basis of \( H \)-eigenstates \( |E,k\rangle \) with eigenvalue \( E \) where \( k \) is a discrete label that removes any remaining degeneracy. In general, these may not represent normalizable states, but only states that are delta-function normalizable. We take \( \langle E_1, k | E_2, k_2 \rangle = \delta^{(c)}(E_1 - E_2) \delta_{k_1, k_2} \) where this \( \delta^{(c)}(E_1 - E_2) \) is to be interpreted as a delta-function or a Kronecker delta as appropriate.
Consider the matrix elements of \( \frac{\omega(t)}{N(t)} \) between any two states of this type. Note that
\[
\langle E_1, k_1 \mid \frac{\omega(t)}{N(t)} \mid E_2, k_2 \rangle = \exp \left( i (E_1 - E_2) \int_{t'}^t dt' n(t) \right) \langle E_1, k_1 \mid \frac{\omega(t')}{N(t')} \mid E_2, k_2 \rangle
\]
so that we have
\[
\langle E_1, k_1 \mid \Omega \mid E_2, k_2 \rangle = 2\pi \delta(E_1 - E_2) \langle E_1, k_1 \mid \frac{\omega(t')}{N(t')} \mid E_2, k_2 \rangle,
\]
using (3.13). The delta-function in \( E_1 - E_2 \) guarantees that our operator preserves the spectral subspaces of \( H \), and therefore that

- \( [\Omega, H] = 0 \) when (3.9) converges weakly.

The reader may be concerned by the presence of the delta-function in \( E_1 - E_2 \) for the case where the spectrum of \( H \) is discrete. This concern appears to be valid and will be discussed in section VI. Here, however, we will only be interested in applying these techniques to the case where the spectrum of \( H \) is purely continuous (at least near the zero eigenvalue).

We now return to observables of the form (3.8). Our first task will be to address the factor ordering of the integrand as \( \frac{\partial}{\partial t} Q(t) \) will typically involve \( P(t) \) and therefore fail to commute with \( Q(t) \) and \( \delta(Q(t) - \tau) \). From (3.22) and (3.24), we see that any symmetric ordering of the factors \( \frac{\partial}{\partial t} Q(t), Q(t), \) and \( A(t) \) will produce a Hermitian gauge invariant that we may take to be a “quantization” of \( [a]_{q=\tau} \). However, experience shows that the ordering
\[
[A]_{Q=\tau} = \frac{1}{2} \int_{-\infty}^\infty dt \{ A(t), \frac{\partial}{\partial t} \theta(Q(t) - \tau) \}_+
\]
is particularly convenient and leads to tractable calculations and analyses. As opposed to other factorizations that might be chosen \(^{1} \), it has the reassuring property (see [V.B]) that \([\text{sign}(p_0)]_{x^0=\tau} \) is the identity operator for the free relativistic particle. Here, \( \{X,Y\}_+ = XY + YX \) is the anticommutator and \( \theta(Q(t) - \tau) \) is the projection onto the positive part of the spectrum of \( Q(t) - \tau \). We thus take (3.15) as the definition of \( [A]_{Q=\tau} \) in what follows.

\(^{1}\text{Note that this is the correct result as it is this operator that counts “the number of times that } x^0 = \tau.” \) Thus, \([\text{sign}(p_0)]_{x^0=\tau} = 1 \) in the classical case and \([1]_{x^0=\tau} = \text{sign}(p_0) \).
Before deriving further results, let us reflect for a moment on the two definitions of “observable” mentioned above. Within our scheme, the canonical idea that an “observable” is an object that commutes with the constraint (the Hamiltonian, \(H\)) does not capture the entire notion of “gauge invariant” (see related comments in [8,9]). For example, the object \(N(t)\) commutes with the constraint but does not correspond to a gauge-invariant quantity. Also, note that the commutator of an operator \(\mathcal{O}\) with \(H\) is not in general gauge invariant so that this definition is itself “gauge dependent.” For example, an argument similar to that of 3.13 and 3.14 shows that any object of the form \(\int_{-\infty}^{\infty} dt A(t)\), where \(A(t)\) is an algebraic combination of \(Q_i(t)\) and \(P_j(t)\), commutes with the Hamiltonian in a representation for which \(n(t) = 1\). However, for more general choices of lapse, it does not commute with \(H\). (This problem can be avoided by requiring that \([\mathcal{O}, H] = 0\) in all irreducible representations and not just be zero in the representation used.) However, we have seen that reparametrization invariant operators do commute with the Hamiltonian. Thus, we take reparametrization invariance as the more fundamental notion of observable.

Finally, we give a few more definitions and useful results. In order to study the case where \(A(t)\) does not commute with both \(Q(t)\) and \(\frac{\partial}{\partial t}Q(t)\), we introduce the operators:

\[
[A]_Q^L = \int_{-\infty}^{\infty} dt A(t) \left( \frac{\partial}{\partial t} \theta(Q(t) - \tau) \right)
\]

and

\[
[A]_Q^R = \int_{-\infty}^{\infty} dt \left( \frac{\partial}{\partial t} \theta(Q(t) - \tau) \right) A(t)
\]

which satisfy

\[
([A]_Q^L) = [A]_Q^R,
\]

\[
[A]_Q = \frac{1}{2}([A]_Q^L + [A]_Q^R),
\]

and, if \([A(t), \frac{\partial}{\partial t} \theta(Q(t) - \tau)] = 0\), we have \([A]_Q = [A]_Q^L = [A]_Q^R\).

The convenient expressions

\[
[A]_Q^L |E, k; t\rangle = 2\pi i \sum_{k^*} |E, k^*; t\rangle \langle E, k^*; t'|A(t')[H, \theta(Q(t') - \tau)]|E, k; t'\rangle
\]
and

$$[A]_{Q=\tau}^R |E; k; t'] = 2\pi i \sum_{k^*} |E, k^*; t'] \langle E, k^*; t'[H, \theta(Q(t') - \tau)]A(t')|E, k; t'\rangle$$  \hspace{1cm} (3.20)$$

for the actions of these operators follow from 3.14 since $\frac{1}{\hbar} \partial_t \theta(Q(t) - \tau) = i[H, \theta(Q(t) - \tau)]$. Here, we have again assumed that $E$ lies in the continuous spectrum of $H$. In [IVB] and [V] these relations will be used to study $[A]_{Q=\tau}$.

**C. The Hilbert Space**

Equation 3.14 is also sufficient for us to determine the physical inner product. In the spirit of [13], we wish to choose this inner product such that all $\Omega$ of the form 3.9 are Hermitian (or at least symmetric) when $\omega(t)$ is hermitian. Thus, we require

$$\overline{(\langle |E = 0; k_1\rangle, \Omega |E = 0, k_2\rangle)_{phys}} = (\langle |E = 0; k_2\rangle, \Omega |E = 0, k_1\rangle)_{phys}$$  \hspace{1cm} (3.21)$$

where the overline denotes complex conjugation and (.)$_{phys}$ is the physical inner product. But, assuming that the spectrum of $H$ is continuous, we may rewrite 3.14 as

$$\Omega |E_1, k_1\rangle = \sum_{k_2} |E_1, k_2\rangle \langle E_1, k_2| \frac{\omega(t')}{N(t')} |E_1, k_1\rangle$$  \hspace{1cm} (3.22)$$

and we see that 3.21 is satisfied if

$$\langle |E = 0; k_2\rangle, |E = 0, k_1\rangle_{phys} = \delta_{k_2, k_1}$$  \hspace{1cm} (3.23)$$

since

$$\overline{(E = 0, k_1 \frac{\omega(t')}{N(t')} |E = 0, k_2\rangle} = \langle E = 0, k_2| \frac{\omega(t')}{N(t')} |E = 0, k_1\rangle. \hspace{1cm} (3.24)$$

We conclude that

- All (convergent) observables of the form 3.9 are symmetric on $\mathcal{H}_{phys}$ with the inner product 3.23.

