Mode decomposition and unitarity in quantum cosmology

Franz Embacher
Institut für Theoretische Physik, Universität Wien,
Boltzmanngasse 5, A-1090 Wien
E-mail: fe@pap.univie.ac.at

UWThPh-1996-67
gr-qc/9611055

Abstract

Contrary to common belief, there are perspectives for generalizing the notion of positive and negative frequency in minisuperspace quantum cosmology, even when the wave equation does not admit symmetries. We outline a strategy in doing so when the potential is positive. Also, an underlying unitarity structure shows up. Starting in the framework of the Klein-Gordon type quantization, I am led to a result that relies on global features on the model, and that is possibly related to structures encountered in the refined algebraic quantization scheme.

1 INTRODUCTION

The basic ingredients of minisuperspace quantum cosmology are an $n$-dimensional (minisuperspace) manifold $\mathcal{M}$, endowed with a metric $ds^2 = g_{\alpha\beta} dy^\alpha dy^\beta$ of Lorentzian signature $(-,+,\ldots,+)$ and a potential function $U$ (which is assumed to be positive). The wave equation (the minisuperspace version of the Wheeler-DeWitt equation) reads

$$\left(-\nabla_\alpha \nabla^\alpha + U\right) \psi = 0.$$  \(1\)

There are several mathematical structures associated with these ingredients, and accordingly one may take several routes when "solving" this equation, giving the solutions some sense as "quantum states" of the (mini)universe and making contact to the mathematical structures of conventional quantum mechanics.

There are two candidate scalar products available,

$$g(\psi_1,\psi_2) = \int_\mathcal{M} d^n y \sqrt{-g} \psi_1^* \psi_2$$  \(2\)

and

$$Q(\psi_1,\psi_2) = -\frac{i}{2} \int_\Sigma d^\Sigma \alpha \left(\psi_1^* \nabla_\alpha \psi_2\right),$$  \(3\)

where $\Sigma$ is a spacelike hypersurface (of sufficiently regular asymptotic behaviour, if necessary). The old-fashioned Klein-Gordon quantization \[\] is based on the observation that the indefinite scalar product $Q$ is independent of $\Sigma$ if both functions $\psi_{1,2}$ satisfy the wave equation. It benefits from the mathematical similarity of the quantum cosmological framework to the quantization of a scalar particle in a curved space-time background $(\mathcal{M}, ds^2)$ and an external positive potential $U$. One of the key paradigms along this road is that — in the generic case — it is not possible to decompose the space $\mathcal{H}$ of wave functions into two subspaces $\mathcal{H}^\pm$ consisting of positive and negative frequency modes \[\] (within which $Q$ would be positive and negative definite, respectively). A possible reaction to this fact is the point of
view that the mathematics of quantum mechanics (in particular a positive definite scalar product) emerges only at an approximate level in a semiclassical context. Other routes to quantization start from the positive definite scalar product $q$, in particular the refined algebraic quantization [4], regarding $(L^2(M), d^n y \sqrt{-g})$ as an auxiliary Hilbert space from which the space of physical states is constructed by distributional techniques.

Here, I would like to begin with the conservative point of view of Klein-Gordon quantization and ask whether a preferred decomposition $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$ of the space of wave functions may be constructed. I will not attempt to define positive and negative frequencies (in the sense of $\psi_\pm \sim e^{\mp i\omega t}$ with respect to some time coordinate) but try to generalize this concept. During the procedure, I will be led towards non-local features in a quite natural way. It may be applied is not very well known. However, it gives a hint how different quantization methods, relying on the two scalar products $q$ and $Q$, might be related in terms of some underlying structure. The details of the computations outlined here may be found in Ref. [3].

