Decomposition and unitarity in quantum cosmology

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Abstract

Considering quantum cosmological minisuperspace models with positive potential, we present evidence that

(i) despite common belief there are perspectives for defining a unique, naturally preferred decomposition of the space $\mathcal{H}$ of wave functions into two subspaces $\mathcal{H}^\pm$ that generalizes the concept of positive and negative frequency, and that

(ii) an underlying unitary evolution within these two subspaces exists and may be described in analogy to the representation of a geometric object in local coordinates: it is associated with the choice of a congruence of classical trajectories endowed with a suitable weight (such a setting is called WKB-branch).

The transformation properties of various quantities under a variation of the WKB-branch provide the tool for defining the decomposition. The construction leads to formal series whose actual convergence seems to require additional conditions on the model (related to global geometric issues and possibly to analyticity). It is speculated that this approach might relate to the refined algebraic quantization program.

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1 Introduction

Minisuperspace quantum cosmology bears some formal similarity to the quantization of a scalar particle on a curved space-time background. The Wheeler-DeWitt equation in the former corresponds to the Klein-Gordon equation in the latter type of models. Therefore, concepts, methods and experiences that have originally emerged in particles quantization issues are often taken over to quantum cosmology. One of the most prominent statements that have a clear meaning in particle quantization is that in the generic case, i.e. if the wave equation does not admit any symmetries, there is no unique decomposition of wave functions into positive and negative frequency subspaces. This statement has been transferred to quantum cosmology although in this field it is much less clear what positive and negative frequencies are and what other concepts might serve as generalizations thereof. Also, it is often believed that the space of wave functions cannot — in a natural way — be decomposed into a direct sum such that the Klein-Gordon scalar product is positive definite on one and negative definite on the other subspace. However, strictly speaking, this type of belief is true only if one refers to the construction of a decomposition by means of underlying local symmetries.

The purpose of this article is to show that (assuming the potential in the wave equation to be positive) there are still perspectives in a number of models for the construction of a preferred decomposition generalizing the concept of positive and negative frequency. In any model admitting the application of the procedure proposed here, this decomposition is not based on a local symmetry but rather on global issues. It gives rise to a Hilbert space structure at the fundamental level of solutions to the (minisuperspace) Wheeler-DeWitt equation. Furthermore, in situations where such a preferred decomposition exists, a unitary evolution within the two subspaces is exhibited in a local context, depending on the choice of a classical action $S$ and a weight function $D$. Calling the pair $(S, D)$ a ”WKB-branch”, the hermitean evolution operator emerges in some analogy to the way tensor components appear in coordinate systems, namely as representatives of some mathematical ”object”. The proposal we formulate is understood as a general strategy whose realization in concrete models will face specific problems that might be easy or hard (or even impossible) to solve.

A further goal of this article is to speculate on the relation between the preferred decomposition and structures that appear in the context of other quantization methods, in particular the refined algebraic quantization. This method incorporates global issues from the outset and ends up with a positive definite inner product on the space of physical states. Uncovering a relation to the more conventional quantization in terms of the Klein-Gordon scalar product could eventually lead to a more fundamental and unified understanding of what happens when one ”quantizes” a theory.

The paper is organized as follows: In Section 2, we write down the wave equation
and the two scalar products (Klein-Gordon and \(L^2\)) at hand. Also, we briefly review how congruences of classical trajectories in minisuperspace are described by the Hamilton-Jacobi equation and its solutions. After a discussion of the decomposition issue and the refined algebraic quantization for the case of the Klein Gordon equation in flat space-time, we formulate the general problem.

Section 3 is devoted to the detailed presentation of a formalism serving to analyze the wave equation in a novel way. Any WKB-branch may be used as a "background structure" with respect to which many decompositions are possible, each one associated with a solution of a differential equation for an operator called \(H\). This differential equation basically states that in each of the two subspaces the wave equation is of the Schrödinger equation type, \(H\) serving as evolution operator. The key idea of this procedure is to generalize the notion of outgoing and incoming orientation of classical trajectories to the quantum case. At first sight, this construction is not unique, and we end up with a variety of ways to do so.

In Section 4, we analyze the transformation properties of various quantities when the WKB-branch used as "background structure" is changed infinitesimally. Section 5 is devoted to the formulation of our proposal. At a formal level we show that — within each WKB-branch — one may choose a solution \(H\) of the above-mentioned differential equation such that all decompositions emerging in different WKB-branches agree with one another. This opens the perspective to unambiguously single out one preferred decomposition of the space of wave functions. The question whether the formal (power series) solution for \(H\) actually convergences (or may consistently be regularized) is addressed to the concrete models upon which the strategy shall be applied. We explicitly display the first few terms in the expansion of \(H\) (and some redefined version \(K\) which makes explicit the unitarity of the evolution). In semiclassical contexts, these terms may be expected to approximate the actual solution and should thus unambiguously describe the decomposition and the underlying unitarity.

In Section 6, we comment on the structure exhibited by the formal solution of the decomposition problem and give some speculations on its nature. It is clear that — whenever it exists — the solution refers to the global structure of minisuperspace (possibly by means of some average over all possible decompositions), and there are hints that some analyticity structure might play a role as well. In Section 7, we display simple examples for which the operator \(H\) may be expressed in terms of known functions. Furthermore, using a toy-model situation, we show that the obvious heuristic argument against a preferred decomposition (the difference of asymptotic incoming and outgoing decompositions on a time-dependent background) does not necessarily apply. Section 8 is devoted to speculations about relations of our proposal to the refined algebraic quantization scheme. We give a heuristic argument (whose basic ingredients date back to the literature of the Sixties) that the mere coexistence of the positive definite physical inner product constructed in this approach with the indefinite Klein-Gordon scalar product on the space of wave functions sin-
gles out a preferred decomposition. It is however not clear whether it coincides with
the decomposition emerging from our proposal or whether it is yet another "natural" solution of the decomposition problem. Finally, in Section 9, we comment on
possible generalizations to the case of not necessarily positive potential and point
out that this issue might touch upon the significance of analytic continuation and
the role of the so-called Euclidean domains in minisuperspace.

Summarizing, our approach intends to clarify the relation between structures
emerging in different quantization schemes. At a formal level, we can offer a proce-
dure that starts from the conventional setting of the Klein-Gordon scalar product on
the space solutions to the wave equation but transcends this framework and exhibits
a Hilbert space structure at the fundamental level, without making use of semiclassical
techniques and other approximations. Although constructed in a local context,
this structure is likely to be based on global issues, and it might be related (or even
identical) to the physical Hilbert space as constructed in the more advanced refined
algebraic quantization method.

In order to improve the readability of this article, we list the most important
notations used:

\((S, D)\) Classical action and wave function prefactor, defined in (2.5)
and (3.6). The pair \((S, D)\) is called WKB-branch.

\(t = -S\), classical evolution parameter along trajectories, serving
as a coordinate in minisuperspace \(\mathcal{M}\).

\(Q\) Indefinite Klein-Gordon type scalar product defined in (2.8).

\(\langle \cdot | \cdot \rangle\) Positive definite scalar product, defined by (3.13)
in terms of a WKB-branch.

\(\mathcal{H}\) Suitably defined vector space of solutions to the wave equation
(2.2), such that \(Q\) exists on \(\mathcal{H}\).

\(\mathcal{H}^\pm\) Subspaces of \(\mathcal{H}\), generalizing the notion of positive/negative
frequency.

\(h\) Operator characterizing the wave equation in the form (3.3),
defined in (3.10)–(3.11).

\(H\) Operator in the evolution equation (3.23) for wave functions
in \(\mathcal{H}^+\), subject to the system of equations (3.18)–(3.20).

\(\mathcal{K}\) Hermitian evolution operator in the Schrödinger type equation
(3.38) for wave functions in \(\mathcal{H}^+\), defined in (3.40).

\(\epsilon\) Formal book-keeping parameter which can be inserted into most
equations of this paper; its actual value is 1, and it is introduced
in Section 5.

\(\mathcal{H}_{\text{phys}}\) Physical Hilbert space as constructed by the refined algebraic
quantization method.

\(\langle \cdot | \cdot \rangle_{\text{phys}}\) Positive definite inner product as constructed by the refined
algebraic quantization method.
2 Klein-Gordon type wave equation with positive potential — the problem

The basic mathematical ingredients for quantum cosmological minisuperspace models as well as for scalar particle quantization in a background space-time are an n-dimensional differentiable manifold $\mathcal{M}$ together with a metric $ds^2$ of pseudo-Riemannian signature $(-,+,+,...,+)$ and a real-valued function $U$ on $\mathcal{M}$. In many practical cases, these objects will be $C^\infty$ or even (real) analytic, and we postpone further specification of their differentiability properties to speculations in Sections 5 and 6. In local coordinates $y \equiv (y^\alpha)$ we can write

$$ds^2 = g_{\alpha\beta}(y) dy^\alpha dy^\beta. \quad (2.1)$$

In quantum cosmological models, $\mathcal{M}$ (the minisuperspace) consists of the spatial degrees of freedom of geometry and matter, $ds^2$ is the DeWitt metric and $U$ the potential, stemming from the spatial curvature as well as the matter couplings. In the scenarios of scalar particle quantization in a background, $\mathcal{M}$ is the space-time manifold and $ds^2$ its metric. The massive (Klein-Gordon) case is given by constant potential $U = m^2$, but more general potentials are admissible as well.

We require in addition that there exists a foliation of $\mathcal{M}$ by spacelike hypersurfaces. (The words "spacelike" and "timelike" shall refer to the "causal structure" provided by the metric $ds^2$. In quantum cosmology, this is of course not the causal structure of space-time). As will be pointed out below in this Section, it will be necessary in some models to impose asymptotic conditions, e.g. to choose a foliation consisting of Cauchy hypersurfaces. In any case, we can assign each local light cone a future and a past orientation in a globally consistent way. Any smooth oriented timelike curve in $\mathcal{M}$ is either future- or past-directed. In the case of quantum cosmology, one could call these two orientations "outgoing" and "incoming", respectively. The hypersurfaces providing the foliation can be labelled as $\Gamma_\lambda (\lambda \in \mathbb{R})$, with future (outgoing) orientation being equivalent to (or, likewise, being defined by) increasing $\lambda$, past (incoming) orientation by decreasing $\lambda$.

As an important restriction for what follows we require that the potential $U$ is everywhere positive on $\mathcal{M}$. In quantum cosmology this implies that any classical trajectory (representing a complete space-time with matter configuration) is everywhere timelike, i.e. either always outgoing or always incoming. Returning trajectories and turning points are excluded, as we shall see shortly. For a particle in a background this condition guarantees that the classical motion (i.e. a world-line in the space-time manifold $\mathcal{M}$) respects the causal structure provided by the metric in that the four-velocity is always timelike (for generality, we admit both future- and past-oriented trajectories). In the massive case $U = m^2$, this condition is obviously satisfied for real $m$. In Section 9 we will speculate about the perspectives to relax the condition $U > 0$. 

4
Denoting by $\nabla_\alpha$ the covariant derivative with respect to the metric, the basic wave equation is given by

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

its solutions $\psi \equiv \psi(y)$ being denoted as wave functions, or "wave functions of the universe". They may be considered as representations of the quantum states of the system. In quantum cosmology (2.2) is the (minisuperspace version of the) Wheeler-DeWitt equation, whereas in the particle quantization models it may be called the Klein-Gordon equation in a background space-time with external potential.