\textsuperscript{2}This inner product has been independently introduced several times in related contexts. See [10,11] for the cases known to the author.
Uniqueness of this inner product can be guaranteed by enforcing Eq. (3.21) for sufficiently many $\Omega$, such as those $(\Omega_{\pm}^{j_1j_2})$ defined by any set of one-forms for which

$$\langle E = 0, k_2 | \frac{\omega_{j_1j_2}(t')}{N(t')} | E = 0, k_1 \rangle = (\delta_{k_1,j_1} \delta_{k_2,j_2} \pm \delta_{k_1,j_2} \delta_{k_2,j_1})i^{(1+1)/2}$$

(3.25)

However, finding a set of physically interesting operators whose Hermiticity makes Eq. (3.23) unique is a more difficult goal which we will not pursue here.

**IV. SIMPLE EXAMPLES**

We now present two simple examples to illustrate how the formalism of Eq. (II) may be applied and to show that it produces reasonable results. These test cases show that the methods of Eq. (II) give the usual results for “already deparametrized systems” (IV A) and lead to a familiar Hilbert space for the relativistic free particle (IV B). These results validate the methods so that we may then apply them to cosmological models in V.

In the examples we will see that our approach in fact provides an “overcomplete set” of quantum observables. By this we mean a set of observables whose classical counterparts are overcomplete (see, for example [13]) on the (constrained) phase space.

**A. Already Deparametrized Systems**

A standard testing ground for ideas regarding quantization of time reparametrization invariant systems is the class of systems that have been deparametrized (i.e., for which a time function has been identified [1]) or, what is nearly equivalent, systems that (in the language of canonical quantization) have a Hamiltonian constraint of the form

$$p_0 + h_1 = 0$$

(4.1)

where $p_0$ is some momentum and $h_1$ is independent of $p_0$. For such systems, the coordinate $q^0$ conjugate to $p_0$ effectively acts as a clock and the system may be regarded as “already deparametrized” by the intrinsic time $q^0$. A typical example is a parametrized nonrelativistic
particle \([14]\) in which case \([4.1]\) describes such a system with Hamiltonian \(h_1\) and Newtonian time function \(q^0\). Note that \(h_1\) may involve \(q^0\), in which case the corresponding Newtonian Hamiltonian is time-dependent. We will see that the approach of \([11]\) gives the usual quantization of nonrelativistic particles when applied to systems of this form.

We wish to evaluate matrix elements of \([A]\) \(Q_{0}=\tau\) and begin by noting that \(Q_{0}(t) = Q_{0}(t') + T(t)\) where \(T(t) = \int_{t'}^{t} N(t)\) for some fixed \(t'\). Thus, we find

\[
\langle q_{1},k_{1};t'|[A]Q_{0}=\tau|q_{2},k_{2};t'\rangle = \langle q_{1},k_{1};t'|A\tau-q_{1}|q_{2},k_{2};t'\rangle \tag{4.2}
\]

where \(t_{\tau-q_{1}}\) is the time \(t\) when \(T(t) = \tau - q_{1}\). Equation \(4.2\) can be used directly to show that \([A]\) \(Q_{0}=\tau\) preserves physical states, but this already follows from the general arguments of \([11]\).

From \(4.2\), we see that \([A]Q_{0}=\tau|\psi\rangle\) has components

\[
\langle q_{1} = \tau - T(t), k_{1}; t|[A]Q_{0}=\tau|\psi\rangle = \langle q_{1} = \tau - T(t), k_{1}; t|A(t)|\psi\rangle \tag{4.3}
\]

on the \(Q_{0}(t) = \tau - T(t)\) subspace. Now, if \(|\psi\rangle\) is an eigenstate of \(H\) with eigenvalue \(E\), so is \(|\psi'\rangle = [A]Q_{0}=\tau|\psi\rangle\) and it satisfies

\[
-i\frac{\partial}{\partial q_{1}^0}\langle q_{1},k_{1};t|\psi'\rangle + \langle q_{1},k_{1};t|H(t)|\psi'\rangle = E\langle q_{1},k_{1};t|\psi'\rangle \tag{4.4}
\]

It is therefore completely determined by the components given in \(4.3\), much as is the case in, for example, \([12]\). Since the action of \([A]Q_{0}=\tau\) on \(|\psi\rangle\) is determined through \(4.3\) and \(4.4\), it follows that, for any \(Z_{1}(t), Z_{2}(t)\) built from the \(Q(t)\)’s and \(P(t)\)’s, if \([Z_{1}(t), Z_{2}(t)] = Z_{3}(t)\) then we have

\[
[[Z_{1}]Q_{0}=\tau, [Z_{2}]Q_{0}=\tau] = [Z_{3}]Q_{0}=\tau. \tag{4.5}
\]

We can also derive

\[
-i\frac{\partial}{\partial \tau}[Z_{1}]Q_{0}=\tau = [\tilde{H}_{1}(\tau), [Z_{1}]Q_{0}=\tau] \tag{4.6}
\]

by considering the matrix elements:
\[ \langle q_0^1 = \tau - T(t), k_1; t | - i \frac{\partial}{\partial \tau} [A|Q^\alpha = \tau|\psi] \]
\[ = -i \frac{\partial}{\partial \tau} \left( \langle q_0^1 = \tau - T(t), k_1; t | [A|Q^\alpha = \tau|\psi] \rangle - \langle q_0^1 = \tau - T(t), k_1; t | P_0(t)[A|Q^\alpha = \tau|\psi] \rangle \right) \]  

(4.7)

and using \([H_1(t), Q^0(t)] = 0, [P_0(t), A(t)] = 0, P_0(t) = H(t) - H_1(t), \) and \([H(t), [A|Q^\alpha = \tau|\psi] = 0.\]

In 4.6, \( \hat{H}_1(\tau) \) is the operator built from the \([Q]Q^\alpha = \tau\)'s and the \([P]Q^\alpha = \tau\)'s in the same way that \( H_1 \) is built from the \( Q(t)\)'s and the \( P(t)\)'s. Thus, we have reproduced the usual results at the level of algebras. Since the states \( |E, k_1\rangle \) which satisfy \( H|E, k_1\rangle = E \) and \( \langle q^0, k_1|E, k_2\rangle = e^{iq^0E}\delta_{k_1,k_2} \) form a basis for \( \mathcal{H} \), this also follows at the level of the physical Hilbert space from our use of 3.23.

**B. The Relativistic Free Particle**

Though hardly a sufficient test of a quantization scheme, every procedure for quantizing reparametrization invariant systems should be applicable to the relativistic free particle. We therefore take this as our next special case and discuss the convergence of the integrals 3.16 and 3.17 and the operators they define. We will also see that the inner product 3.23 is unique, provided that a simple set of observables are required to be symmetric.

We consider here a relativistic free particle in a flat Minkowski spacetime of an arbitrary number of dimensions. Because the equations of motion can be solved easily, we can explicitly write the desired algebra as:

\[ [X^\mu(t), X^\nu(t')] = \frac{i}{m} \eta^{\mu\nu} \int_t^{t'} dt N(t), \quad [N(t), X^\mu(t')] = 0 \]  

(4.8)

where \( \eta^{\mu\nu} \) is the Minkowski metric. This follows from 3.3 in the form

\[ \frac{d}{dt} P_\mu(t) = 0, \quad \frac{d}{dt} X_\mu = \frac{N(t)}{m} P_\mu \]  

(4.9)

\[^3\text{Note that a “deparameterized algebra” based on gauge fixing } x^0 = t \text{ may also be introduced for this system and can be used in place of 4.8 to construct the operators 3.8. A brief comparison of these two possibilities, as well as some of the calculations below, appeared in 12.}\]
so that $P_\nu(t) = P_\nu$. The constraint is given by $H = P^2 + m^2 = 0$. As in (3), $N(t)$ is some function $n(t)$ times the identity operator.