## 2 Unitarity and Preferred Decomposition

I will use a congruence of hypersurface orthogonal classical trajectories as background structure with respect to which the wave equation is further analyzed. In what follows I will assume that all quantities are defined in domains large enough to allow for the existence of the integrals appearing below. Let $S$ be a solution of the Hamilton-Jacobi equation

$$\hat{\nabla}_\alpha S(\nabla^\alpha S) = -U \tag{4}$$

and $D$ a positive solution of the conservation equation

$$\nabla_\alpha (D^2 \nabla^\alpha S) = 0. \tag{5}$$

The action function $S$ generates a congruence of classical trajectories by means of the differential equation

$$\frac{1}{N} \frac{dy^\alpha}{dt} = \nabla^\alpha S, \tag{6}$$

with $N$ an arbitrary lapse function, and $D$ provides a weight on the set of trajectories, thus specifying the scalar product defined in (12) below. The pair $(D, S)$ is called a WKB-branch (although I will not impose any approximations here). The (“time”) evolution parameter is defined by $t = -S$, and one may choose coordinates $\xi^a$ labelling the trajectories. This corresponds to the lapse function $N = U^{-1}$ in (6), and the metric becomes

$$ds^2 = -\frac{dt^2}{U} + \gamma_{ab} d\xi^a d\xi^b. \tag{7}$$

By $\partial_t$ (or a dot) I denote the derivative along the trajectories (in the coordinates $(t, \xi^a)$ it is just the partial derivative with respect to $t$).

Given a WKB-branch, any wave function may be written as

$$\psi = \chi De^{iS}, \tag{8}$$

by which the wave equation (1) becomes

$$i \partial_t \chi = \left( \frac{1}{2} \partial_\alpha + h \right) \chi, \tag{9}$$

where

$$h = H_{\text{eff}} - \frac{1}{2} D(D^{-1})\cdot. \tag{10}$$

and

$$H_{\text{eff}} = \frac{1}{2D\sqrt{U}} D_a \frac{1}{\sqrt{U}} D^a D, \tag{11}$$

$D_a$ denoting the covariant derivative with respect to the metric $\gamma_{ab}$ (acting tangential to the hypersurfaces $\Sigma_t$ of constant $t$). The scalar product

$$\langle \chi_1 | \chi_2 \rangle \equiv \langle \chi_1 | \chi_2 \rangle_t = \int_{\Sigma_t} d\Sigma \sqrt{U} D^2 \chi_1^* \chi_2, \tag{12}$$

with $d\Sigma$ the (scalar) hypersurface element on $\Sigma_t$, serves to define the (formal) Hermitean adjoint $A^\dagger$ of a linear operator $A$, and the complex conjugate of an operator is defined by $A^* \chi = (A \chi)^*$.
\[ \hat{A} = [\partial_t, A]. \] The operator \( h \) satisfies \( h^1 = h^* = h \) and \( [h, S] = 0. \)

Consider now the following differential equations for an operator \( H \)
\[ i\dot{H} = 2h - 2H - H^2, \quad (13) \]
with the additional conditions
\[ [H, S] = 0 \quad H^1 = H^*. \quad (14) \]
Whenever such an operator is given, any solution of the Schrödinger type equation
\[ i\partial_t \chi = H\chi \quad (15) \]
satisfies the wave equation (13). The function \( \chi \) thus corresponds to a solution \( \psi \) of (1). Denoting the space of wave functions obtained in this way by \( \mathcal{H}^+ \) (and its complex conjugate by \( \mathcal{H}^- \)), the system of equations for \( H \) implies that the space of wave functions decomposes as a direct sum \( \mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^- \) under the relatively mild assumption that
\[ A = 1 + \frac{1}{2}(H + H^) \quad (16) \]
is a positive operator. Moreover, the Klein-Gordon scalar product \( Q \) is positive (negative) definite on \( \mathcal{H}^+ \) (\( \mathcal{H}^- \)). When wave functions are rescaled once more as
\[ \eta = A^{1/2} \chi, \quad (17) \]
we find
\[ Q(\psi_1, \psi_2) = \langle \eta_1 | \eta_2 \rangle \quad (18) \]
for \( \psi_{1,2} \in \mathcal{H}^+ \) and
\[ Q(\psi_1, \psi_2) = -\langle \eta_1 | \eta_2 \rangle \quad (19) \]
for \( \psi_{1,2} \in \mathcal{H}^- \), whereas \( Q(\psi_1, \psi_2) = 0 \) if \( \psi_1 \in \mathcal{H}^+ \) and \( \psi_2 \in \mathcal{H}^- \). Defining the operator
\[ K = A^{1/2} H A^{-1/2} + i (A^{1/2}) A^{-1/2}, \quad (20) \]
which is Hermitean, \( K^* = K \), and acts tangential to \( \Sigma_t, [K, S] = 0 \), the Schrödinger type equation (15) becomes
\[ i\partial_t \eta = K\eta \quad (21) \]
for \( \psi \in \mathcal{H}^+ \) (and an analogous equation for \( \mathcal{H}^- \)). Thus, with any choice \((S, D, H)\) there is associated a decomposition of \( \mathcal{H} \) and a unitary evolution of wave functions.