We should now make more explicit what we consider to be the underlying classical dynamics. A classical evolution of the system under consideration is provided by an oriented trajectory $y(t)$ in $\mathcal{M}$ satisfying the equations of motion generated by the action

$$
S = \frac{1}{2} \int dt \left( \frac{1}{N} g_{\alpha\beta} \dot{y}^\alpha \dot{y}^\beta - NU \right) .
$$

The "lapse function" $N$ serves as a Lagrangian multiplier and thus does not have a dynamical evolution equation. Its appearance in the action expresses reparametrization invariance, i.e. it reflects the fact that the evolution parameter $t$ has no physical significance (except for its orientation, which is achieved by restricting $N$ to be positive). After variation with respect to the variables $(N, y^\alpha)$, it may be chosen as a function $N \equiv N(y)$, thereby fixing the evolution parameter $t$. We will not write down the equations of motion explicitly but just note that the momenta $p_\alpha$ are related to the "velocities" by

$$
\frac{1}{N} \frac{dy^\alpha}{dt} = g^{\alpha\beta} p_\beta ,
$$

and variation of $S$ with respect to $N$ yields the constraint $p_\alpha p^\alpha = -U$, whose quantum version is the wave equation (2.2). Sometimes, for $n \geq 3$, when passing from the classical to the quantum theory, the original classical potential $U^{cl}$ is modified by adding a curvature term, $U = U^{cl} + \xi R[g]$, where $\xi = \frac{1}{4}(n-2)/(n-1)$ and $R[g]$ is the Ricci-scalar of the DeWitt metric [1]. This makes the wave equation invariant under redefinitions of the lapse $N = \Omega^2(y)N$, which amounts to a conformal transformation $\tilde{g}_{\alpha\beta} = \Omega^2 g_{\alpha\beta}$, a rescaling of the classical potential $\tilde{U}^{cl} = \Omega^{-2} U^{cl}$ and a rescaling of the wave function $\tilde{\psi} = \Omega^{(n-2)/2} \psi$. In such a case the quantity $U$ in (2.3) shall denote the modified potential, as it appears in the wave equation, and when talking about classical trajectories, we understand the dynamics generated by the action (2.3) with precisely the same potential $U$. In other words, classical and quantum theory are both formulated in terms of the same fundamental objects $ds^2$ and $U$, the latter everywhere positive. In some cases with not everywhere positive potential, it is possible to achieve $U = U^{cl} + \xi R[g] > 0$ after a transformation of the type given above. When trying to find an appropriate conformal factor $\Omega^2$, one has to make use of the conformal transformation properties of the Ricci-scalar. One
should however agree on a definite choice of $U$ to work with, because the formalism
to be developed in this paper is not conformally invariant in an obvious way. (This
would be an interesting issue to pursue, but we will not raise it here).

In what follows we will not make use of single classical trajectories but of con-
gruences generated by solutions of the Hamilton-Jacobi equation. The latter reads
\[ S_\alpha S^\alpha = -U , \] (2.5)

whereby we use the abbreviation $S_\alpha \equiv \nabla_\alpha S$, $S^\alpha \equiv \nabla^\alpha S$. Once having chosen a real
solution $S(y)$ (which in general may exist only in a region $\mathcal{G}$ of $\mathcal{M}$), one may identify
its gradient $S_\alpha$ with the momentum $p_\alpha$ of a family of oriented curves. Having fixed
$N$ to be some positive function on $\mathcal{M}$, (2.4) plays the role of the differential equation
\[ \frac{1}{N} \frac{dy^\alpha}{dt} = S^\alpha \] (2.6)

for $y^\alpha(t)$, the general solution being a congruence (i.e. a non-intersecting ($n - 1$)-
parameter family) of solutions to the classical equations of motion. Redefining
$N$ just rescales the evolution parameter $t$ along the trajectories (in an orientation-
preserving way). Choosing a particular function $N$ eliminates the reparametrization
invariance, and thus has the status of fixing a gauge. A Hamilton-Jacobi function $S$
is sometimes called ”classical action”. This is because $S$ agrees with (2.3) when the
integration is carried out along the according trajectories (and all lower integration
bounds lie on a fixed hypersurface of constant $S$).

The tangent vectors of all trajectories in the congruence are, by construction,
orthogonal to the hypersurfaces $S = \text{const}$. Due to the positivity of the potential,
the trajectories are timelike, the hypersurfaces of constant $S$ are spacelike. The
trajectories belonging to some $S$ are either all outgoing or all incoming. Thus, any
$S$ may be associated with one of these two possible classical modes of orientation.
Accordingly, $S' = -S$ generates the identical congruence, but with all trajectories
reversed in orientation. Whenever different trajectories intersect each other (e.g. on
a caustic), or whenever the congruence contains a sequence approaching a lightlike
curve, $S$ develops a singularity. (An example of this latter type is provided by
$ds^2 = -d\tau^2 + dx^2$, $U = 1$ and $S = \sqrt{\tau^2 - x^2}$). This causes Hamilton-Jacobi functions
$S$ in general to be defined only in some region $\mathcal{G}$ of $\mathcal{M}$ (although the analytic
continuation of $S$ across the boundary of $\mathcal{G}$ plays a role in certain approaches to
quantum cosmology).

After having summarized how the classical evolution emerges from the structure
provided by $ds^2$ and $U$, we return to the issue of the quantum problem. There are
two natural candidates for a scalar product, namely
\[ q(\psi_1, \psi_2) = \int_{\mathcal{M}} d\mu \psi_1^* \psi_2 \] (2.7)
and

\[ Q(\psi_1, \psi_2) = -i \frac{1}{2} \int_{\Sigma} d\Sigma^\alpha (\psi_1^* \nabla_\alpha \psi_2), \]  

(2.8)

where \( d\mu \equiv d^n y \sqrt{-g} \) is the covariant volume element on \( \mathcal{M} \), \( \Sigma \) a spacelike hypersurface and \( d\Sigma^\alpha \) the covariant hypersurface element on \( \Sigma \). Both scalar products have been considered in attempts to quantize the system and to interpret solutions of the Wheeler-DeWitt equation in terms of observational physics. The first one, \( q \), is sometimes modified into an integration over a bounded domain of \( \mathcal{M} \) and in this form intended to be the basis for computing relative (conditional) probabilities for "finding" the configuration variables in the respective domain. It is associated with what is sometimes called "naive interpretation" of quantum cosmology and has been advocated by Hawking and Page [2]. It is also the starting point for the "refined algebraic quantization" program that is used in the more recent versions of the Ashtekar approach [3] and about which we will say a few words below. The second (Klein-Gordon type) indefinite expression \( Q \) is especially designed for the case that \( \psi_1 \) and \( \psi_2 \) satisfy the wave equation (2.2) (in which case its integrand is a conserved current) and is the starting point for another range of approaches to quantum cosmology, such as the Bohm interpretation [4] and the semiclassical (WKB) interpretation as proposed, among others, by Vilenkin [5]. By replacing \( \psi_1^* \rightarrow \psi_1 \) and omitting the prefactor \( i \) in (2.8), it is sometimes viewed as a symplectic structure on the space of real wave functions. Some results have been achieved on the relation between the two scalar products \( q \) and \( Q \) [2, 6, 7], but they either involve approximations or refer to very specific situations and are thus not very conclusive at the fundamental level.

The formalism to be developed in this article starts from the "conservative" point of view that some appropriately defined space \( \mathcal{H} \) of solutions of the wave equation (2.2) is endowed with the structure \( Q \), and that the physical significance of a wave function should be expressed in terms thereof. One could call this point of view "Klein-Gordon quantization" (cf. Ref. [8]). When proceeding, non-local and non-causal issues will appear, and we will frequently speculate on relations of our formalism to schemes that are based on \( q \), in particular the refined algebraic quantization that was mentioned already above. This method has been developed during the past few years by several authors (see Refs. [3, 6, 7, 9, 10]; also see Refs. [11, 12, 13, 14] for predecessors). In our simple case, the idea is essentially to utilize the "delta function" \( \delta(C) = (2\pi)^{-1} \int d\lambda \exp(i\lambda C) \) where \( C \) is the wave operator in (2.2), the integration actually being related to a group average. Physical states are defined as \( \psi_{\text{phys}} = \delta(C)\psi \), where \( \psi \) is to some extent arbitrary (in particular, it should not satisfy the wave equation). The inner product is given by \( \langle \psi_{\text{phys}} | \phi_{\text{phys}} \rangle_{\text{phys}} = \int d\mu \psi^* \delta(C)\phi \). This naive idea can be made precise in terms of distributions within the framework provided by the "kinematic" (auxiliary) Hilbert space \( L^2(\mathcal{M}, d\mu) \) (see also Ref. [14]). The main condition for the procedure to work is that the wave operator \( C \) is self-adjoint with respect to this structure.

In contrast to \( q \), the Klein-Gordon type scalar product \( Q \) is adequate not only for
quantum cosmology but for the scenario of a scalar field in a space-time background as well, since it does not need information about \( ds^2 \) and \( U \) residing in the future of \( \Sigma \). It is thus compatible with the idea of a field \( \psi \) propagating causally in \( \mathcal{M} \). On the other hand, such a feature is not at all necessary in quantum cosmology, and we will transcend it later. For the moment, however, our procedure may be interpreted in terms of quantum cosmology as well as in terms of a scalar field in a background.

There is a subtlety related to the question which hypersurfaces \( \Sigma \) may be used in (2.8). When both \( \psi_1 \) and \( \psi_2 \) satisfy the wave equation (2.2), the integrand is a conserved current. Hence, whenever at least one of the two wave functions vanishes sufficiently fast in the asymptotic boundary region of two spacelike hypersurfaces \( \Sigma \) and \( \Sigma' \), the complex number \( Q(\psi_1,\psi_2) \) is independent of whether it is computed using \( \Sigma \) or \( \Sigma' \). However, this is a rather vague statement, since we have not presupposed a particular asymptotic structure. One may, for example, think of \( \Sigma \) to be a Cauchy hypersurface, and \( \Sigma' \) to be a spacelike non-Cauchy hypersurface (if \( ds^2 = -d\tau^2 + dx^2 \), it could be of the type \( \tau^2 - x^2 = \text{const} \)). Whether two hypersurfaces differing so much in their global structure give rise to a unique scalar product \( Q \) will highly depend on the model — i.e. on \( (\mathcal{M}, ds^2, U) \) — as well as on the space of solutions to (2.2) admitted. The minimal requirement is that the scalar product \( Q \) is compatible with \( \Sigma \) being any of the hypersurfaces \( \Gamma_\lambda \) defining the foliation of \( \mathcal{M} \). In some models it will thus be necessary to impose additional asymptotic conditions, e.g. to require all \( \Gamma_\lambda \) to be Cauchy hypersurfaces. We assume that a class of "admissible hypersurfaces" has been specified so as to fix \( Q \) unambiguously. Whenever we use a spacelike hypersurface \( \Sigma \) to compute \( Q \), it shall belong to this class.

In the case of the Klein-Gordon equation in a flat background \((ds^2 = -d\tau^2 + dx^2, U = m^2)\), the indefinite nature of \( Q \) gives rise to a decomposition of the space of wave functions \( \mathcal{H} \) into positive and negative frequency subspaces (particle and antiparticle modes), \( \mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^- \). The spaces \( \mathcal{H}^+ \) and \( \mathcal{H}^- \) are orthogonal to each other, and \( Q \) is positive (negative) definite on \( \mathcal{H}^+ (\mathcal{H}^-) \). Complex conjugation maps \( \mathcal{H}^\pm \) into each other. In principle, there are many such decompositions, related to each other by Bogoljubov transformations. However, in flat space-time the existence of a timelike Killing vector field as well as the action of the Lorentz group ensures the standard (Lorentz invariant) decomposition to be singled out as preferred one. Moreover, when a Lorentzian coordinate system has been fixed, the wave equation reduces to a Schrödinger type equation with unitary evolution within each subspace. One thus encounters two Hilbert space structures \((\mathcal{H}^+, Q)\) and \((\mathcal{H}^-, -Q)\) within each of which an evolution of the "ordinary" quantum mechanics type (although with non-local Hamiltonian) takes place. Fixing some Lorentzian coordinate system and writing the wave function as \( \psi(\tau, \vec{x}) = \chi(\tau, \vec{x})e^{-im\tau} \), the evolution in \( \mathcal{H}^+ \) (or likewise the definition of \( \mathcal{H}^+ \)) is given by \( i\partial_\tau \chi = E\chi \) with \( E = (m^2 - \Delta)^{1/2} - m \). This operator may be well-defined in the momentum representation (i.e. by means
of the Fourier transform). The Schrödinger type wave function $\chi$ appears as prefactor of $e^{iS}$ with classical action $S = -m\tau$, which in turn is associated with a congruence of classical particles at rest in the Lorentzian coordinate system chosen. Since this coordinate system was arbitrary, any congruence of particles in parallel uniform motion provides a possible "background" with respect to which a unitary evolution equation may be written down. It should be remarked that this reasoning corresponds to a "one-particle interpretation" and is not the modern way to proceed when treating the quantized scalar particle. However, in quantum cosmology the wave function $\psi$ is usually not promoted into an operator — as long as third quantization is not envisaged — and one may look at it from the point of view of a "one-universe interpretation". We will, in this paper, try to generalize the pattern provided by unitarity and decomposition to non-trivial backgrounds $(\mathcal{M}, ds^2, U)$ as far as possible. If one likes in addition the space $\mathcal{H}$ of wave functions to form a Hilbert space, one may reverse the sign of $Q$ in $\mathcal{H}^-$ and obtain an overall positive definite scalar product. Although such a procedure might seem somewhat arbitrary, it is completely compatible with the Lorentz symmetry. Moreover, the refined algebraic quantization approach \cite{3, 10}, when applied to the Klein-Gordon equation in Minkowski space \cite{7} as well as in a flat space-time with toroidal spatial sections \cite{3} (i.e. $\mathcal{M} = \mathbb{R} \times S^1 \times S^1 \times S^1$ with arbitrary radii for the $S^1$-factors) precisely yields the structure $(\mathcal{H}^+, Q) \oplus (\mathcal{H}^-, -Q)$ as the Hilbert space $(\mathcal{H}_{\text{phys}}, \langle | \rangle_{\text{phys}})$ of physical states.