For each $t$, it is useful to introduce two bases $\{ |x; t\rangle \}$ and $\{ |p; t\rangle \}$ that satisfy

$$X^\mu(t)|x; t\rangle = x^\mu|x; t\rangle, \quad P_\nu|p; t\rangle = p_\nu|p; t\rangle$$

$$\langle x; t|x'; t\rangle = \delta(x - x'), \quad \langle p; t|p'; t'\rangle = \delta(p - p') \exp(i \int_t^{t'} dt' N(t)p_\nu p^\nu)$$

$$\langle x; t|p; t\rangle = \frac{1}{\sqrt{2\pi}} e^{ipx}. \quad (4.10)$$

We then proceed to consider the operators $[A]_{X^0=\tau}$. Inserting complete sets of states and using $\int dE \sum_a |E, a\rangle \langle E, a| = \int dp|p; t\rangle \langle p, t'| \delta(E - E^*) = \delta(p^2 - (p^*)^2)$, and

$$\langle p', t|\theta(X^0(t) - \tau)|p, t\rangle = \delta(p - p') \int_\tau^\infty \frac{dp'^0}{2\pi} e^{ip'^0(p_0 - p'^0)} \tag{4.11}$$

together with (3.19), we find that

$$[A]_{X^0=\tau}^L|p; t\rangle = -2\pi i \int dp' dp^* \delta(p^2 - (p^*)^2) \langle p^*; t'| p^2; t'| A(t')|p'^0, \overline{p}; t'\rangle$$

$$\times \frac{1}{2} e^{i\tau(p'^0 - p_0)} [\delta(p'^0 - p_0) - \frac{i}{\pi (p'^0 - p_0)}]. \tag{4.12}$$

Here, $\overline{p}$ is the collection of spatial components of $p$ so that $p = (p_0, \overline{p})$ and the integration over $x^0$ has been performed in a distributional sense. Note, again, the presence of the energy conserving delta-function which guarantees that our operators commute with the constraint.

The expression (4.12) contains several singular expressions, all of which are regulated by the factor $(p'^2_0 - p_0^2)$ so that we find:

$$[A]_{X^0=\tau}^L|p; t\rangle = \int dp^* dp'_0 |p^*; t'| \delta(p^2 - (p^*)^2) \langle p^*; t| A(t)|p'^0, \overline{p}; t\rangle e^{i\tau(p'^0 - p_0)} [p'_0 + p_0]. \tag{4.13}$$

If $A$ commutes with $P_0$, this simplifies to

$$[A]_{X^0=\tau}^L|p; t\rangle = \int d\overline{p'} \sum_{\epsilon \in \{+,-\}} |\epsilon \tilde{p}_0, \overline{p'}; t'| \overline{\langle \overline{p'}; t'| A(t')| \overline{p}, t'\rangle} e^{i\epsilon(\tilde{p}_0 + p_0)} \frac{[\epsilon \tilde{p}_0 + p_0]}{2 \tilde{p}_0}. \tag{4.14}$$

where we have introduced the reduced matrix elements $\langle \overline{p'}; t'| A(t')| \overline{p}; t'\rangle_p$ that satisfy:

$$\langle p'; t'| A(t')|p; t\rangle = \delta(p'_0 - p_0) \langle p'; t'| A(t')|p; t'\rangle_p \tag{4.15}$$
and where \( \tilde{p}_0 = \sqrt{p_0^2 - \vec{p}^2 + \gamma^2} \). If \( A \) commutes with \( Q^0 \), the reduced matrix elements (4.13) do not depend on \( p_0 \).

Note that the factor of \( \epsilon \tilde{p}_0 + p_0 \) in (4.14) minimizes the amount by which this operator mixes positive and negative frequency states, though some mixing still occurs. Thus, the case of \( A = X_i \) does not correspond to a Newton-Wigner operator (which would leave the positive and negative frequency subspaces invariant). On the other hand, it may be checked that \( [\theta(P_0)\text{sign}P_0X^i]_{X^0=\tau} \) is just the Newton-Wigner operator \( X^i_{\text{NW}}(\tau) \) associated with the coordinate \( X^i \).

It now follows that Hermiticity of a few interesting operators guarantees that the inner product (3.23) is unique. From (4.14), we see that

\[
[P_0 \text{sign}(P_0)]_{X^0=\tau}^L |p; t'\rangle = p_0 |p; t'\rangle
\]

which is hermitian on \( \mathcal{H} \) so that \( [P_0 \text{sign}(P_0)]_{X^0=\tau}^L = [P_0 \text{sign}(P_0)]_{X^0=\tau}^R = [P_0 \text{sign}(P_0)]_{X^0=\tau} \). If we require \( [P_0 \text{sign}(P_0)]_{X^0=\tau} \) to be Hermitian on the physical space (spanned by \( |\epsilon|\vec{p} | p; t'\rangle \)), it follows that the positive and negative frequency subspaces are orthogonal. If we also ask that \( [X_i]_{X^0=\tau} \) and \( [P_j]_{X^0=\tau} \) be symmetric, then the inner product is fixed up to an overall normalization on the positive frequency subspace and a similar normalization on the negative frequency subspace. Additionally, if we require \( [\Theta]_{X^0=\tau} \) to be Hermitian, where \( \Theta \) is the time reversal operator \( (\Theta|p; t\rangle = | - p; t\rangle) \), these normalizations must be identical and the inner product is uniquely determined (up to an overall scale factor) to be:

\[
(|\epsilon|\vec{p} | \vec{p}; t'\rangle, |\epsilon'\vec{p'} | \vec{p'}; t'\rangle)_{\text{phys}} = 2\sqrt{\vec{p}^2 + m^2} \delta(\vec{p} - \vec{p'})\delta_{\epsilon,\epsilon'}
\]

(4.17)

Note that (4.17) agrees with (3.23) since \( dE = 2|p_0|dp_0 \). It therefore follows from (III A) that all operators of the form \( [A]_{B=\tau} \) are symmetric (for Hermitian \( A(t) \) and \( B(t) \)) and we need not have chosen \( x^0 \) as the “intrinsic clock.” Finally, we verify that we have constructed an overcomplete set of observables as densely defined operators on \( \mathcal{H}_{\text{phys}} \). This follows since

\[4\text{A similar calculation verifies that } [\text{sign}(P_0)]_{X^0=\tau} = \mathbb{1} \text{ as claimed.}\]
4.17 shows that \([X_i]_{X^0=\tau}, [P_j]_{X^0=\tau}, [P_0 \text{ sign}(P_0)]_{X^0=\tau}\) and \([\Theta]_{X^0=\tau}\) yield normalizable states when acting on any \(|\psi\rangle \in \mathcal{H}_{\text{phys}}\) for which \((|\epsilon|, \mathcal{P}, t', |\psi\rangle)_{\text{phys}}\) is a sufficiently smooth and rapidly decreasing function of \(\mathcal{P}\) and thus are densely defined.

V. RECOLLAPSING DYNAMICS: SEPARABLE SEMI-BOUND MODELS

The LRS Bianchi IX and Kantowski-Sachs minisuperspaces fall into the class of models that we refer to as “separable and semi-bound.” These are, roughly speaking, models for which the potential is separable and which (classically) describe spacetimes whose homogeneous slices expand, reach a maximum volume, and recontract. They are thus “semi-bound” in the sense that they do not classically reach arbitrarily large size.

Below, we apply the methods of section III to such models. As before, we verify the convergence (V B) of the integrals that define our observables and construct a complete set of densely defined operators on \(\mathcal{H}_{\text{phys}}\) (V C). In addition, we derive quantum analogues of 2.3 and 2.4, showing that our quantization also predicts recollapsing behavior.