This is not a very exciting result, but is becoming a bit more interesting when we ask how the decomposition changes when the WKB-branch \((S, D)\) and the operator \( H \) are varied by an infinitesimal amount \((\delta S, \delta D)\) — compatible with (13) — and \( \delta H \) — compatible with (13)–(14). It turns out that the decompositions of \( \mathcal{H} \) defined in these two branches actually coincide if
\[ \delta H = [H, \frac{\delta D}{D}] + i[H - h, \delta S] + [H, \delta S] (\partial_t + iH). \quad (22) \]
Hence, if we manage to select a solution \( H \) for any WKB-branch such that its variation \( \delta H \) between infinitesimally close neighbours satisfies the above equation, we expect a unique decomposition to be specified. (This should be true at least when any two WKB-branches may be deformed into each other by a sequence of infinitesimally small steps). The big question is whether this can be done in a natural way.

The answer to this question is surprisingly simple, although at a formal level. Rewrite the differential equation (13) as
\[ H = h - \frac{1}{2} H^2 - i \frac{1}{2} \dot{H} \quad (23) \]
and solve it iteratively by inserting it into itself. This corresponds to the sequence
\[ H_0 = 0 \]
\[ H_{p+1} = h - \frac{1}{2} H^2_p - i \frac{1}{2} \dot{H}_p \quad (24) \]
for non-negative integer \( p \). One encounters a formal expression whose first few terms read
\[ H = h - \frac{1}{2} h^2 - \frac{i}{2} \dot{h} + \frac{1}{2} h^3 + \frac{i}{2} \{h, \dot{h}\} - \frac{1}{4} \ddot{h} + \ldots \quad (25) \]
When appropriately keeping track of the various terms appearing in this procedure (for details see Ref. [3]), we can reformulate \( H \) as a formal series, called the "iterative solution". The amazing thing is that it formally satisfies the condition (22) guaranteeing the decomposition to be
unique. However, it is not quite clear in which models this series will actually converge (or, on which wave functions it will converge).

In case of convergence, we have specified a solution \( H \) in any WKB-branch without ever having performed a choice! Due to the appearance of a series containing arbitrarily high time-derivatives of \( h \), we expect \( H \) to rely on global properties of the model, possibly connected with analyticity issues. In Ref. [3], these manipulations have been presented in detail, and there the question is raised whether the structure encountered is related to quantization methods that start from global features, such as the scalar product \( q \) from (2), and some examples for the iterative solution are given.

3 EXAMPLE: FLAT KLEIN-GORDON EQUATION

A first orientation about what can be achieved by this approach is to apply it to the Klein-Gordon equation in flat space \((ds^2 = -dt^2 + dx^2 \text{ and } U = m^2, \text{ which we set equal to } 1)\) as a toy model. In this case \( h = -\frac{1}{2} \Delta \), hence \( \dot{h} = 0 \), and the iterative solution (25) becomes the closed expression

\[
H = \sqrt{1 + 2h - 1}.
\]  

(26)

Note that it is well-defined although (25) does not converge on all wave functions. Similar features may be expected in more general models as well, so that it is not at all obvious how to give the formal solution a mathematically well-defined meaning. The spaces \( \mathbb{H} \pm \) in our example are identical with the standard positive/negative frequency subspaces of \( \mathbb{H} \).