A typical way how the conceptual problems in quantum cosmology arise is that a generic background $(ds^2, U)$ does not admit a preferred frequency decomposition of wave functions in an obvious way. This problem persists even when the potential $U$ is positive, and the notion of outgoing and incoming trajectories (i.e. the classical analogue of mode decomposition) is unambiguously well-defined. Also, the split of the wave equation into two (mutually complex conjugate) unitary evolution equations is usually achieved only in a semiclassical context \cite{5} where some additional assumption such as the division of variables into classical and quantum ones are necessary (see e.g. Ref. \cite{15} and, as a recent contribution touching upon the problem of unitarity, Ref. \cite{16}). This type of problem has plagued early attempts to quantize a scalar particle in curved space-time, and similar obstructions have been encountered when the question was raised how quantum cosmology should be interpreted. It might appear that no "invariant" structure of the ordinary quantum mechanical type — such as Hilbert spaces and unitary evolution — may be constructed at the fundamental level of the wave equation. This expectation has long been common belief, and it relies on the absence of geometric structures such as symmetries that would take over the role of the timelike Killing vector field in the flat Klein-Gordon case \cite{8} (see also Ref. \cite{17} for the full superspace context).

Nevertheless, some efforts have been made to circumvent this type of problems, thereby making use of other than local geometric structures. Recently, proposals have been given that relate a preferred decomposition with the structure of super-
space at small scale factors \[18\] and the structure of minisuperspace at large scale factors \[19\]. Furthermore, the refined algebraic quantization approach envisages the construction of a Hilbert space of physical states quite independent of local geometric considerations. As outlined above, it is based on the scalar product \( q \) from \( (2.7) \) and thus incorporates global issues from the outset. It definitely rejects the interpretation of wave functions to propagate causally in minisuperspace, and hence the use of the Klein-Gordon type product \( Q \) from \( (2.8) \). Nevertheless, as we have already remarked above, its result in the flat Klein-Gordon case consists merely in reversing the sign of \( Q \) in the negative frequency sector. The question whether a similar relation exists in more general models has — to my knowledge — not yet been investigated systematically. All these attempts and strategies provide hints that in addition to the local geometry of (mini)superspace, some other structure may play a fundamental role in the emergence of the mathematical objects of quantum mechanics and the possibility of predictions.

The aim of this article is to provide further evidence that mode decomposition and underlying unitarity might be achieved in a larger class of models than is usually believed. For the moment, our main assumption is the positivity of the potential \( U \), i.e. the clear separation of modes in the classical sense. After developing the formalism necessary in the next two Sections, our proposed solution of the decomposition problem is formulated in Section 5. There and in Section 6 we will encounter hints that the construction of an underlying quantum mechanical structure along our proposal is related to further restrictions, possibly of the type of analyticity properties of the model, and that it relies on global issues. In Section 8 we will speculate on possible relations to the refined algebraic quantization approach, and we give a heuristic argument how to define a preferred decomposition in this framework (although we have to leave open whether this decomposition agrees with the one following from our proposal or whether it may give rise to a different solution of the decomposition problem).

3 Decompositions and unitary evolutions associated with WKB-branches

Our starting point is to choose a Hamilton-Jacobi function \( S \) (i.e. a solution of \( (2.3) \) in some domain \( \mathcal{G} \)) in order to define a geometric background structure with respect to which the wave equation may further be exploited. The question whether some structures are actually independent of this choice will be dealt with in Sections 4 and 5. Hence, for the moment, we consider \( S \) to be fixed. Without loss of generality, we assume \( S^\alpha \) to be a future (outgoing) oriented vector. Adopting the usual notation, we will call \( S \) an "action" function. Since we will compute scalar products of the type \( (2.8) \) with \( \Sigma \) being hypersurfaces of constant \( S \), the domain \( \mathcal{G} \) shall be of the appropriate type. One may construct an action function by choosing any spacelike
hypersurface $\Sigma$ admissible for defining the scalar product $Q$ and imposing $S = 0$ on $\Sigma$. Then the positivity of $U$ ensures the existence of a solution $S$ at least in a neighbourhood of $\Sigma$. The delicate problem of asymptotic spatial boundary conditions for wave functions will depend on the particular model.

The function $S$ locally generates a congruence of outgoing classical trajectories. The natural time parameter along these is given by the action itself. In order to retain the usual convention, we define the time parameter as

$$ t = -S, \tag{3.1} $$

future orientation corresponding to increasing values of $t$. (This is an immediate consequence of equation (2.6), taking the pseudo-Riemannian signature of $ds^2$ and the positivity of the lapse function $N$ into account). The evolution parameter $t$ is not intended to be the physically experienced "time", although we take the freedom to use this word. The derivative along the trajectories with respect to this time parameter shall — in a sloppy way — be denoted as $\partial_t$, and is given by

$$ \partial_t = \frac{S^\alpha}{U} \nabla_\alpha. \tag{3.2} $$

The result of the action of this derivative on a function $f$ is sometimes written as $\dot{f}$. Comparison with equation (2.6) shows that this corresponds to the choice $N = U^{-1}$ of the lapse function. It proves useful to introduce a coordinate system in $\mathcal{G}$ adopted to this situation. Let $\xi^a$ ($a = 1, \ldots, (n-1)$) label the trajectories (i.e. $\xi^a = 0$) and choose $(y^a) \equiv (t, \xi^a)$. It then follows that the metric is given by

$$ ds^2 = -\frac{dt^2}{U} + \gamma^{ab} d\xi^a d\xi^b, \tag{3.3} $$

where the potential is expressed as a function $U(t, \xi)$, and $\gamma^{ab}(t, \xi)$ is the Riemannian (i.e. positive definite) induced metric on the surfaces $\Sigma_t$ of constant $t$ (i.e. of constant action). In this coordinate system, $\partial_t$ is given by the partial derivative $\partial/\partial t$. For any fixed $t$, the functions $\xi^a$ provide a coordinate system on $\Sigma_t$. For later purpose let $\mathcal{D}_a$ denote the covariant derivative with respect to $\gamma^{ab}$. Again, for fixed $t$, this is an object intrinsic to the geometry of $\Sigma_t$. An $n$-covariant version of $\gamma^{ab}$ is provided by

$$ P_{\alpha\beta} = g_{\alpha\beta} - \frac{S_{\alpha}S_{\beta}}{S^\gamma S_{\gamma}} \equiv g_{\alpha\beta} + \frac{S_{\alpha}S_{\beta}}{U}. \tag{3.4} $$

It may also be understood as the projection onto directions tangential to $\Sigma_t$.

We will encounter linear operators $A$ acting on functions $\chi(t, \xi)$ on $\mathcal{M}$ whose action is actually tangential to $\Sigma_t$ (as e.g. any derivative operator composed of $\partial_a \equiv \partial/\partial \xi^a$, such as $A^{ab}(t, \xi)\partial_{ab})$. Such an operator is characterized by

$$ [A, S] = 0, \tag{3.5} $$
the derivative $\dot{A}$ thereof along the trajectories being defined as the commutator $[\partial_t, A]$. (In the example just mentioned this would be $\dot{A}^{ab}(t, \xi)\partial_{ab}$). Taking again the commutator with $\partial_t$, it follows that $[\dot{A}, S] = 0$, i.e. $\dot{A}$ acts tangential to $\Sigma_t$ along with $A$.

We are now in position to develop our formalism. In addition to $S$ we fix a real function $D$ satisfying the conservation equation

$$\nabla_\alpha (D^2 S^{\alpha}) = 0. \tag{3.6}$$

In terms of the coordinates $(t, \xi^a)$, the general solution thereof reads

$$D^2(t, \xi) = \frac{f(\xi)}{\sqrt{\gamma(t, \xi)} \sqrt{U(t, \xi)}}, \tag{3.7}$$

where $f(\xi)$ is an arbitrary function which is constant along each trajectory and which we assume to be chosen strictly positive everywhere in $\mathcal{G}$, and $\gamma$ is the determinant of the metric $\gamma_{ab}$. The function $f$ represents the freedom to re-label the trajectories and defines the measure $d^{n-1}\xi f(\xi)$ (see (3.14) below).

Given $S$ and $D$, we express any wave function as

$$\psi = \chi D e^{iS}. \tag{3.8}$$

This resembles what is usually done in the semiclassical approach. Note however that we require $S$ and $D$ to satisfy the full Hamilton-Jacobi and conservation equation, with all variables $y$ involved. No division of degrees of freedom into classical and quantum has been assumed. Any wave function $\psi$ is associated with a function $\chi$ on the domain $\mathcal{G}$ in which $S$ and $D$ exist. Some wave functions "fit" the background structure $(S, D)$ in a natural way: When $e^{iS}$ varies much faster than $D$ and $\chi$, $\psi$ may be called a WKB-state. Although we will not develop a WKB type formalism here, we simply call the pair $(S, D)$ a WKB-branch. (One could equally well call it Hamilton-Jacobi-branch; it encodes a congruence of classical trajectories whose tangent vector field is hypersurface orthogonal, endowed with a weight represented by $D$. By using the notation admissible WBK-branch we emphasize that in a particular model some asymptotic condition constraining the set of possible action functions $S$ might be appropriate).

Inserting (3.8) into (2.2), the wave equation becomes equivalent to

$$i \partial_t \chi = \left( \frac{1}{2} \partial_{tt} + h \right) \chi, \tag{3.9}$$

where $h$ is an operator acting tangential to $\Sigma_t$, i.e. $[h, S] = 0$. This may be shown either by direct computation or, more elegantly, by using an ADM type $(n-1) + 1$-decomposition of the Laplacian $\nabla_\alpha \nabla^\alpha$. In Ref. [20] the differential equation for $\chi$ has been worked out for more general evolution parameters. (Setting $\mathcal{N} = U^{-1/2}$,
\( N_a = 0 \) in the formalism of Ref. [20] reduces everything to the framework considered here). We just quote the result that \( h \) is given by

\[
h = H^{\text{eff}} - \frac{1}{2} D (D^{-1}) \cdot
\]  

where

\[
H^{\text{eff}} = -\frac{1}{2DU} \nabla_{\alpha} P^{\alpha\beta} \nabla_{\beta} D \equiv -\frac{1}{2D\sqrt{U}} D_{\alpha} \frac{1}{\sqrt{U}} D^a D.
\]  

The derivatives \( \nabla_{\alpha} \) and \( D_a \) are understood in this expression to act on everything to the right of them (e.g. \( \nabla_{\alpha} D \) acting on a function \( \chi \) giving \( \nabla_{\alpha}(D\chi) \)). In Ref. [20] it was argued that in a WKB-context (3.9) is well-approximated by the effective Schrödinger equation

\[
i \partial_t \chi \approx H^{\text{eff}} \chi.
\]

(\( H^{\text{eff}} \) was therefore called ”effective Hamiltonian”).