A. The System and Observables

Separable semi-bound systems are time-reparametrization invariant models that can be described in the canonical formalism with a Hamiltonian constraint of the form \(h = h_0 - h_1 = 0\) where \(h_0\) is of the form \(p_0^2 + V_0(q^0)\) for some canonically conjugate pair \((p_0, q^0)\) which take values in \((-\infty, \infty)\), \(h_1\) does not involve either \(p_0\) or \(q_0\), and \(h_1\) is a Hamiltonian of the type appropriate to a nonrelativistic particle. Thus, we consider the case where the configuration space \(\mathcal{Q}\) is of the form \(\mathbb{R} \times \mathcal{Q}_1\) and the phase space is \(T^* \mathcal{Q} = T^* \mathbb{R} \times T^* \mathcal{Q}_1\). In addition, we will ask that \(V(q^0)\) be smooth, that \(V_0(q^0) \rightarrow -\infty\) as \(q^0 \rightarrow +\infty\), \(V_0(q^0) > 0\), and \(V_0(q^0) < W e^{\alpha q_0}\) for some positive \(W\) and \(\alpha\). This last condition is important only for large negative \(q^0\). This leads to the following:
• **Definition:** A separable semi-bound system is a Hilbert space $H_{aux} = L^2(\mathbb{R}) \otimes \mathcal{H}_1$ together with a self-adjoint operator $H = H_0 - H_1$ such that $H_1 = \mathbb{1} \otimes \tilde{H}_1$ for some $\tilde{H}_1$ and $H_0 = \tilde{H}_0 \otimes \mathbb{1}$ for $\tilde{H}_0 = -\frac{\partial^2}{\partial (q^0)^2} + V(q_0)$ and a potential $V(q^0)$ which satisfies (on every semi-bounded interval $(-\infty, \tilde{q}^0)$) the bound $V(q^0) < W e^{-\alpha q^0}$ for some $W, \alpha > 0$, but for which $V(q^0) \to \infty$ as $q^0 \to \infty$.

These conditions imply that, when viewed as an operator on the Hilbert space $L^2(\mathbb{R})$ in a "$q^0$ - coordinate representation,” the spectrum of $H_0$ is purely continuous. The condition that $V_0(q^0) \to \infty$ will allow us to work with convergent expressions that require no regularization or careful treatment. From [15], we see that when described by the appropriate variables and with a rescaled Hamiltonian, the LRS Bianchi IX and Kantowski-Sachs models may be placed in this form with $q^0 = \ln(\det g)$ where $g$ is the 3-metric of a homogeneous slice.

As described in [[IIA]], we use the auxiliary Hilbert space $L^2(Q)$ to carry a representation of the algebra defined by 3.2 and 3.3 and require that $H = H_0 - H_1$ be a Hermitian factor ordering of $h$ on this space (and similarly for $H_0$ and $H_1$). From this and the above conditions, it follows that $H$ has a purely continuous spectrum with $\sigma_c(H) = (-\infty, \infty)$. Note that $H$ is time independent and that, since they commute, $H_0$ and $H_1$ are time independent as well.

As before, we will make use of a basis in this auxiliary space that is tailored to our system. This basis will consist of (delta-function normalizable) states $\{|E_0, E_1, k\rangle\}$ that are eigenvectors of $H_0$ with eigenvalue $E_0$ and that are eigenvectors of $H_1$ with eigenvalue $E_1$. The (discrete) label $k$ is to remove any remaining degeneracy in our description. Thus, $H|E_0, E_1, k\rangle = (E_0 - E_1)|E_0, E_1, k\rangle$. Note that this set of labels leads to a decomposition of our auxiliary Hilbert space as a direct product $\mathcal{H} = \mathcal{H}_0 \otimes \mathcal{H}_1$ through $|E_0, E_1, k\rangle = |E_0\rangle \otimes |E_1, k\rangle$ since, for systems of this type, the spectral subspaces of $H_0$ on $L^2(q^0)$ are nondegenerate.

Also as in [[IIA]], the (constrained) Hamiltonian $H$ and the lapse $N(t)$ define a parameter time evolution that, for the canonical variables, is given by

$$A(t) = \exp(iH \int_t^t dt N(t)) A(t') \exp(-iH \int_t^t dt N(t)).$$

(5.1)
In irreducible representations, \( N(t) \) is proportional to the identity: \( N(t) = n(t)\mathbb{1} \) and we assume that (3.6) holds. Also, for each \( t \), our representation has a set of states \( |q; t\rangle \) labeled by points \( q \) in the configuration space \( Q \) that define a “configuration representation at time \( t \)” and satisfy \( \langle q; t|q'; t\rangle = \delta(q, q') \). As in the case of the relativistic free particle, it will be convenient to introduce a family of “energy bases” \( \{|E_0, E_1, k; t\rangle\} \) (also labeled by \( t \)), where

\[
|E_0, E_1, k; t\rangle = \left( \exp[i(E_0 - E_1) \int_{t'}^{t} dt N(t)] \right) |E_0, E_1, k; t'\rangle
\]

so that inner products of the form \( \langle q; t|E_0, E_1, k; t\rangle \) are independent of \( t \). The arbitrary phase in the definition of \( |E_0, E_1, k\rangle \) may be used to set \( |E_0, E_1, k\rangle = |E_0, E_1, k; t'\rangle \) for any \( t' \).

Since the spectrum of \( H \) includes zero, the set of physical states that are delta-function normalizable in the auxiliary inner product and satisfy \( H|\psi\rangle = 0 \) is not empty. They are of the form \( |E_0 = E_1, E_1, k; t'\rangle \) where \( E_1 \) ranges over the spectrum of \( H_1 \) and \( k \) ranges over its full set of values. From (3.23), the physical inner product is just

\[
(|E_1^*, E_1^*, k^*; t'), |E_1, E_1, k; t')\rangle_{phys} = \delta^{(2)}(E_1^*, E_1)\delta_{k^*, k}
\]

where the \( \delta^{(2)}(E_1^*, E_1) \) is to be interpreted as a delta-function or Kronecker delta as appropriate to the spectrum of \( H_1 \).

A few brief comments are now in order before deriving the rigorous convergence and recollapse results. We again wish to consider the action of the operators \([A]_{B=\tau}\). Let us suppose that \( B \) is, in fact, a configuration variable. Note that

\[
\langle E_0', E_1', k'; t|\theta(B(t) - \tau)|E_0, E_1, k; t\rangle = \int_{Q_{\theta(q)>\tau}} dq \langle E_0', E_1', k'; t|q; t\rangle \langle q; t|E_0, E_1, k; t\rangle
\]

so that we may write

\[
\langle E_0^*, E_1^*, k^*; t| [A]_{B=\tau}^L |E_0, E_1, k; t\rangle
\]

\[
= -i2\pi \delta(E_0 - E_1 - E_0^* + E_1^*) \int dE_0' \sum_{E_1', k'} (E_0 - E_1 - E_0' + E_1')
\]

\[
\times \langle E_0^*, E_1^*, k^*; t|A(t)|E_0', E_1', k'; t\rangle \int_{Q_{\theta(q)>\tau}} dE_0' dq \langle E_0', E_1', k'; t|q; t\rangle \langle q; t|E_0, E_1, k; t\rangle
\]

(5.5)
and, similarly for \([A]_{B=\tau}^R\).

Two cases are now of interest. The first occurs when the spectrum of \(H_1\) is entirely discrete. Then, the factor states \(|E_1\rangle\) are normalizable and the wavefunctions \(\langle E'_0, E'_1, k'; t|q; t\rangle\) fall off rapidly in the directions in which \(Q\) is not compact and \(q^0\) remains constant. Furthermore, because of the assumption that \(V_0(q^0) \to \infty\) as \(q^0 \to \infty\), these wavefunctions also fall off in the positive \(q^0\) direction. Thus, if \(b(q)\) is any configuration variable for which \(q^0\) is bounded from below in the region of \(Q\) with \(b(q) \geq \tau\), this factor represents a convergent expression. At the other extreme, if the spectrum of \(H_1\) is purely continuous (as in IV B), then this integral will converge only in a distributional sense, as is appropriate. Note that convergence of these integrals guarantees that the matrix element in (5.5) (and correspondingly for \([A]_{Q^0=\tau}^R\)) vanishes in the large \(\tau\) limit, verifying the recollapsing behavior of 2.4 in a weak sense.

**B. Rigorous Convergence and Recollapse Results**

We now present two results concerning the convergence of the sums in expressions 3.19 and 3.20. These results will show rigorously that a quantum analogue of 2.4 holds. As usual, the stronger result follows for the simpler case.