4 DISCUSSION

Given that the procedure described in Section 2 goes through in a particular model without symmetries, the question arises what structure one has touched upon. Due to the existence of a preferred decomposition, there is a natural positive definite scalar product on the space of wave functions, provided by \((\mathbb{H}, Q_{\text{phys}}) \equiv (\mathbb{H}^+, Q) \oplus (\mathbb{H}^-, -Q)\). In the case of the Klein-Gordon equation in flat space, this just amounts to reverse the sign of \( Q \) in the negative frequency sector. On the other hand, the refined algebraic quantization program arrives at a Hilbert space \((\mathcal{H}_{\text{phys}}, \langle | \rangle)\) which, for the flat Klein-Gordon equation, agrees with our construction [4]. Hence, it is natural to ask whether this relation carries over to more general cases. In Ref. [3], an independent argument is given that the mere coexistence of the indefinite Klein-Gordon scalar product \( Q \) and the physical inner product \( \langle | \rangle \) make the existence of a preferred decomposition very likely.

Unitarity shows up in our approach only in the context of WKB-branches. This resembles the way tensor components show up in coordinate systems. Consequently, there is not "the" unitary evolution, although one has the feeling to deal with a fundamental structure. Maybe the expression "covariance with respect to WKB-branches" is appropriate to describe this point of view.

In a semiclassical context, the operator \( h \) is expected to be "small", so that the first few terms in (25) may be regarded as numerically approximating the exact solution \( H \). Using physical units, in a typical quantum cosmological setting we have \( H \approx h + \text{Planck scale corrections} \). The first few terms of the operator (16) defining the redefinition (17) are given by

\[
\mathcal{A} = 1 + h - \frac{1}{2} h^2 + \frac{1}{2} h^3 - \frac{1}{4} \dot{h} + \ldots,  
\]  

(27)

which might in a concrete model serve to justify the assumption that \( \mathcal{A} \) is positive. The Hermitian operator (20) defining the unitary evolution (21) is given by

\[
\mathcal{K} = h - \frac{1}{2} h^2 + \frac{1}{2} h^3 - \frac{i}{8} [h, \dot{h}] - \frac{1}{4} \ddot{h} + \ldots  
\]  

(28)

It is not claimed here that (21) is "the" Schrödinger equation with \( t \) as the physically experienced time, but our result opens the perspective of deriving conventional quantum physics within the context of the familiar mathematical framework of quantum mechanics.
5 ACKNOWLEDGMENTS

Work supported by the Austrian Academy of Sciences in the framework of the "Austrian Programme for Advanced Research and Technology".

References

[1] K. Kuchař, "Canonical methods of quantization", in: C. J. Isham, R. Penrose and D. W. Sciama (eds.), Quantum Gravity 2. A Second Oxford Symposium, Clarendon Press (Oxford, 1981); "General relativity: Dynamics without symmetry", J. Math. Phys. 22, 2640 (1981).

[2] A. Ashtekar, J. Lewandowski, D. Marolf, J. Mourão and T. Thiemann, "Quantization of diffeomorphism invariant theories of connections with local degrees of freedom", J. Math. Phys. 36, 6456 (1995); D. Marolf, "Refined algebraic quantization: Systems with a single constraint", preprint gr-qc/9508015, to appear in Banach Center Publications.

[3] F. Embacher, "Decomposition and unitarity in quantum cosmology", preprint UWThPh-1996-64, also gr-qc/9611007.

[4] D. Marolf, "Quantum Observables and Recollapsing Dynamics", Class. Quantum Grav. 12, 1199 (1995); A. Higuchi, "Linearized quantum gravity in flat space with toroidal topology", Class. Quantum Grav. 8, 2023 (1991).