Here we will proceed without approximation instead. We first compute the scalar product (2.8) for two wave functions of the form (3.8), (i.e. within the same WKB-branch (S,D)) for hypersurfaces \( \Sigma = \Sigma_t \). (Due to our assumptions, there exists at least an interval of values for \( t \) such that \( \Sigma_t \) is admissible for computing \( Q \)). The orientation of the hypersurface element is fixed by

\[
d_{\Sigma} \equiv -\frac{1}{U^{1/2}} S^a, \quad n^a = -U^{-1/2} S^a \text{ is the unit normal (} n_a n^a = -1 \text{)}, \quad \text{and } d\Sigma \text{ is the (positive definite) scalar hypersurface element (in the coordinate system } (t,\xi^a) \text{ we have } n^0 < 0 \text{ and } d\Sigma = d^{a-1} \xi \sqrt{\gamma}.\]

Making use of (3.2), the definition of \( n^a \) and the fact that \( D \) is real, the result is easily seen to be

\[
Q(\psi_1, \psi_2) = \int_{\Sigma_t} d\Sigma \sqrt{U} D^2 \left( \chi_1^* \chi_2 + \frac{1}{2} \left( \chi_1^* (i\partial_t \chi_2) + (i\partial_t \chi_1)^* \chi_2 \right) \right).
\]  

(3.12)

By construction, it is independent of \( t \). The first part of this expression amounts to introduce the (positive definite) scalar product for each hypersurface \( \Sigma_t \) within a WKB-branch

\[
\langle \chi_1 | \chi_2 \rangle = \int_{\Sigma_t} d\Sigma \sqrt{U} \chi_1^* \chi_2 = \int_{\Sigma_t} d\Sigma \sqrt{U} D^2 \chi_1^* \chi_2.
\]  

(3.13)

In the coordinate system \( (t,\xi^a) \) this reduces to

\[
\langle \chi_1 | \chi_2 \rangle = \int d^{n-1} \xi \sqrt{\gamma} \sqrt{U} D^2 \chi_1^* \chi_2 = \int d^{n-1} \xi f(\xi) \chi_1^*(t,\xi) \chi_2(t,\xi).
\]  

(3.14)

It thus has the Leibnitz rule property

\[
\frac{d}{dt} \langle \chi_1 | \chi_2 \rangle = \langle \dot{\chi}_1 | \chi_2 \rangle + \langle \chi_1 | \dot{\chi}_2 \rangle.
\]  

(3.15)

In the following we will make use of the formal hermitean conjugate \( A^\dagger \) of an operator \( A \), defined by

\[
\langle \chi_1 | A \chi_2 \rangle = \langle A^\dagger \chi_1 | \chi_2 \rangle.
\]  

(3.16)
In case of differential operators, it is found by formally carrying out the usual pro-
cedures of partial integration and omitting all terms stemming from the (asymptot-
ic) boundary of $\Sigma_t$. The conditions necessary to make them (and statements
like $A = A^\dagger$) rigorous are addressed to concrete models to which this formalism is
applied. The complex conjugate $A^*$ of an operator $A$ is defined by

$$A^* \chi = (A\chi)^*.$$  \hfill (3.17)

Complex conjugation satisfies $(AB)^* = A^*B^*$, $(A\chi)^* = A^*\chi^*$ and $(A^*)^\dagger = (A^{\dagger})^*$. The operator $h$ from (3.10) is hermitean and real ($h^\dagger = h^* = h$), and the same is true for the effective Hamiltonian $H_{\text{eff}}$ from (3.11) as well as for the action $S$ (as multiplication operator). The latter fact implies that the hermitian conjugate $A^\dagger$ and the complex conjugate $A^*$ of an operator $A$ satisfying (3.5) both act tangential to $\Sigma_t$ along with $A$. The dot operation $A \rightarrow \dot{A} \equiv [\partial_t, A]$ commutes with both * and $^\dagger$.

The wave equation in the form (3.9) is not of the Schrödinger type, but rather a
differential equation of second order in the classical evolution parameter $t$. However,
let us try to assume that there exists an operator $H$ such that any solution of the
differential equation $i\partial_t \chi = H\chi$ automatically satisfies (3.9). Differentiating this
equation with respect to $t$ and inserting $i\partial_t \chi$ and $\partial_{tt}\chi$ into (3.9), one finds that
the operator $C \equiv i\dot{H} - 2h + 2H + H^2$ must annihilate all functions $\chi$ subject to
$i\partial_t \chi = H\chi$. We would like in addition that $H$ acts tangential to $\Sigma_t$, which implies
$C\chi = 0$ for all $\chi$ defined on $\Sigma_t$, hence $C = 0$. Moreover, a short computation reveals
that the space of all wave functions $\psi$ such that $\chi$ evolves as $i\partial_t \chi = H\chi$ is orthogonal
under $Q$ to its complex conjugate if $H^\dagger = H^*$. The reasoning sketched in these few
lines shall now be reversed.

In view of the brief arguments given above, we write down the differential equa-
tion for an operator $H$,

$$i\dot{H} = 2h - 2H - H^2,$$  \hfill (3.18)

together with two additional requirements,

$$[H, S] = 0.$$  \hfill (3.19)

and

$$H^\dagger = H^*.$$  \hfill (3.20)

A further requirement will be imposed later (see (3.33) below). As is easily shown
using $[h, S] = 0$ and $h^\dagger = h^*$, the two constraints (3.19)–(3.20) are propagated by
the evolution (3.18). Whenever they are satisfied for one particular value $t = t_0$,
they are valid for all $t$. Hence, the system (3.18)–(3.20) is consistent and well-posed.

It is useful to introduce some more notation. For any solution $H$ of the system
let

$$H + 1 \equiv \mathcal{P} \equiv A + iB,$$  \hfill (3.21)
where $A \dagger = A^* = A$, $B \dagger = B^* = B$ and $[A, S] = [B, S] = 0$. The operators $A$ and $B$ provide the decomposition of $H + 1$ into its hermitian and anti-hermitian (and at the same time into its real and imaginary) part. These operators are uniquely determined to be

$$A = 1 + \frac{1}{2}(H + H^\dagger) \quad \quad B = \frac{i}{2}(H^\dagger - H).$$

(3.22)

It is in particular the first of these operators that will play an important role later on. Moreover we note that, if $H$ is a solution, the operator $\tilde{H} = -(H^* + 2)$ (which is identical to $-(H^\dagger + 2)$ on account of (3.20)) is a solution as well, the associated quantities being given by $\tilde{P} = -P^*$, $\tilde{A} = -A$ and $\tilde{B} = B$.

We assume now that a solution $H$ of (3.18)–(3.20) has been chosen. Recalling the motivation for considering this system of equations, we state the following property: Any solution of the equation

$$i \partial_t \chi = H\chi$$

(3.23)

gives rise to a solution of the wave equation in the form (3.9), or by virtue of (3.8), in the original form (2.2). This follows from the differential equation (3.18). Let us denote the space of wave functions obtained in this way by $IH^*$. Accordingly, any solution of the equation

$$i \partial_t \chi = -(H^* + 2)\chi$$

(3.24)

gives rise to a solution of the wave equation as well. This is because $\tilde{H} = -(H^* + 2)$ satisfies the differential equation (3.18) along with $H$. The space of wave functions obtained in this way shall be denoted by $IH^-$. We have thus defined two subspaces $IH^\pm$ of the total space $IH$ of wave functions (whereby we assume appropriate fall-off conditions to hold at the boundaries of $\Sigma_t$, if necessary).

Turning to the question how these three spaces are related to each other, we observe that $IH^\pm$ are complex conjugate to each other, i.e. $(IH^\pm)^* = IH^\mp$. In order to see this it is important to recall that we have chosen a WKB-branch $(S, D)$ with respect to which any wave function $\psi$ is traced back to a function $\chi$. The relation between $\psi$ and $\chi$ is always provided by (3.8). Hence, if the complex conjugate $\psi^* = \chi^* D e^{-iS}$ of a wave function $\psi$ shall be represented in terms of the WKB-branch $(S, D)$, it must be rewritten as $\psi^* = \chi_c D e^{i\delta}$, with $\chi_c = \chi^* e^{-2i\delta} \equiv \chi^* e^{2i\delta}$ being the associated function. (In contrast, the original expression $\psi^* = \chi^* D e^{-iS}$ refers to the WKB-branch $(-S, D)$ instead). Complex conjugation $\psi \rightarrow \psi^*$ of wave functions is thus represented as $\chi \rightarrow \chi_c$. It is now an easy task to show that $\chi$ satisfies the evolution equation (3.23) if and only if $\chi_c$ satisfies (3.24). The number 2 in the operator $-(H^* + 2)$ thus represents the separation between the two WKB-branches $(\pm S, D)$ by a total relative phase factor $e^{-2i\delta}$. This can be illustrated by a heuristic argument: In a semiclassical (WKB) context one may expect $H$ to be "small" as compared to unity, and thus (3.23) to describe a slowly varying function $\chi$. As a consequence, (3.8) is dominated by the phase factor and represents a WKB type state. Its complex conjugate is a WKB type state as well (with respect to the
WKB-branch ($-S, D$), i.e. with reversed trajectories), but the associated function $\chi_c$ — the representation of $\psi^*$ in the WKB-branch ($S, D$) — is now rapidly varying!

Since the two spaces $\mathcal{H}^\pm$ are complex conjugate to each other, whatever can be stated about $\mathcal{H}^+$ and the evolution equation (3.23) has a counterpart in terms of $\mathcal{H}^-$ and the evolution equation (3.24). It is thus natural to ask whether $\mathcal{H}^+$ and $\mathcal{H}^-$ have a non-trivial intersection, and whether their sum spans the space $\mathcal{H}$ of all wave functions. The answer to these questions depends on the properties of the operator $A$. It proves useful to insert (3.21) into (3.18). The differential equation for $H$ becomes equivalent to

$$i\dot{P} + P^2 = 1 + 2h.$$ (3.25)

Separating real and imaginary parts, we find the system

$$\dot{A} = -\{A, B\}$$ (3.26)

$$\dot{B} = A^2 - B^2 - 1 - 2h,$$ (3.27)

where $\{A, B\}$ denotes the anticommutator $AB + BA$. (Let us note en passant that yet another equivalent form of (3.18) is achieved by setting $P = i\dot{u} u^{-1}$. The resulting equation for the operator $u$ is linear,

$$\ddot{u} + (1 + 2h) u = 0,$$ (3.28)

which is not a surprise since $H$ stems from a linear problem. We will make use of this result later on). Equation (3.26) may formally be solved: Let $A_0$ be the action of $A$ on some ”initial” hypersurface $\Sigma_{t_0}$. Since $A$ acts tangential to all $\Sigma_t$ (i.e. $[A, S] = 0$), one may imagine to represent $A$ as a $t$-dependent operator acting on functions $\chi(\xi)$, and then insert $t = t_0$. This makes $A_0$ an operator for functions $\chi(y)$, i.e. at the same footing as all other operators considered so far. The solution to (3.26) is given by

$$A = UA_0 U^\dagger$$ (3.29)

where $U$ is the operator satisfying the differential equation $\dot{U} = -BU$ and the initial condition $U_0 = 1$. Its hermitean conjugate thus satisfies $\dot{U}^\dagger = -U^\dagger B$, and (3.29) is easily seen to be the unique solution to (3.26), once $B$ is known. Hence, whenever there is a function $\chi_0$ on some $\Sigma_{t_0}$ such that $A_0\chi_0 = 0$ on $\Sigma_{t_0}$, it follows that there is a function $\chi$ in the region on which $A$ acts, such that $A\chi = 0$. This ensures that there exist solutions $H$ such that $A$ is invertible (or positive). As an example, one may choose $H_0 = 0$.

There is another way to make this explicit. If $\psi \in \mathcal{H}^+$, i.e. $\chi$ satisfies (3.23), then $\mu = A\chi$ satisfies $i\partial_t \mu = H^\dagger\mu$. Likewise, if $\psi \in \mathcal{H}^-$, i.e. $\chi$ satisfies (3.24), then $\mu = A\chi$ satisfies $i\partial_t \mu = -(H + 2)\mu$. If $A_0\chi_0 = 0$ on a hypersurface $\Sigma_{t_0}$, we promote $\chi_0$ into a solution of (3.23). Then $\mu = A\chi$ vanishes on $\Sigma_{t_0}$ and satisfies
a Schrödinger type equation. As a consequence $\mu = 0$, i.e. $A\chi = 0$ everywhere. In other words, the existence of functions annihilated by $A$ cannot be restricted to a single hypersurface $\Sigma_{t_0}$. In this sense, the character of $A$ as an invertible (or positive) operator is propagated by the evolution provided by (3.18).

Subtracting (3.24) from (3.23), we infer that a common element of both $IH^+$ and $IH^-$ satisfies $A\chi = 0$. We require that this equation has no non-trivial solution. In a particular model, one must refer to the asymptotic boundary conditions defining $IH$ in order to exclude the existence of a non-trivial $\chi$. We assume that this can be done and end up with $IH^+ \cap IH^- = \{0\}$. Consequently, one may consider the direct sum $IH^+ \oplus IH^-$ and ask whether it coincides with $IH$. Given any $\psi \in IH$, we consider its "initial data" $(\chi, \dot{\chi})$ at some hypersurface $\Sigma_{t_0}$. $\psi$ is the sum of two wave functions $\psi^\pm \in IH^\pm$ if the system of equations $\chi^+ + \chi^- = \chi, H\chi^+ - (H^* + 2)\chi^- = i\dot{\chi}$ may be solved with respect to $\chi^\pm$ on some $\Sigma_{t_0}$. The propagation of $\chi^\pm$ off $\Sigma_{t_0}$ is then provided by (3.23) and (3.24). Eliminating $\chi^+$ from these equations, one arrives at the single equation $2A\chi^- = (H - i\partial_t)\chi$, which has to be solved with respect to $\chi^-$ on $\Sigma_{t_0}$. Since $\chi$ and $\dot{\chi}$ may arbitrarily be prescribed on $\Sigma_{t_0}$ (up to the required fall-off behaviour at the asymptotic boundary), the decomposition of $\psi$ into a sum of $\psi^\pm$ may always be achieved if $A$ has a sufficiently well-behaved inverse.