Let us begin by assuming that \(B = Q^0\) and that \(A(t)\) commutes with both \(Q^0(t)\) and \(P_0(t)\) so that \([A]_{Q^0=\tau}^L = [A]_{Q^0=\tau}^R = [A]_{Q^0=\tau}\). Thus, we may again introduce the reduced matrix elements \(\langle E'_1, k'|\tilde{A}|E_1, k\rangle\) that satisfy

\[
\langle E'_0, E'_1, k'; t'|A(t)|E_0, E_1, k; t\rangle = \delta(E'_0 - E_0)\delta(E'_1 - E_1)\langle E'_1, k'|\tilde{A}|E_1, k\rangle \tag{5.6}
\]

and are independent of \(E_0\). Note that (5.6) defines a “reduced operator” \(\tilde{A}\) on the factor space \(\mathcal{H}_1\). The action of \([A]_{Q^0=\tau}\) now takes the form:

\[
[A]_{Q^0=\tau}|E_0, E_1, k; t\rangle = -i2\pi \sum_{E_1^*, k^*} \langle E_1^* - E_1|E_0 - E_1 + E_1^*, E_1^*, k^*; t\rangle_1 \langle E_1^*, k^*|\tilde{A}|E_1, k\rangle_1 \\
\times \int_{q_0 > \tau} dq_0 \langle E_0 - E_1 + E_1^*|q_0\rangle_0 \langle q_0|E_0\rangle_0 \tag{5.7}
\]
where bras and kets with subscripts 0 and 1 refer to states in $\mathcal{H}_0$ and $\mathcal{H}_1$ respectively. Note that while all terms in this sum are finite it remains to show that the sum itself represents a normalizable state in the physical space. Note that this sum will be at best delta-function normalizable in the auxiliary space since $|E_0, E_1, k\rangle$ is only delta-function normalizable.

In order to discuss the convergence of the sum in (5.7), we would like to find a bound $M(\tau, E)$ such that $|I(E, E^*, \tau)| \leq M(\tau, E)$ where

$$I(E, E^*, \tau) = \int_{q^0 \geq \tau} \langle E_0 = E^* | q^0 \rangle \langle q^0 | E_0 = E \rangle.$$  

(5.8)

We use the fact that the states are delta-function normalized so that $I(E, E^*, \tau) = \delta(E - E^*) - \int_{q^0 \leq \tau} \langle E^* | q^0 \rangle \langle q^0 | E \rangle$. Because the potential $V_0(q^0)$ is exponentially small for large negative $q^0$, we approximate the function $\langle q^0 | E \rangle$ by plane waves through the expression:

$$\langle q^0 | E \rangle = \frac{1}{\sqrt{4\pi p}} (e^{iq^0} + \alpha_E e^{-iq^0}) + \frac{1}{\sqrt{p}} \Delta_E(q)$$  

(5.9)

for the appropriate $\alpha_E$ with $|\alpha_E| = 1$ and some $\Delta_E$ which we expect to be small. Here, we have set $p = \sqrt{E}$. Note that we have chosen to normalize the plane waves in a manner consistent with the normalization $\langle E | E' \rangle = \delta(E - E') = \frac{1}{2p} \delta(p - p')$.

Thus, we may expand $I$ as

$$I = \delta(E - E^*) - \frac{1}{2p} \delta(p - p^*) + \frac{i}{4\pi (p + p^*)} \frac{e^{i\tau(p+p^*)} \alpha_E - e^{-i\tau(p+p^*)} \alpha_E^*}{\sqrt{pp^*}}$$

$$+ \frac{i}{4\pi (p^* - p)} \frac{e^{i\tau(p^*-p)} - e^{-i\tau(p^*-p)} \alpha_E \alpha_E^*}{\sqrt{pp^*}}$$

$$- \frac{1}{\sqrt{4\pi pp^*}} \left( \tilde{\Delta}_E^\tau(-p^*) + \alpha_E \tilde{\Delta}_E^\tau(p^*) + \Delta_E^\tau(-p^*) + \alpha_E \Delta_E^\tau(p) \right)$$

$$- \int_{q_0 \leq \tau} dq_0 \frac{\Delta_E \Delta_E^*}{\sqrt{pp^*}}$$  

(5.10)

where the bars denote complex conjugation and

$$\tilde{\Delta}_E^\tau(p^*) = \int_{q^0 \leq \tau} e^{iq^0p^*} \Delta_E(q^0)$$  

(5.11)

The first two terms in (5.10) cancel.

The bound on the potential may now be used to verify that $\Delta_E$ can be regarded as small. By the usual arguments, it follows that $\Delta_E$ satisfies

$$\Delta_E^\tau(p) = \int_{q^0 \leq \tau} e^{iq^0p} \Delta_E(q^0)$$  

(5.11)
\[ \left( \frac{\partial^2}{\partial(q^0)^2} + E \right) \frac{\Delta_E}{\sqrt{p^2}} = V_0(q^0) \langle q_0|E \rangle \]  

(5.12)

which has the solution

\[ \Delta_E(q^0) = \sqrt{\rho} e^{ipq^0} \int_{-\infty}^{q^0} dq^{0} e^{-2ipq^{0}} \int_{-\infty}^{q^0} dq^m e^{2ipq^{m0}} V_0(q^{m0}) \]  

(5.13)

since, for the right choice of \( \alpha_E \), \( \Delta_E \) satisfies the boundary conditions \( \Delta_E \to 0 \) and \( \frac{\partial}{\partial q} \Delta_E \to 0 \) as \( q^0 \to -\infty \). Let us rewrite this expression using (5.3):

\[ \Delta_E(q^0) = \frac{e^{ipq^0}}{\sqrt{4\pi}} \int_{-\infty}^{q^0} dq^{0} e^{-2ipq^{0}} \int_{-\infty}^{q^0} dq^m e^{2ipq^{m0}} V_0(q^{m0}) + e^{ipq^0} \int_{-\infty}^{q^0} dq^{0} e^{-2ipq^{0}} \int_{-\infty}^{q^0} dq^m \alpha_E V_0(q^{m0}) + e^{ipq^0} \int_{-\infty}^{q^0} dq^{0} e^{-2ipq^{0}} \int_{-\infty}^{q^0} dq^m e^{ipq^{m0}} \Delta(q^{m0}) V_0(q^{m0}) \]  

(5.14)

Let \( \beta_1(E) \) and \( \beta_2(E) \) be the maximum values of the first and second terms in (5.14) for \( q^0 \in (-\infty, \tau] \), which exist since \( V(q^0) \) is smooth and bounded on this interval by \( W e^{\alpha q^{m0}} \).

Note that \( \beta_1(E), \beta_2(E) \to 0 \) as \( E \to \infty \) since both describe integrals of fixed \( L^p(-\infty, \tau) \) functions against oscillating exponentials. Here, the integral over \( q^0 \) is highly oscillatory in the definition of \( \beta_2(E) \) and the integral over \( q^{m0} \) is relevant for \( \beta_1(E) \).