The structure of the scalar product for elements of $IH^\pm$ depends on the properties of $A$ as well. If $\psi_1, 2 \in IH^+$, a straightforward use of (3.12) reveals

$$Q(\psi_1, \psi_2) = \langle \chi_1 | A\chi_2 \rangle,$$

(3.30)

whereas for $\psi_1, 2 \in IH^-$ we find

$$Q(\psi_1, \psi_2) = -\langle \chi_1 | A\chi_2 \rangle.$$

(3.31)

If $\psi_1 \in IH^+$ and $\psi_2 \in IH^-$, the scalar product is

$$Q(\psi_1, \psi_2) = \frac{1}{2} \langle \chi_1 | (H^+ - H^-)\chi_2 \rangle,$$

(3.32)

which vanishes on account of (3.20).

In view of these results we impose an additional requirement on the solutions $H$ of the system (3.18)–(3.20). We assume that $A$ is a positive operator, symbolically

$$A > 0.$$

(3.33)

As a consequence, the Klein-Gordon type scalar product $Q$ is positive (negative) definite on $IH^+$ ($IH^-$), and the total space of wave functions is a direct orthogonal sum

$$IH = IH^+ \oplus IH^-.$$

(3.34)

Thus, if all steps we have presented in a rather formal way go through in a particular model, any choice of a WKB-branch $(S, D)$ and any choice of $H$ subject to the above...
restrictions gives rise to two Hilbert spaces of wave functions. Note that for this construction to fix \( \mathcal{H}^\pm \) uniquely, it is sufficient that the basic objects, \( S \) and \( H \), exist in a neighbourhood of some hypersurface \( \Sigma_{t_0} \). The key role of \( H \) is thus to fix the initial data of \( \psi^\pm \). At the boundary of the domain on which \( S \) and \( D \) exist, the relation (3.8) between \( \psi \) and \( \chi \) breaks down, thus leading to a singular behaviour of \( \chi \) and \( H \), while \( \psi \) remains well-behaved.

We have already mentioned that in a WKB-context the operator \( H \) can be considered as much "smaller" than unity. In such a context, a solution of (3.23) may be viewed to be a WKB type state "built" mainly around outgoing trajectories. Analogously, a solution of (3.24) may be viewed to be associated with incoming trajectories. Thus, the spaces \( \mathcal{H}^\pm \) provide generalizations of the classical modes of "outgoing" and "incoming" evolution to the quantum level. In this sense, we can talk about a "mode" decomposition. Note however that, so far, there is considerable freedom in defining such a decomposition. In Section 5 we will examine the perspectives for making it unique.

The practical use we will now make of the positivity property of \( \mathcal{A} \) is that there exists a positive square root \( \mathcal{A}^{1/2} \) and its inverse \( \mathcal{A}^{-1/2} \). So far, we have constructed two Schrödinger type equations (3.23)–(3.24), but the evolution operators \( H \) and \(- (H^* + 2)\) are in general not hermitean. This may easily be cured by redefining the wave functions once more. If the WKB-branch \((S, D)\) is fixed, equation (3.8) defines a one-to-one correspondence between \( \psi \) and \( \chi \). Having chosen \( H \), we define for any wave function

\[
\eta = \mathcal{A}^{1/2} \chi. \tag{3.35}
\]

For \( \psi_{1,2} \in \mathcal{H}^+ \) we thus find

\[
Q(\psi_1, \psi_2) = \langle \eta_1 | \eta_2 \rangle, \tag{3.36}
\]

whereas for \( \psi_{1,2} \in \mathcal{H}^- \) we have

\[
Q(\psi_1, \psi_2) = -\langle \eta_1 | \eta_2 \rangle. \tag{3.37}
\]

For completeness we recall that \( Q(\psi_1, \psi_2) = 0 \) if \( \psi_1 \in \mathcal{H}^+ \) and \( \psi_2 \in \mathcal{H}^- \). Since (3.35) applies for any state, the decomposition of a given wave function with respect to \( \mathcal{H}^\pm \) reads \( \eta = \eta^+ + \eta^- \).

The evolution equations (3.23)–(3.24) may now easily be re-written in terms of \( \eta \). If \( \psi \in \mathcal{H}^+ \) we find

\[
i \partial_t \eta = \mathcal{K} \eta, \tag{3.38}
\]

which replaces (3.23), and for \( \psi \in \mathcal{H}^- \) we have

\[
i \partial_t \eta = -(\mathcal{K}^* + 2) \eta, \tag{3.39}
\]

which replaces (3.24). The operator \( \mathcal{K} \) appearing here is given by

\[
\mathcal{K} = \mathcal{A}^{1/2} H \mathcal{A}^{-1/2} + i (\mathcal{A}^{1/2})^* \mathcal{A}^{-1/2}. \tag{3.40}
\]
It is hermitean,

\[ K^\dagger = K, \quad (3.41) \]

and acts tangential to \( \Sigma_t \), i.e. \([K, S] = 0\). Note that in general \( K^\dagger \neq K^* \). The same properties hold for the evolution operator of (3.39), in particular \(- (K^* + 2)^\dagger = -(K^* + 2)\). (The way how properties of \( K \) carry over to properties of \(- (K^* + 2)\) may be inferred analogously to the case of the operators \( H \) and \(- (H^* + 2)\): If a wave function \( \psi \) is represented in the WKB-branch \((S, D)\) by the function \( \eta \), then the complex conjugate wave function \( \psi^* \) is represented by \( \eta_c = \eta^* e^{-2iS} \). By using (3.21), (3.26), the time derivative of the identity \( A = A^{1/2} A^{1/2} \), and the fact that \((A^{1/2})^\dagger = A^{1/2}\), we can write down another expression for \( K \),

\[ K = A - 1 + \frac{i}{2} A^{-1/2} \left( [A, B] + [A^{1/2}, (A^{1/2})^\cdot] \right) A^{-1/2}, \quad (3.42) \]

which makes its hermiticity property (3.41) explicit. In this formula, one may insert \([A, B] = \frac{i}{2} [H, H^\dagger]\).

Both (3.38) and (3.39) represent (at least at the formal way we are treating things here) a unitary evolution with respect to the (negative of the) classical action \( S \) as time parameter. The coordinates \( \xi^a \) labeling the trajectories play the role of standard quantum mechanical variables. For a given wave function \( \psi(y) \), the function \( \eta(t, \xi) \) may thus in a sense be considered as the "true" representation of the quantum state with respect to the background structure \((S, D, H)\).

### 4 Variations between WKB-branches

The WKB-branch \((S, D)\) as well as the operator \( H \) used in the previous Section have not yet been specified but have been chosen arbitrarily. Here, we will examine what happens when a wave function is analyzed with respect to two WKB-branches.

Let \((S, D)\) and \((S', D')\) be two infinitesimally close WKB-branches. They can be assumed to be defined in the same domain, which thus contains a family of hypersurfaces \( \Sigma_t \) as well as a family of hypersurfaces \( \Sigma'_t \). One may imagine these two families of hypersurfaces to be small deformations of each other. We will denote variations at fixed points of the manifold \( \mathcal{M} \) by \( \delta S = S' - S, \delta D = D' - D \) etc. The background quantities are of course unchanged (in particular \( \delta U = 0 \), and \( \delta \) commutes with \( \nabla_\alpha \)). Finite variations can in principle be constructed from infinitesimal ones, as long as the initial and the final WKB-branch are not separated by some barrier of global type.

The variation is characterized by \( \delta S \) and \( \delta D \), which have to respect the Hamilton-Jacobi (2.5) as well as the conservation equation (3.6). These quantities are easily seen to be constrained by

\[ (\delta S)^\cdot = 0 \quad (4.1) \]
It is convenient to write down these objects in terms of the original ("unperturbed") WKB-branch \((S, D)\). In a coordinate system \((y^\alpha) \equiv (t, \xi^a)\), the first equation states that \(\delta S(\xi)\) is an arbitrary function, and \(\delta D(t, \xi)\) can be found by integration along the trajectories of \(S\), the freedom to choose the initial value \(\delta D(t_0, \xi)\) corresponding to the expected freedom for \(D'\). The variation of the derivative operator (3.2) is given by

\[
\delta(D) = -\frac{1}{2U} \nabla_\alpha(D^2 \delta S^\alpha).
\] (4.2)

This is a derivative operator purely tangential to \(\Sigma_t\) (i.e. \([\nabla, S] = 0\)) illustrating the change in the direction of the trajectories (and thus the variation of the hypersurfaces of constant action).

Since the operator \(h\) from (3.10) is uniquely defined in each WKB-branch, its variation is already fixed. Nevertheless, straightforward application of \(\delta\) gives an awkward expression that may be simplified in a somewhat lengthy computation. On that way, one uses identities like \(P^{\alpha\beta} \delta S_\beta = \delta S^\alpha\), \(S_\beta \delta P^{\alpha\beta} = -\delta S^\alpha\) and \([\delta h, S] = -[h, \delta S]\) (which follows from the fact that \([h, S] = 0\)). After performing some operator algebra involving (anti)commutators with \(\partial_t\), one may get rid of several inconvenient terms stemming from the second contribution in (3.10) and containing derivatives of \(D\). Denoting

\[
\mathcal{E} = \frac{\delta D}{D} + i \delta S,
\] (4.4)

the result is

\[
\delta h = [h, \mathcal{E}] + i \left( \nabla - \dot{\mathcal{E}} \right) - \frac{1}{2} [\partial_t, \nabla - \dot{\mathcal{E}}] + [h, \delta S] \partial_t.
\] (4.5)

Due to (4.1), one may insert \(\dot{\mathcal{E}} = (D^{-1} \delta D)'\). Another expression for this variation is

\[
\delta h = [h, \frac{\delta D}{D}] + \frac{1}{2} \left[ [\partial_t, \delta S] + [h, \delta S] \partial_t \right],
\] (4.6)

where one may replace \([\dot{h}, \delta S]\) by \([\partial_t, [h, \delta S]] \equiv [h, \delta S]'\). Also note that \([h, \delta S] = -\nabla + \dot{\mathcal{E}}\). This form is particularly suitable for computing the variation of \(\dot{h}\) and higher derivatives. The most beautiful and comprimed formula is

\[
\delta h = [h, \frac{\delta D}{D}] + \frac{1}{2} \left( \partial_t, [h, \delta S] \right).
\] (4.7)

In all these expressions, the appearance of \(\partial_t\) as an operator acting directly on wave functions signals the variation of the trajectories. Although \(h'\) contains only derivatives with respect to the coordinates \(\xi'^a\), it attains derivatives \(\partial_t\) when re-written in terms of \((t, \xi^a)\).
Having made explicit how the basic quantities defining a WKB-branch transform, we turn to the case of $H$. In both WKB-branches, we have the system of equations `(3.18)–(3.20)` for $H$ and $H'$, respectively. In principle, both $H$ and $H'$ may be chosen completely independent of each other, as long as they satisfy their respective equations (we just assume that they differ only by an infinitesimal operator $\delta H$). One may of course take the variation of `(3.18)` — thereby using $\delta \dot{H} \equiv \delta ([\partial_t, H]) = (\delta H)' + [\nabla, H]$ — in order to obtain a linear inhomogeneous differential equation for $\delta H$ that has to be satisfied anyway. (It states that, if $H$ obeys `(3.18)`, then $H'$ obeys its respective differential equation as well). Also, one may vary `(3.19)` and `(3.20)`, whereby in the latter case one must take into account the subtlety that $\delta$ does not commute with $\partial_t$.

We will however restrict the freedom in choosing $H$ and $H'$ independently. We require that the mode decompositions induced by these two operators are identical, i.e. $IH^+ = I'H^+$ and $IH^- = I'H^-$. Any wave function can be re-written in terms of the two WKB-branches as $\psi = \chi De^{iS} = \chi' D'e^{iS'}$. If $\psi$ is an element of both $IH^+$ and $I'H^+$, we encounter two evolution equations $i \partial_t \chi = H \chi$ and $i \partial_t \chi' = H' \chi'$. Expressing $\chi$ and $\partial_t$ in terms of $\chi'$ and $\partial_t'$ and assuming $\delta H \equiv H' - H$ to be infinitesimal, a simple calculation reveals that the variation of $H$ must be of the form

$$\delta H = [H, \mathcal{E}] + i (\nabla - \mathcal{E}) + \mathcal{O} ,$$

where $\mathcal{E}$ is given by `(4.4)` and $\mathcal{O}$ is an operator satisfying $\mathcal{O} \chi = 0$ for all $\chi$ such that $i \partial_t \chi = H \chi$. Taking into account that `(3.13)` is valid in both WKB-branches (hence $[\delta H, S] + [H, \delta S] = 0$), it follows that $\mathcal{O} = [H, \delta S](\partial_t + iH)$. Thus, $\delta H$ is completely fixed, once $H$ has been chosen. (Supposing that $\mathcal{O}$ has an additional contribution $\mathcal{O}^{add}$, we must have $[\mathcal{O}^{add}, S] = 0$ and $\mathcal{O}^{add} \chi = 0$ for all $\chi$ such that $i \partial_t \chi = H \chi$. Since $\mathcal{O}^{add}$ acts tangential to $\Sigma_t$, and the “initial value” of $\chi$ on some $\Sigma_{t_0}$ is arbitrary, we infer that $\mathcal{O}^{add} \chi = 0$ for all $\chi$, hence $\mathcal{O}^{add} = 0$). In other words, $H$ and $H'$ must be such that their (infinitesimal) difference is given by

$$\delta H = [H, \mathcal{E}] + i (\nabla - \mathcal{E}) + [H, \delta S](\partial_t + iH) .$$

Inserting $\nabla - \mathcal{E} = -[h, \delta S]$, we obtain

$$\delta H = [H, \frac{\delta D}{D}] + i [H - h, \delta S] + [H, \delta S](\partial_t + iH) .$$

This condition is equivalent to the equality $IH^+ = I'H^+$. Complex conjugation implies the equality $IH^- = I'H^-$. We have now a simple criterion whether the decompositions defined in terms of two overlapping WKB-branches are equal. Our idea is that the whole of the manifold $\mathcal{M}$ is covered by all admissible WKB-branches of the previous type. Furthermore we assume that this set of admissible WKB-branches is connected in the sense that any two branches may be deformed into each other by a family of infinitesimal variations.
Whether this idea may rigorously be formulated will depend on the details of the particular model, its asymptotic structure and on how ”admissible” is defined. Here, we assume that it is the case.

As a consequence, one could try to choose the operator $H$ within any WKB-branch such that for infinitesimal neighbours the condition (4.10) holds. This in turn gives rise to a unique decomposition. One may, for example, start with any decomposition of $\mathcal{D}H$ and define $H$ in each WKB-branch such that it generates the pre-assumed decomposition. Then (4.10) will surely hold for close neighbours. This argument shows the existence of such constructions. However, in doing so, nothing would be gained. Our actual goal is to single out a preferred decomposition.

At this step we must make a difference between the two possible interpretations of the wave equation (2.1) as a quantized scalar particle and as a quantum cosmological model. In the first interpretation, the idea of a wave function propagating causally is natural if not necessary. This provides the main motivation for using the Klein-Gordon type scalar product $Q$ rather than the $L^2$-product $q$ from (2.7) in quantum field theory on curved space [21]. On the other hand, no such feature is necessary in quantum cosmology. When trying to select a solution of the differential equation (3.18), we will accept a result that lacks causality and locality properties and thus transcends the quantized particle picture.

5 Perspectives for uniqueness: the iterative solution

In this Section we will tackle the problem whether a preferred decomposition $\mathcal{D}H = \mathcal{D}H^+ \oplus \mathcal{D}H^-$ may be defined in a natural way. According to the formalism developed in the two foregoing Sections, we have to choose an operator $H$ within each admissible WKB-branch $(S,D)$, satisfying the differential equation (3.18) and the additional conditions (3.19)–(3.20). For any two infinitesimally close WKB-branches, the variation shall satisfy the equation (4.10). This guarantees that the decompositions associated with the two WKB-branches are identical. As already mentioned, we assume the global structure of the set of all admissible WKB-branches to imply the statement that, no matter which WKB-branch is used to define the decomposition, the result is alway the same.

Thus, the next step in our program is to make an appropriate choice of the operator $H$, once $(S,D)$ are given. This choice has to be ”natural”, and should thus not refer to additional objects (such as a prescribed decomposition). Since (3.18) is a differential equation, one might think of fixing the ”initial value” of $H$ on some hypersurface $\Sigma_{t_0}$. Two possible guesses might be $H = 0$ or $H = h$ at $t = t_0$. However, a simple computation reveals that the solutions of (3.18) defined by these choices cannot satisfy (4.10). The reason is that two WKB-branches differing merely
by a rigid translation $t \to t + \text{const}$ must be considered different (with $\delta S = \text{const}$). In other words, the value $t = t_0$ does not have an invariant significance, and any choice of a solution $H$ based on initial conditions will fail. Let us add that the attempt to use initial conditions for selecting $H$ is in spirit related to the scalar particle quantization picture of our problem. The impossibility in doing so reflects the fact that no preferred decomposition may be singled out in a causal and local way. This may be viewed as a justification of the point of view that a unique mode decomposition is not the appropriate thing to look for in quantum field theory in a curved background. However, we are mainly interested in quantum cosmology, where new possibilities arise.

We will now present a formal solution to the problem. It is ”formal” in the sense that a power series emerges whose actual convergence (possibly in some regularized sense) may depend on the particular model. The procedure described in the following is thus understood as a general strategy whose application to concrete models or classes of models will raise a number of questions by its own.

The starting point is to rewrite (3.18) as

$$H = h - \frac{1}{2} H^2 - \frac{i}{2} \dot{H}. \quad (5.1)$$

This equation may be iterated, i.e. the two terms $H^2$ and $\dot{H}$ may be replaced by the square and the time-derivative of $h - \frac{1}{2} H^2 - \frac{i}{2} \dot{H}$, followed by the same substitution whenever $H$ appears in this new equation, and so forth. One obtains an expression

$$H = h - \frac{1}{2} h^2 - \frac{i}{2} h + \frac{1}{2} h^3 + \frac{i}{2} \{h, \dot{h}\} - \frac{1}{4} \ddot{h} + \ldots \quad (5.2)$$

in which the dependence of the rhs on $H$ has disappeared. Only expressions involving $h$ and its derivatives remain. Whenever this series converges (in a suitable topology on the space of operators) it defines a solution of (5.1). Also, the constraints (3.19)–(3.20) will be satisfied on account of the properties of $h$ and the operations $\dagger$, $\ast$ and $\partial_t$. Surprisingly, this solution — if it exists — solves the decomposition problem, as we will now show.

When iterating (5.1), it is useful to introduce a formal book-keeping parameter $\epsilon$ whose actual value is 1, and which keeps track of the ”order” of terms appearing in (5.2). By replacing $h \to \epsilon h$, $H \to \epsilon H$ and $\partial_t \to \epsilon \partial_t$, the differential equation (5.1) becomes

$$H = h - \frac{1}{2} \epsilon H^2 - \frac{i}{2} \epsilon \dot{H}. \quad (5.3)$$

This reflects the structure of the iteration and allows to think of $\epsilon$ as a ”small” expansion parameter. The rescaling of quantities by insertion of appropriate powers of $\epsilon$ could have been achieved from the outset by using the evolution parameter $t^{\text{new}} = \epsilon t \equiv -\epsilon S$ and the operators $h^{\text{new}} = \epsilon^{-1} h$, $H^{\text{new}} = \epsilon^{-1} H$ instead of $t$, $h$ and $H$, and thereafter removing the superscript $\text{new}$. As a consequence, the according
We remark here for completeness that the insertion of \( \epsilon \)'s along the lines described above changes the the wave equation (3.9) into
\[ i\partial_t \chi = \left( \frac{1}{2} \epsilon \partial_{tt} + h \right) \chi, \]
whereas the definition (3.21) becomes \( \epsilon H + 1 \equiv \mathcal{P} \equiv \mathcal{A} + i\mathcal{B} \). The formula (3.40) for the operator \( K \) as well as the unitary evolution equations (3.38)–(3.39) remain as they stand (if one rescales \( K \rightarrow \epsilon K \)). Equation (3.25) takes the form \( i\epsilon \dot{\mathcal{P}} + \mathcal{P}^2 = 1 + 2\epsilon h \). The linear differential equation (3.28) will be re-written below (equation (5.16)).

Returning to (5.3), the iteration procedure generates a power series

\[ H = \sum_{p=0}^{\infty} \mathcal{H}_p \epsilon^p, \tag{5.4} \]

by which we mean that, for any given order \( p \), a finite number (actually \( p + 1 \)) of iterations generates the operators \( \mathcal{H}_0, \ldots, \mathcal{H}_p \). Any further iteration leaves these operators unchanged (i.e. acts only on \( \mathcal{H}_{p+1}, \mathcal{H}_{p+2}, \ldots \)). When the iteration procedure leads to a convergent result, it should be identical to (5.4), evaluated at \( \epsilon = 1 \). There are two ways to formulate this situation in terms of sequences of well-defined operators. The first one is to consider the iterative scheme

\[
\begin{align*}
H_0 &= 0 \\
H_{p+1} &= h - \frac{1}{2} \epsilon H_p^2 - \frac{i}{2} \epsilon \dot{H}_p
\end{align*} \tag{5.5}
\]

for non-negative integer \( p \). After an appropriate number of steps, the operators \( \mathcal{H}_p \) may be read off. The iterative solution to the differential equation (5.3) is formally given by \( \lim_{p \to \infty} H_p \).

An alternative formulation is to insert (5.4) as an ansatz into (5.3) and separate orders of \( \epsilon \). This generates the iterative scheme

\[ \mathcal{H}_0 = h \]
\begin{equation}
H_{p+1} = -\frac{1}{2} \sum_{q=0}^{p} \mathcal{H}_q \mathcal{H}_{p-q} - \frac{i}{2} \mathcal{H}_p
\end{equation}

for non-negative integer \( p \). The corresponding solution \( H \) of (5.3) is given by the series (5.4). The first few terms are

\begin{align*}
\mathcal{H}_1 &= -\frac{1}{2} h^2 - \frac{i}{2} \dot{h} \\
\mathcal{H}_2 &= \frac{1}{2} h^3 + \frac{i}{2} \{h, \dot{h}\} - \frac{1}{4} \ddot{h},
\end{align*}

(5.7)

and they clearly fit the structure of (5.2). In view of this scheme one could say that the series (5.4) is the (unique) solution to (5.3) which is analytic in \( \epsilon \).

The convergence of the sequence (5.5) implies the convergence of the series (5.4). However, the converse does not seem to be necessarily true: it is conceivable that the limit of the sequence \( (H_p)_{p=0}^{\infty} \) does not exist on account of effects produced at very large orders in \( \epsilon \), while the operators \( \mathcal{H}_p \) do not "feel" these effects and combine into a convergent series. (A toy-example of such a situation is given by the scheme \( H_0 = 1, \ H_{p+1} = 2\epsilon H_p \), where the result is \( H_p = (2\epsilon)^p \), which does not converge as \( p \to \infty \) if \( \epsilon = 1 \), but whose analogue to (5.4) yields \( \mathcal{H}_p = 0 \), hence \( H = 0 \). We also note that a modification of the scheme (5.5) by admitting some non-zero starting value \( H_0 \) would change the higher order behaviour of the \( H_p \), while leaving the \( \mathcal{H}_p \) unchanged). The actual convergence of \( \lim_{p \to \infty} H_p \) would thus imply these higher order effects to become successively negligible. The principle possibility of a situation in which they are not negligible becomes clear when one tries to define precisely what the dots in (5.2) mean. All of our considerations will concern statements given for some arbitrary but finite order in \( \epsilon \). For this type of statements, both procedures are equivalent, but what we mean by "the" iterative solution \( H \) is — in case of doubt — the series (5.4) rather than the limit of (5.5). Nevertheless, the iteration (5.5) is more appealing as a fundamental issue because it does not even require the parameter \( \epsilon \) to be different from 1. In contrast, the procedure (5.6) relies on a particular book-keeping of terms which is controlled by \( \epsilon \). Thus, our hope is that these two procedures are in fact equivalent, the parameter \( \epsilon \) merely being a technical tool in computations that could as well be omitted.