Further, since \( \langle q|E \rangle \) is smooth and bounded as \( q \to -\infty \), \( |\Delta_E| \) takes some maximal value \( \Delta_E^M \) on \( (-\infty, \tau) \) by (5.13) and we see that \( \Delta_E^M \leq \beta_1(E) + \beta_2(E) + \gamma \Delta_E^M \), where \( \gamma = \frac{W}{\alpha \tau} e^{\alpha \tau} \) is independent of \( E \). Let us suppose for the moment that \( \gamma < 1 \) so that

\[ \Delta_E^M \leq \frac{\beta_1(E) + \beta_2(E)}{1 - \gamma}. \]  

(5.15)

Thus,

\[ |\Delta_E(q^0) - \frac{e^{ipq^0}}{\sqrt{4\pi}} \int_{-\infty}^{q^0} dq^{0} e^{-2ipq^{0}} \int_{-\infty}^{q^0} dq^m (e^{2ipq^{m0}} + \alpha_E) V_0(q^{m0})| \leq \frac{(\beta_1(E) + \beta_2(E)\gamma}{1 - \gamma}. \]  

(5.16)

Since \( \beta_1 + \beta_2 \to 0 \), this estimate is accurate in the \( E \to \infty \) limit and \( \Delta_E(q^0) \to 0 \). A similar argument using (5.14) and (5.15) demonstrates that

\[ \int_{-\infty}^{\tau} dq^{0} \frac{\Delta_E^*(q^0)}{\sqrt{p^2}} \to 0 \]  

(5.17)
in the $E^* \to \infty$ limit and that the $L^2$ norm of $\frac{\Delta E}{\sqrt{p^*}}$ on $(-\infty, \tau)$ is finite and also vanishes for large $E^*$. It follows that $I(E, E^*, \tau) \to 0$ as $E^* \to 0$ and thus that there exists a bound $M(E, \tau) \geq |I(E, E^*, \tau)|$. To see this, recall that we know that $I(E, E, \tau)$ is finite so that we may ignore the apparent divergences in $5.10$ for $p^* = \pm p$. Now, for $p \neq p^*$ $I$ is a continuous function of $E^*$ by $5.10$ and $5.13$. The first two terms in $5.10$ cancel and the next two terms are explicitly decreasing for large $p^*$. The pair of terms involving $\tilde{\Delta}^E_\tau(\pm p^*)$ are bounded by a multiple of $5.17$ and the terms $\tilde{\Delta}^E_\tau(\pm p^*)$ vanish as they are the integral of a smooth $L^2$ function against a rapidly oscillating exponential. The last term is bounded by the product of $\Delta_M^E$ and $5.17$. Thus, we have derived the existence of a bound (and in fact of a maximal value) for $|I(E, E^*, \tau)|$, assuming $\gamma < 1$.

We now consider the more general case and show that, by repeating the approximation described by $5.14$, we can follow a similar proof without assuming $\gamma < 1$. Note that if we iterate this approximation $n$ times, replacing at each step the $\Delta_E$ that appears in the integral on the right hand side of $5.14$ with the entire right hand side, then the term on the right hand side that still contains $\Delta_E$ can be bounded by an expression of the form:

$$\Delta_E^M \int_{\tau \leq q_1 \leq q_2 \leq q_3 \leq \ldots \leq q_{2n}} d^{2n}q \prod_{j=1}^{n} V(q_{2j}) \leq \frac{W^n}{(n!)^2 \alpha^2 \gamma^2 n \tau} \Delta_E^M$$

and so approaches zero as $n \to \infty$. Hence, for any $V_0$ of the form specified, there is some finite $n$ such that the bound in $5.18$ (which we will call $\gamma_n \Delta_E^E$) is less than $\Delta_E^E$ so that $\gamma_n < 1$. A bound of the form $5.15$ again follows with $\gamma$ replaced by $\gamma_n$ and $\beta_1, \beta_2$ replaced by the appropriate $\beta_{1,n}$ and $\beta_{2,n}$ which also vanish in the $E \to \infty$ limit. The rest of the argument proceeds as before, and we conclude that $I(E, E^*, \tau)$ is a bounded function of $E^*$; that is,

- There is a function $M(E, \tau)$ such that $M(E, \tau) \geq |I(E, E^*, \tau)|$.

From $5.7$ and our bound $M(E, \tau)$, we now see that $[A]_{Q=\tau}|E_0, E_1, k; t\rangle$ is a normalizable state for any $A$ such that

$$\sum_{E_1, k} (E_1^* - E_1)^2 |\langle E_1^*, k^*|\tilde{A}|E_1, k\rangle|^2 \leq \infty,$$ i.e., such that $||[\tilde{A}, \tilde{H}_1]|E_1, k\rangle||_{\mathcal{H}_1} < \infty$. (5.19)
where \(|\langle |\psi\rangle\rangle|_{\mathcal{H}_1}\) represents the norm of the state \(|\psi\rangle\) in the factor space \(\mathcal{H}_1\). This allows us to conclude the following result:

- **Result 1:** Let \(A\) be a densely defined operator of the form \(1 \otimes \tilde{A}\) on \(\mathcal{H}_{aux}\) of a separable semi-bound system. Further, let \(A(t)\) be the one parameter family of operators defined through (5.4) with \(A(0) \equiv A\), and let \([A]_{Q^0=\tau}\) be the one parameter family of operators on \(\mathcal{H}_{phys}\) defined by (3.18), (3.19), and (3.20). Note that our construction (3.23) of \(\mathcal{H}_{phys}\) identifies \(\mathcal{H}_{phys}\) with \(\mathcal{H}_1\) at \(t = 0\). Then, under this identification, if \(|\psi\rangle\in \mathcal{H}_1\) lies in the domain of \([\tilde{A},H_1]\), it also lies in the domain of \([A]_{Q^0=\tau}\). In particular, if \([\tilde{A},H_1]\) is densely defined, so is \([A]_{Q^0=\tau}\).

It now follows that quantization of “separable semi-bound models” captures the classical notion of “recollapse” expressed through (2.4) for \(a(t)\) independent of \(q^0(t)\) and \(p_0(t)\). As in (7), this is to be expected since we have used the auxiliary space \(L^2(Q)\). Below, we show that the norms of all states of the form \([A]_{Q^0=\tau}\langle E_0, E_1, k; t'\rangle\) vanish in the large \(\tau\) limit and thus that the operator \([A]_{Q^0=\tau}\) converges strongly to zero.

Note that we may take the bound \(M(E, \tau)\) on the integral \(I\) to be given by the maximum value of \(I(E, E^*, \tau)\) over \(E^*\), which exists by our previous argument. Thus, \(M(E, \tau)\) is also given by an expression of the form \(|\int_{q^0 \geq \tau} f(E)|\) for \(f \in L^1(\tau, \infty)\). Since this integral converges, it must vanish in the large \(\tau\) limit and, since the norm of \([A]_{Q^0=\tau}\langle E_0, E_1, a; t'\rangle\) in \(\mathcal{H}_{phys}\) is bounded by the product of \(M^2\) and the norm given in (5.19), we find

- **Result 2:** For \(A\) as in Result 1, \([A]_{Q^0=\tau}\rightarrow 0\) as \(\tau \rightarrow \infty\) in the sense of convergence on a dense set of states; that is, \([A]_{Q^0=\tau}\) converges strongly to the zero operator.

Unfortunately, considering only operators \(A\) that commute with \(Q^0\) and \(P_0\), is not sufficient to conclusively demonstrate recollapsing behavior. Recall that if a classical spacetime \(s\) expands smoothly and then recollapses, \([a]_{Q^0=\tau}(s)\) represents a difference of a term associated with the expansion and a term associated with the collapse. Thus, our discussion to
this point leaves open the possibility that this quantization should be interpreted as describing pairs of contracting and expanding spacetimes such that the appropriate terms cancel for large $\tau$. It would be comforting to find that operators insensitive to the expansion or contraction of the universe vanish in the large $\tau$ limit as well.

As suggested in section II, we would like to study the operator $[\text{sign}(P_0)]_{Q=\tau}$. However, for technical reasons we will instead work with

$$O_\tau \equiv \left[ \frac{1}{H_0 + 1} \theta(Q^0 - \tau') \text{sign}(P_0) \frac{1}{H_0 + 1} \right] Q^0 = \tau \quad \text{(5.20)}$$

and derive the analogue of (2.4) for this operator. Note, first, that the factors of $\theta(Q - \tau')$ are completely irrelevant classically for $\tau' < \tau$. Despite this, they will greatly simplify the details in what follows. Also, $H_0$ is time independent and the classical $h_0$ is constant along a solution. Thus, (5.20) is nearly as satisfactory as $[\text{sign}(P_0)]_{Q=\tau}$ since, if the corresponding classical observable approaches zero along a solution for large $\tau$, it tells us that the spacetime in question does not reach arbitrarily large values of $q^0$.