In the sense elaborated above, it is clear that the series (5.4) qualifies as a formal solution of the differential equation (5.3) or, after setting \( \epsilon = 1 \), of (3.18). In case of convergence, it will be an actual solution. The same applies to the conditions (3.19)–(3.20). The really interesting question, to which we will now pay our attention, is whether it satisfies equation (4.10) which guarantees the uniqueness of the decomposition. In order to investigate this question in a most economic way, we re-write the equations (4.6) and (4.10) by rescaling \( h \), \( H \) and \( \partial_t \) by a factor \( \epsilon \), while leaving \( \delta S \) and \( \delta D \) unchanged. The variation of \( h \) thus becomes

\begin{equation}
\delta h = [h, \frac{\delta D}{D}] + \frac{1}{2} \epsilon \{\dot{h}, \delta S\} + \epsilon [h, \delta S] \partial_t,
\end{equation}

(5.8)
and the uniqueness condition (4.10) reads
\[ \delta H = [H, \frac{\delta D}{D}] + i [H - h, \delta S] + \epsilon [H, \delta S] (\partial_t + iH). \] (5.9)

We also display the variation of the differential equation (5.3),
\[ \delta H = \delta h - \frac{1}{2} \epsilon \{H, \delta H\} + \frac{i}{2} \epsilon [\{h, \delta S\}, H] + \frac{i}{2} \epsilon [H, (\frac{\delta D}{D})] - i \epsilon (\delta H), \] (5.10)

where the variation of \( \partial_t \) has been performed as shown in Section 4. We understand that \( \delta h \) in this equation stands for the expression (5.8). The variation of the formal iterative solution \( H \) may be computed either directly (by using explicit expressions like (5.7)), or by using the iterative scheme (5.6), or by simply iterating (5.10) (i.e. successively re-inserting (5.3) and (5.10) for \( H \) and \( \delta H \)). All these procedures generate the coefficients of
\[ \delta H = \sum_{p=0}^{\infty} \delta H_p \epsilon^p \] (5.11)
to any desired order. The problem under consideration may now be treated using (5.3) and (5.8)–(5.10), without any further reference to the structure of \( h \). As mentioned above, this is an immediate consequence of how we insert powers of \( \epsilon \). Although we treat \( h \) as independent of \( \epsilon \), the variation \( \delta h \) involves \( \epsilon \). This is just an artefact of how we group terms consistently. (We recall that the wave equation (3.9) is rescaled as \( i \partial_t \chi = (\frac{1}{2} \epsilon \partial_{tt} + h) \chi \), which provides another explanation for the \( \epsilon \)-dependence of \( \delta h \)).

Once having the above formulae at hand, the argument we need is surprisingly simple. It is based on the observations that

(i) inserting \( \delta H \) from the uniqueness condition (5.3) into the variation (5.10) of the differential equation gives an identity (because (5.3) guarantees that \( H' = H + \delta H \) satisfies its respective differential equation along with \( H \)), that

(ii) the converse of this, i.e. inserting the variation (5.11) of the iterative solution into the uniqueness condition (5.9), or, likewise, inserting and re-inserting \( \delta H \) from (5.10) into (5.9), is just the equation we would like to prove, and that

(iii) the iterative structure of our problem implies that (i) and (ii) and essentially identical! Note that the statements (i) and (ii) hold for arbitrary order in \( \epsilon \), due to the overall consistency of the way the various factors \( \epsilon \) have been inserted.

Let \( \delta H_4 \) denote the rhs of (5.9) and \( \delta H_5 \) the rhs of (5.10). We consider the equation \( \delta H_4 = \delta H_5 \), which still contains \( H \) and \( \delta H \). In all steps we understand that for \( H \) the iterative solution is inserted. Technically, this is achieved by inserting and re-inserting (5.3) until the desired order in \( \epsilon \) is achieved. In the case of the remaining \( \delta H \)'s, we have two possibilities: Inserting \( \delta H = \delta H_4 \) gives the identity mentioned in observation (i), whereas inserting \( \delta H = \delta H_5 \) iteratively gives the equation of interest, mentioned in observation (ii), that we want to prove.
We proceed iteratively and begin with $O(\epsilon^0)$. To this order, the equation $\delta H_{[5.9]} = \delta H_{[5.10]}$ reduces to the identity $[h, \frac{\delta H}{\delta D}] = [h, \frac{\delta H}{\delta D}]$. The terms containing $\delta H$ are of order $O(\epsilon)$, hence to not contribute. In other words, no matter which of the two possibilities for inserting $\delta H$ is chosen, we find that $\delta H_{[5.9]} = \delta H_{[5.10]}$ is true to $O(\epsilon^0)$.

Now we consider the equation $\delta H_{[5.9]} = \delta H_{[5.10]}$ at $O(\epsilon)$. The remaining $\delta H$’s enter only with their $O(\epsilon^0)$ part, and at this order both possible choices give the same result, as we have shown above. Hence, we infer that $\delta H_{[5.9]} = \delta H_{[5.10]}$ is true to $O(\epsilon)$. The following steps proceed exactly along the same lines. Using all previous orders, we may establish the equation $\delta H_{[5.9]} = \delta H_{[5.10]}$ to hold to arbitrary order $O(\epsilon^p)$. The crucial point is that it is not necessary to specify whether we have to insert $\delta H_{[5.9]}$ or $\delta H_{[5.10]}$ for the remaining $\delta H$’s, because the equality of both alternatives has been shown in the foregoing step. In other words: The uniqueness condition (5.9), with the iterative solution (5.4) inserted, precisely yields (5.11). We have thus proven the

**Theorem:** The formal solution (5.4) and its variation (5.11) satisfy the uniqueness condition (5.9) to any finite order in $\epsilon$.

The explicit check thereof for the first few orders is in principle straightforward, but rather time-consuming. Before the general pattern of the proof has become clear, we have explicitly done the computation for $O(\epsilon)$ by hand and for $O(\epsilon^2)$ and $O(\epsilon^3)$ using Mathematica 2.2.

This is our proposal for solving the decomposition problem. Applying the scheme to concrete models, one will have to make sure that the the series (5.4) makes sense. In Section 7, a number of examples is discussed.

We are now in position to give the first few terms in the expansion of the quantities $A$, $B$ and $K$ which have proven to determine the unitary (Schrödinger type) evolution within the spaces $IH^\pm$ with respect to a WKB-branch. Using the hermiticity property of $h$ and its time-derivative, it is easy to compute $H^1$. Then (5.22) immediately yields (taking into account the rescaled definition $\epsilon H + 1 = A + iB$)

$$A = 1 + \epsilon h - \frac{1}{2} \epsilon^2 h^2 + \epsilon^3 \left( \frac{1}{2} h^3 - \frac{1}{4} \ddot{h} \right) + O(\epsilon^4) \quad (5.12)$$

$$B = -\frac{1}{2} \epsilon^2 \dot{h} + \frac{1}{2} \epsilon^3 \{h, \dot{h} \} + O(\epsilon^4). \quad (5.13)$$

The first of these equations could provide the key for the question whether the positivity property (3.33) of $A$ that was necessary to write down the unitary evolution equations (3.38)–(3.39) actually holds in concrete models. Proceeding formally, the operator $A^{1/2}$ defining the effective wave function by (3.35) becomes

$$A^{1/2} = 1 + \frac{1}{2} \epsilon h - \frac{3}{8} \epsilon^2 h^2 + \epsilon^3 \left( \frac{7}{16} h^3 - \frac{1}{8} \dot{h} \right) + O(\epsilon^4), \quad (5.14)$$
the inverse of which as well as the commutator with \( \partial_t \) being readily computed. Inserting the results into into (3.40), the evolution operator \( \mathcal{K} \) takes the form

\[
\mathcal{K} = h - \frac{1}{2} \epsilon \hbar^2 + \epsilon^2 \left( \frac{1}{2} \hbar^3 - \frac{i}{8} [h, \dot{h}] - \frac{1}{4} \ddot{h} \right) + O(\epsilon^3),
\]

(5.15)

whose hermiticity is evident. Whenever the position of \( \epsilon \) characterizes quantities that are actually small (e.g. in a semiclassical context), these expressions may be used as approximations.

Let us at the end of this Section comment on an alternative formulation specifying our proposed solution (5.4). Recall that the differential equation for \( H \) is related to the linear problem (3.28) which now reads

\[
\epsilon^2 \ddot{u} + (1 + 2\epsilon \hbar) u = 0.
\]

(5.16)

Any solution thereof provides a solution to (5.3) by \( P \equiv 1 + \epsilon H = i\epsilon \dot{uv}u^{-1} \). It is easy to show that any solution \( u \) of the form

\[
u = v e^{-it/\epsilon} \quad \text{with} \quad v = \sum_{q=0}^{\infty} v_q e^{qq}
\]

(5.17)

provides the iterative solution (5.4) by

\[
H = i \dot{v} v^{-1}.
\]

(5.18)

Here it is of course understood that the coefficient operators \( v_q \) do not depend on \( \epsilon \). Although the solution of the form (5.17) is not unique, all possible freedom cancels in (5.18) so as to make \( H \) unique. (If \( \hbar \) were a c-number function of \( t \), one could state that (5.17) is unique up to multiplication by an analytic function of \( \epsilon \).) At the formal level (5.18) reproduces the coefficients of the power series (5.4). The differential equation satisfied by \( v \) turns out to be

\[
i \dot{v} = \hbar v + \frac{1}{2} \epsilon \ddot{v},
\]

(5.19)

which may be used to compute the coefficients \( v_q \) by iteratively solving the linear inhomogeneous differential equations \( i\dot{v}_0 = h v_0, i\dot{v}_{q+1} = h v_{q+1} + \frac{1}{2} \ddot{v}_q \) (and choosing arbitrary integration constants). The formal series emerging from this procedure is nothing but the WKB-expansion associated with the differential equation (5.16) to all orders in \( \epsilon \) (which serves as the "small" \( \hbar \)-type parameter). This analogy becomes even more appealing by the fact that (5.16) formally resembles a one-dimensional time-independent Schrödinger equation, with \( t \) being the position coordinate and \(-1 - 2\epsilon \hbar \) playing the role of the potential. In a sense, the computation of \( H \) is traced back to a problem within the framework of conventional quantum mechanics. We may thus be confident that in a large number of concrete models our proposed
solution $H$ actually exists (i.e., that the formal power series for $v$ and $H$ belong to analytic operator valued functions).

In the literature, the general solution of a differential equation of the type $\ddot{u} + Vu = 0$ is sometimes given as a linear combination $ve^{-it} + we^{it}$ or $r \sin t + s \cos t$. However, the requirement that $u$ is of the form (5.17) is not an attempt to say something about the time-dependence of $u$ for finite $\epsilon$, neither is it an asymptotic condition for large $|t|$ mimicking "positive frequency" (we do not even suppose the coordinate $t$ to extend over all real values). There is no fall-off condition for $v$ involved. It may happen, for example, that for some finite $\epsilon$ the oscillatory factor $e^{-it/\epsilon}$ in $u$ is numerically almost irrelevant as compared to $v$. An illustration of this type of solution is provided by Example 2 in Section 7 where $H$ is computed for $h = a + bt$ and $v$ turns out to behave oscillatory and bounded in the domain $h \gg 0$ but oscillatory and exponentially unbounded in the domain $h \ll 0$. The nature of $v$ as defined in (5.17) without any further condition is absolutely crucial in our construction: for generic time-dependence of $h$, one would not expect a solution of the form (5.17) to exist if $v$ was supposed to be "small" or "slowly varying". The behaviour of the quantities $u$, $v$ and $H$ should not be confused with that of wave function (despite the fact that (5.19) is of the same form as the wave equation (3.9)).

There is another interesting feature related to (5.17). Suppose the time dependence of $h$ is $C_0^\infty$, i.e., $h$ vanishing identically outside an interval $t_0 < t < t_1$ but being non-zero inside and $C^\infty$ for all $t$. As a consequence, $u$ from (5.17) is purely "positive frequency" outside the interval ($u = c_\pm e^{-it/\epsilon}$ for $t < t_0$ and $t > t_1$ with $c_\pm$ being independent of $t$). On the other hand, (5.17) is a differential equation that can be integrated once $u = c_\pm e^{-it/\epsilon}$ for $t < t_0$ is known, and the result will in general be such that $u \neq c_\pm e^{-it/\epsilon}$ for $t > t_1$. This tells us that there will be no solution $u$ of the required type. (This is actually the argument against the existence of a preferred standard-type separation into positive and negative frequencies in the non-stationary case). Since $v$ and $H$ may in any case be generated as formal power series, we conclude that in the case of $h$ being $C_0^\infty$ in $t$, these formal series will not converge and cannot be associated with analytic functions in a unique way. Similar effects can be expected when the basic ingredients of the model ($ds^2$ and $U$) involve $C_0^\infty$ quantities. It is not quite clear what the correct conditions on the model are in order to make sense of the series (5.4), but it is conceivable that they have to do with analyticity.

6 Discussion & Speculations

Let us make some speculations concerning the structure we have possibly touched upon. One appealing feature of the iteration procedure defining $H$ (preferably in the version (5.5), although version (5.6) is technically simpler) is that a (formal)
solution is specified "without ever having made a choice". The procedure as such just consists in shifting the unwanted $H$-dependence at the rhs of (5.3) to arbitrarily large orders in $\epsilon$. The key criterion for solving the problem is the uniqueness condition (5.9). Nevertheless, one would like to know what is behind such a procedure. The whole situation is a bit reminiscent of the idea of general covariance, stating that the geometric objects used to formulate physical laws can be described in terms of coordinates, but still have their right own as "objects". The different descriptions (e.g. of a tensor field in various coordinates) must match (i.e. obey appropriate transformation laws) so as to allow for an "object"-interpretation (e.g. as a tensor). Considering this as an analogy to our situation, one is tempted to talk about "covariance with respect to WKB-branches". The WKB-branch $(S, D)$ thus plays the role of a coordinate description of a geometric structure. The corresponding structure in our case encodes not only the (unique) decomposition, but also leads to the unitary evolution equations (3.38) and (3.39) within the two subspaces $\mathcal{H}^\pm$ of wave functions. These equations show up only in the context of WKB-branches, i.e. there is no unique hermitean operator, just as a scalar field is not given by a unique function of its coordinates unless the coordinate system is specified. Nevertheless, the structures emerging in WKB-branches, such as decomposition and unitarity, match in a beautiful way.