Now, for an operator $A$ (such as (5.20)) that is constructed only from $Q^0$ and $P_0$, the matrix element $\langle E_0^*, E_1^*, k^*; t'|A(t')|E_0, E_1, k; t' \rangle$ must vanish unless $E_1^* = E_1$ and $k^* = k$. Thus, $[A]_{Q^0=\tau}|E_0, E_1, k; t' \rangle$ must be again proportional to $|E_0, E_1, k; t' \rangle$. From (3.19) and (3.20), we see (if the spectrum of $H_1$ is discrete) that in fact

$$[A]_{Q^0=\tau}|E_0, E_1, k; t' \rangle = 2\pi |E_0, E_1, k; t' \rangle \times \text{Im} \langle E_0, E_1, k; t'|A(E_0 - H_0)\theta(Q^0(t') - \tau)|E_0, E_1, k; t' \rangle \quad \text{(5.21)}$$

where $\text{Im}$ denotes the imaginary part. If the spectrum of $H_1$ is continuous, the action of $[A]_{Q^0=\tau}$ on $|E_0, E_1, k; t \rangle$ will not, of course, produce a state that is normalizable in the physical inner product. However, essentially the same analysis follows by considering wave packets and using the fact that $A(E_0 - H_0)\theta(Q - \tau)$ is of the form $O \otimes \mathbb{1}$ with respect to the decomposition $\mathcal{H} = \mathcal{H}_0 \otimes \mathcal{H}_1$.

Thus, our task is to show that this expectation value is finite and vanishes as $\tau \to \infty$. Note that $\theta(Q^0(t') - \tau)|E_0, E_1, k; t' \rangle$ is actually normalizable in the auxiliary inner product
since $\langle q^0|E \rangle$ decays faster than exponentially for large positive $q^0$. We may express the expectation value in 5.21 for the case where $A = \frac{1}{H_{0_t + 1}} \theta(Q - \tau') \text{sign}(P_0) \theta(Q - \tau')$ as

$$\frac{1}{E_0 + 1} \langle \psi(\tau') | \text{sign}(P_0(t')) \theta(Q^0(t') - \tau) \frac{E_0 - H_0}{H_0 + 1} | \psi(\tau) \rangle$$

(5.22)

where $|\psi(\tau)\rangle = \theta(Q^0(t') - \tau) |E_0, E_1, k; t'\rangle$ and similarly for $|\psi(\tau')\rangle$. Note that 5.22 is the matrix element of a bounded operator between two normalizable states and is therefore finite and bounded by some multiple of the norm of $|\psi(\tau)\rangle$. Again, $[A]_{Q=\tau}$ is densely defined on our physical Hilbert space. Also, the norm of $|\psi\rangle$ decreases to zero as $\tau \to \infty$, so the action of $[A]_{Q=\tau}$ vanishes in this limit on any finite combination of the states $|E_0, E_1, a; t'\rangle$. Thus we find:

- **Result 3:** $\mathcal{O}_\tau$ of 5.20 is densely defined and converges strongly to zero as $\tau \to \infty$.

The statement that there may be states to which this does not apply (i.e., that are not in the appropriate dense set) is of the same type as the statement that there are states in nonrelativistic quantum mechanics with infinite expectation value of the energy. For this reason, we feel justified in saying that when $Q^0$ has the interpretation of a scale factor for a cosmology, our quantization predicts that such spacetimes recollapse. Note that this rules out the possibility of an “evolution law” of the type 4.6. There is no exact unitary evolution in $\tau$-time for semi-bound separable systems, just as there is no corresponding exact Hamiltonian evolution at the classical level.

**C. A Complete Set of Operators**

Our final result will be that a complete set of densely defined quantum observables can be constructed by the techniques presented above. In order to prove this general result, we consider operators defined somewhat differently than in 3.16 and 3.17. We will also assume that, for each $E_0, E_1$, the label $k$ takes only a finite set of values. This is the case for both LRS Bianchi IX and the Kantowski-Sachs Model.
For any operator $B(t) = B(Q(t), P(t))$ bounded on $\mathcal{H}$, consider the objects
\[
[B]^L_{Q^0=\tau} = \int_{-\infty}^{\infty} dt f(H_0) \frac{1}{H+i} \theta(Q^0(t) - \tau') B(t) \theta(Q^0 - \tau') \frac{1}{H-i} \left( \frac{\partial}{\partial t} \theta(Q^0 - \tau) \right) f(H_0)
\]
\[
[B]^R_{Q^0=\tau} = \int_{-\infty}^{\infty} dt f(H_0) \left( \frac{\partial}{\partial t} \theta(Q^0 - \tau) \right) \frac{1}{H+i} \theta(Q^0(t) - \tau') B(t) \theta(Q^0 - \tau') \frac{1}{H-i} f(H_0)
\]
and note that these satisfy the analogues of (3.18) when $B(t)$ is Hermitian on $\mathcal{H}$. Here, $f$ is an as yet unspecified real function that will serve to regulate the above expression. Note that the factors of $\frac{1}{H+\pm i}$ combine to have no effect in the corresponding classical expression and that the $\theta$-functions in $Q^0 - \tau'$ are classically irrelevant for $\tau > \tau'$. Thus, the classical objects $[b]_{q^0=\tau}$ and $[\tilde{b}]_{q^0} = \tau$ differ only by the factor $1/f(h_0)^2$. It follows that as $B$ ranges over all bounded operators built from the $Q(t)$’s and $P(t)$’s, $[b]_{q^0=\tau}$ ranges over an overcomplete set of functions on the space of solutions.

The usual calculation shows that convergence of the action of our operator on some given state rests in the behavior of the matrix elements
\[
\langle E_0^s, E_1^s | [B]^L_{Q^0=\tau} E_0, E_1 = E_0, k \rangle \rangle_{\text{phys}} = 2\pi f(E_0^s) f(E_0)
\times \langle E_0^s, E_1^s | \theta(Q^0 - \tau') B \theta(Q^0 - \tau') \frac{H}{H-i} \theta(Q^0 - \tau) | E_0, E_1 = E_0, k \rangle
\]
When the spectrum of $H_1$ is discrete, $\theta(Q^0 - \tau) | E_0, E_1 = E_1, a \rangle$ is some normalizable state $|\psi(E_0, a, \tau)\rangle$ in $\mathcal{H}$ with norm $z_{\tau}(E_0)$ which is a monotonically decreasing function of $\tau$ and does not depend on $a$. We will use this function to choose an appropriate $f$. The case where $H_1$ has continuous spectrum can be dealt with in much the same way, using wave packets and the factorization $\mathcal{H} = \mathcal{H}_0 \otimes \mathcal{H}_1$, but we will not do so explicitly.

For the discrete case, fix $\tau' < \tau$ and let $n(E_1)$ be an enumeration of the energy levels of $H_1$ such that if $n = n(E_1)$, the $n$-th energy level has eigenvalue $E_1$. Similarly, let $m(E_1)$ be the dimension, which we have assumed to be finite, of the subspace of $\mathcal{H}_1$ with eigenvalue $E_1$. Now, extend the functions $n(E_1)$ and $m(E_1)$ which until now were defined only on the spectrum of $H_1$ to all of $\mathbb{R}$, say by defining them to be linear for $E_1$ not in the spectrum of $H_1$, and let $f$ be any function such that
\[
|f(E_0)| \leq \frac{1}{n(E_0) \sqrt{m(E_0) z_{\tau'}(E_0)}}.
\]
It then follows that
\[
|\langle E_0^*, E_1^* = E_0^*, k^* \rangle, [\tilde{B}]^{L}_{Q^0 = \tau}, E_0, E_1 = E_0, k \rangle_{\text{phys}}|^2 \leq \frac{4\pi^2||B||^2 z^2_\tau(E_0)}{n(E_0)n(E_0)\sqrt{m(E_0)m(E_0)z^2_\tau(E_0)}}
\]  
(5.26) 
and
\[
|\langle E_0^*, E_1^* = E_0^*, k^* \rangle, [\tilde{B}]^{R}_{Q^0 = \tau}, E_0, E_1 = E_0, k \rangle_{\text{phys}}|^2 \leq \frac{4\pi^2||B||^2 z^2_\tau(E_0^*)}{n(E_0)n(E_0)\sqrt{m(E_0)m(E_0^*)z^2_\tau(E_0)}}
\]  
(5.27) 
where \(||B||\) is the operator norm of \(B\) on \(H\). Summing over \(E_0^*\) and \(k^*\), it follows that the norm of the actions of \([\tilde{B}]^{L}_{Q^0 = \tau}\) and \([\tilde{B}]^{R}_{Q^0 = \tau}\) on \(|E_0, E_1 = E_0, k\rangle\) is bounded by
\[
||[\tilde{B}]^{L}_{Q^0 = \tau} |E_0, E_1 = E_0, k\rangle||^2_{\text{phys}} \leq \frac{4\pi^2||B||^2 z^2_\tau(E_0)}{\sqrt{m(E_0)n(E_0)z^2_\tau(E_0)}} \sum_{n^*} \frac{1}{(n^*)^2}
\]  
(5.28) 
and
\[
||[\tilde{B}]^{L}_{Q^0 = \tau} |E_0, E_1 = E_0, k\rangle||^2_{\text{phys}} \leq \frac{4\pi^2||B||^2}{\sqrt{m(E_0)n(E_0)}} \sum_{n^*} \frac{z^2_\tau(E^*)}{z^2_\tau(E^*)(n^*)^2}
\]  
(5.29) 
where \(n^*\) and \(E^*\) are related by \(n^* = n(E^*)\). Thus, we have

- **Result 4** Let \(B\) be a bounded operator on \(H_{aux}\) of a separable semi-bound system and let \(B(t)\) be the associated one parameter family of operators on \(H_{aux}\) defined through \(5.1\) with \(B(0) = B\). Then, for some function \(f\) which may depend on the system but is independent of the choice of \(B\), the operator
\[
[\tilde{B}]_{Q^0 = \tau} = \frac{1}{2}([\tilde{B}]^{L}_{Q^0 = \tau} + [\tilde{B}]^{R}_{Q^0 = \tau})
\]  
(5.30) 
given by \(5.23\) defines a bounded operator with domain \(H_{phys}\). Furthermore, if \(B\) is self-adjoint, then so is \([\tilde{B}]_{Q^0 = \tau}\).

In particular, \(B\) may be of the form \(B = (A \text{sign}(P_0) + \text{sign}(P_0) A)\) for some bounded \(A\) that commutes with both \(P_0\) and \(Q_0\) or we may have \(B = A\) for such an \(A\). It follows that we have constructed a set of bounded operators \([\tilde{B}]_{Q^0 = \tau}\) on \(H_{phys}\) whose classical counterparts \([b]_{Q^0 = \tau}\) form a complete set of functions on the classical space of solutions (or on the classical phase space) of the system. We thus say that
• The $[\mathcal{B}]_{Q^0=\tau}$ form a complete set of bounded quantum observables.

Note that the bound in 5.20 becomes zero as $\tau \to \infty$ since $z_\tau(E_0) \to 0$ and that the bound in 5.21 also vanishes since the sum in 5.21 converges absolutely and each term is a monotonically decreasing positive function of $\tau$. Thus, we also have

• Result 5: The $[\mathcal{B}]_{Q^0=\tau}$ of Result 5 converge strongly to zero as $\tau \to \infty$.

VI. DISCUSSION

We have seen that the construction of gauge invariants through integration over manifolds can be combined with Hamiltonian methods for constrained systems to build a complete set of gauge invariant operators that are densely defined in a physical Hilbert space for a number of time reparametrization invariant models. A physical inner product was identified and this approach was shown to predict the collapse of spacetimes for the appropriate Bianchi cosmologies. The primary method discussed involved the use of an auxiliary Hilbert space of the form $L^2(Q)$, that is, containing functions that are square integrable over the configuration space $Q$.

While the approach can be stated for an arbitrary finite dimensional reparametrization invariant model, questions of convergence and spectral analysis have only been addressed in narrower contexts. The most general rigorous results were obtained for already deparametrized systems (IV A), the free relativistic particle (IV B), and the separable semi-bound models of V. Results for other systems remain formal, but a forthcoming paper [16] will address the full Bianchi IX model.

Although only finite dimensional models were discussed in this work, it might be hoped that similar ideas could be applied to full quantum gravity. However, a number of issues would have to be faced. These include the choice of representation (which may be constrained by the parameterized dynamics of 3.3 in analogy with unconstrained field theory [47,48]), the choice of algebra itself (see [34]), and the definition of the products of operators that
appear in our integrands (ultraviolet divergences). On the other hand, another interesting extension would be to apply these ideas at the \((C^\ast)\) algebraic level without introducing a Hilbert space at all.

Several interesting open problems also remain within the current framework of finite dimensional models. These include the search for a general characterization of the convergence of the integrals 3.16 and 3.17 and for the self-adjointness (as opposed to just symmetry) of the resulting operators on \(\mathcal{H}_{phys}\). It would also be useful to show that such operators form a complete set in some inherently quantum mechanical sense (such as that the resulting representation on \(\mathcal{H}_{phys}\) is irreducible) and to find a simple set of physically interesting operators whose Hermiticity guarantees the uniqueness of the physical inner product.

Before concluding, a few remarks are in order about the limitations of this approach and the delta-functions in 3.14. The point is that while the technique of introducing an auxiliary Hilbert space of the form \(L^2(\mathcal{Q})\) is quite general and can (in principle) be applied to any system which has a classical canonical description, technical difficulties may prevent this method from being *useful*. The result may be trivial in two ways. First, it may be that when the Hamiltonian constraint is chosen to be a Hermitian operator in the auxiliary space its spectrum may not contain the value zero. That is, there may be no solutions to the constraint equation that are even delta-function normalizable. The other difficulty is that the integral by which we would like to define our gauge invariants may diverge on physical states. We have seen that the matrix elements are of the form \(\langle E, k|[A]_{Q^0=\tau}|E', k'\rangle = \delta(E - E')f(E, E'k, k')\) for eigenstates \(|E, k\rangle\) of \(H\) with eigenvalue \(E\) and some function \(f\) so that, if zero lies in the point spectrum of \(H\) and a solution to the constraint is actually normalizable in the auxiliary space, the action of \([A]_{Q^0=\tau}\) on \(|E, q^0\rangle\) contains a divergent factor. While it is possible that this divergence is regulated by the factor \(f\), this seems unlikely as we shall shortly see that this divergence has a physical interpretation.

Note that both of these features tend to occur when the spectrum of \(H\) is discrete, such as in the models [19] where the constraint represents a difference of two harmonic oscillator Hamiltonians or in minisuperspace models that recollapse in a finite amount of proper time.
$(\int N(t)dt)$. This is the case for the LRS Bianchi IX and Kantowski-Sachs models if the usual lapse of general relativity is used instead of our “rescaled lapse.” A similar feature occurs in the recollapsing models of [20]. However, discrete spectra are associated with confining potentials as in [19,20] and, if the dynamics is complete, such systems will generally have solutions for which $q^0(t) = \tau$ at an infinite number of times in which case $[a]_{q^0=\tau}$ may diverge as well. For such systems, one might imagine replacing the integral over $t$ with

$$
\lim_{t_\pm \to \pm \infty} \frac{1}{T(t_+) - T(t_-)} \int_{t_-}^{t_+} dt
$$

(6.1)

and hope to obtain a finite result. Equivalently, we may take 3.22 as the definition of the operator $\Omega$ instead of 3.9.

If, however, in a gravitational model, we take as one of our coordinates the parameter $\alpha = \ln(\det g)$, then, because gravity classically admits gravitational collapse, we know that the “potential” is not confining in the $\alpha \to -\infty$ direction. Thus, at least after a proper scaling of the Hamiltonian constraint (in minisuperspace models) we expect that this constraint may be turned into a Hermitian operator for which zero lies in the continuous spectrum of $H$ in the auxiliary Hilbert space so that the methods of III will be applicable.

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