We should emphasize here that we have not dealt with the question how the evolution parameters $t$ relate to what we experience as time, nor have we suggested a complete scheme how to reconstruct standard quantum physics and "the" Schrödinger equation. We merely suggest that, whenever the decomposition problem may be solved positively (i.e. the series for $H$ can be given a sense) the mathematical structures of standard quantum mechanics (positive definite scalar product, Hilbert space, unitarity and the possibility of writing down probability-type expressions) begin to come into our reach. It is thus conceivable that the further steps necessary in deriving quantum mechanics from the Wheeler-DeWitt equation proceed within this familiar mathematical framework.

The most difficult of the questions raised seem to be the technical aspects of the convergence properties of the formal solution (5.4). Without trying to go into the details here, we note that time-derivatives of $h$ of arbitrarily large order are involved. Thus we expect the solution $H$, whenever it exists, to rely on the global structure of the model and the WKB-branch. As we have pointed out at the end of the preceding Section it might be some kind of analyticity condition that ensures convergence of the series. We have seen that at least $C^\infty$ is likely not to be the appropriate differentiability class of $(ds^2, U)$. On the other hand, it is conceivable that the need for analyticity is just a technical tool at some stage in order to give the operator $H$ as provided by the formal series (5.4) a definite meaning, and that this condition disappears when the action of $H$ is maximally extended. This might be in analogy to the attempt to define the operator $U = \exp(\epsilon \frac{d}{dx})$ by means of its formal power series. As an intermediate step, one encounters analytic functions, but
in the end, the action of $\mathcal{U}$ may be extended to the whole of the Hilbert space $L^2(\mathbb{R})$, without any reference to analyticity. If this analogy holds, the structure responsible for the preference of a decomposition would be of global (geometric) nature, rather than relying on analyticity, and the class of models to which our formalism applies can be expected to be rather large.

In any case, our proposal seems to transcend the standard local differential geometric framework (within which we know the solution of the generic decomposition problem to be negative [8]). As we will illustrate for the case of a toy-model in the next Section (Example 7), a naive treatment of the series (5.2) or (5.4) leads to an argument against the existence of the unique decomposition that might be erroneous though intuitively appealing. Maybe one could state that, despite the lack of a local geometric structure (such as a symmetry) specifying a unique decomposition, some underlying global or analytic structure does the job. In the latter case our proposal might give a hint towards a subtle role, not yet completely understood, played by analyticity in the proper formulation of the laws of nature at the fundamental level.

The major difference between the picture suggested by a quantized scalar particle and the picture due to a quantum cosmological model has already been addressed above: In the former, one thinks about the wave function $\psi$ as of a field propagating causally in space-time, and the interpretational framework, such as a decomposition of the space of wave functions, should be in accordance with this point of view. Thus, whatever the significance of such a decomposition is, it should be determined locally on (or near) some spacelike hypersurface and not depend on what will happen to the background $(\mathcal{M}, ds^2, U)$ in the far future. The local character of the standard frequency decomposition in generic backgrounds refers to such a situation. In contrast, the appearance of a formal series in our proposal destroys this causal picture. The decomposition of $\mathcal{H}$ into $\mathcal{H}^\pm$ is determined by global issues in that it cannot be inferred from knowing $(ds^2, U)$ only near some hypersurface. The scalar particle picture can at best lead to locally defined decompositions, e.g. associated with spacelike hypersurfaces. It is conceivable that our proposed unique decomposition is related to all these local decompositions by some kind of average. (We can even imagine that the actual well-posedness of such an average is tied to the convergence of the series for $H$. This would trace back the convergence problem to the existence of, say, an appropriate measure). Since the idea of causal propagation of the wave function is no longer crucial in quantum cosmology, these considerations are not necessarily objections against our approach but might help to uncover the structure which it is based upon. Also, there might be relations to the refined algebraic quantization scheme, on which we will speculate in Section 8. There we will give a heuristic argument that this approach seems to require the existence of a preferred decomposition (whose relation to ours remains open).

In order to get some feeling for the way how the formal solution may become an actual one, we consider the simple case in which $\dot{\hbar} = 0$. In terms of the coordinate
system \((t, \xi)\) this means that the operator \(\hat{h}\) does not depend on \(t\). The flat Klein-Gordon equation \((ds^2 = -d\tau^2 + d\vec{x}^2, U = m^2, S = -m\tau \equiv -t, D = 1)\) is a special case, with \(\hat{h} = -\frac{1}{2m^2}\Delta\). (We note that \(D = \text{const}\) is not a general consequence of \(\dot{\hat{h}} = 0\). In two-dimensional models, \(n = 2\), one can show that \(\dot{\hat{h}} = 0\) implies \(\dot{D} = 0\), but even in this case \(D\) may depend on \(\xi\). For a general situation with \(\dot{\hat{h}} = 0\), the iteration procedure generates a formal solution with \(\dot{\hat{H}} = 0\). Thus, (5.3) reduces to a quadratic equation for \(\hat{H}\). One may easily check that the series (5.4)

\[
H = h - \frac{1}{2} \epsilon h^2 + \frac{1}{2} \epsilon^2 h^3 - \frac{5}{8} \epsilon^3 h^4 + O(\epsilon^4)
\]

(6.1) is just the power series of the closed expression

\[
H = \frac{1}{\epsilon} \left( \sqrt{1 + 2\epsilon h} - 1 \right)
\]

(6.2) around \(\epsilon = 0\). Since one has to insert \(\epsilon = 1\), this expression makes sense if \(h - \frac{1}{2}\) is a non-negative operator, the symbol \(\sqrt{\cdot}\) being understood as providing the (unique) non-negative square root. In the case of the flat Klein-Gordon equation (6.2) leads to the expression \(mH = (m^2 - \Delta)^{1/2} - m\), which was already mentioned in Section 2 (and denoted \(E\) there). It may be well-defined in terms of the Fourier representation, where \(-\Delta\) just becomes \(\vec{k}^2\).

In more general models one will encounter generalizations of this positivity condition. We do not expect these to create major problems, and as a hint we note that the condition \(h - \frac{1}{2} \geq 0\) is likely to hold in realistic models. (In the semiclassical context one even has \(h^2 \ll 1\); see Ref. [20].) In general, the structure of (3.10)–(3.11) tells us that \(H^{\text{eff}}\) is (at least at the formal level at which we are treating such issues here) a non-negative operator, and whenever the ”potential term” \(-\frac{1}{2}D(D^{-1})\cdot\cdot\cdot\) in (3.11) is bounded from below, we can expect \(h\) to share this property.

The results obtained for the case \(\dot{\hat{h}} = 0\) shed new light on the nature of the parameter \(\epsilon\) and the way how to re-insert \(\epsilon = 1\). If \(h\) were a number, the series (6.1) would converge only if \(|2\epsilon h| < 1\). However, the symbol \(h\) actually stands for all numbers contained in the spectrum of the operator \(h\). This situation may be illustrated in the flat Klein-Gordon case \(h = -\frac{1}{2m^2}\Delta\). Applying \(h\) on a function

\[
\chi(\vec{x}) = \int dk \ e^{i\vec{k} \vec{x}} \tilde{\chi}(\vec{k})
\]

(6.3) it effectively acts as \(\frac{1}{2m^2}\vec{k}^2\). Thus, the closed expression (6.2) leads to the appearance of \(\sqrt{1 + \epsilon \vec{k}^2/m^2}\). The power series thereof converges only if \(|\epsilon \vec{k}^2| < m^2\). Thus, we may apply the series (6.1) to a function \(\chi(\vec{x})\) whose Fourier transform \(\tilde{\chi}(\vec{k})\) has support inside a bounded interval \(-k_0 < k < k_0\). Choosing \(0 < \epsilon < m^2/k_0^2\), the series converges and agrees with (6.1). Although \(\epsilon = 1\) may lie outside the domain of convergence, it is always possible to analytically continue the result unambiguously.
along the real line to \( \epsilon = 1 \). This procedure may be performed for all functions with bounded support in momentum space. Since the set of these functions is dense in any reasonable topology considered for this situation, the action of (6.2) may be reconstructed from the series (6.1) although it will not converge on any function. Thus, it might be the case that in more general situations the structure of the series (6.4) should first be analyzed for small \( \epsilon \), restricted to an appropriate set of states for which it converges. The original value \( \epsilon = 1 \) would then be achieved by means of analytic continuation.

The above considerations seem to imply a suggestion how to proceed in more general cases. One could define, as a preliminary space, the set of all wave functions \( \chi \) for which there exists a non-zero \( \epsilon \) (and hence a non-trivial interval of \( \epsilon \)'s) such that

\[
\sum_{p=0}^{\infty} \epsilon^p \langle H_p \chi \rangle
\]

(6.4)

converges in a reasonable sense. The action of the power series operator (5.4) should then be constructed by analytic continuation and an appropriate extension to (discrete or continuous) linear combinations. This is of course only a schematic sketch, and in practice various technical problems may occur.

In case the series (6.4) for \( H \) turns out not to converge on a sufficiently large number of states (or even on none), one might think of applying a regularization scheme. In this case one would have to check the branch-independence of the regularized decomposition. One might also speculate on the existence of some mathematical structure that is poorly accounted for by our power series for \( H \), with the effect that the first few terms give reasonable results, whereas the thing as a whole diverges. (Note that a similar issue arises for the perturbation expansion in ordinary quantum field theory). A minimalist point of view would, by the way, consider the operator \( K \) as the most important object for practical computations. In case there are models in which its formal power series (i.e. (5.15) to all orders) makes sense, whereas (5.4) does not, one might be tempted to accept non-regularizable infinities in \( H \).

Let us close this Section by another speculative remark. We can imagine that procedures other than the one leading to (5.4) exist and solve the decomposition problem at a formal level. (Such procedures could e.g. be based on differently defined iteration schemes, due to alternative way to group terms by means of a book-keeping parameter \( \epsilon \)). It is not clear whether different schemes effectively lead to the same result. In case they do not, all of these non-equivalent schemes would provide a setting within which the ”natural” construction of a unique decomposition is possible. They would be regarded as different realizations of what was called ”co-variance with respect to WKB-branches” above (just as different tensor fields might solve some geometric theory), and should be considered as inequivalent solutions to the decomposition problem. The naturalness of the construction of a decomposition (lacking reference to external structures) may be regarded to bear some analogy to,
say, the problem of finding tensor fields built merely from a metric. Since the actual existence of our proposed solution seems to rely on further conditions, as discussed above, the number of different "natural" solutions might depend on the model as well. Whether all these may in principle be "realized" (just as different metrics solving Einstein’s field equations may realize space-time) or whether one of them is singled out fundamentally, is of course at the moment impossible to answer for us.

7 Examples

Whenever a WKB-branch \((S, D)\) has been chosen and the operator \(h\) is known, the key procedure in our framework is to evaluate the formal solution (5.4) of the differential equation (5.3) and to determine whether (and on which functions) it actually converges. This justifies the consideration of (5.3) in situations in which the operator \(h\) is simple. The property of \(h\) being a second order differential operator in the coordinates \(\xi^a\) may even be ignored to some extent, and emphasis may be laid on its dependence on the evolution parameter \(t\). In the following we list some simple cases that can be treated exactly, and a scenario illustrating a class of models within which our proposal may directly be confronted with the standard frequency decomposition picture.

Example 1: \(\dot{h} = 0\)

This is the simplest case, and it has already been studied in Section 6. The power series (5.4) corresponds to the closed expression (5.2). Due to the simplicity of this situation, non-commutativity of operators does not play any role here. In the case of the flat Klein-Gordon equation \(h\) is proportional to \(-\Delta\), and \(H\) may be given a definite meaning, as outlined in Section 6.

Example 2: \(\ddot{h} = 0\) and \([h, \dot{h}] = 0\)

This is the special case \(h = a + b t\), where the operators \(a\) and \(b\) do not depend on \(t\) and commute with each other. We will treat them as numbers, and in particular assume that \(b\) is invertible and \(|b|\) exists. The general solution of the linear differential equation (5.16) can be expressed in terms of Airy functions (Ref. [22], p. 446). Using their asymptotic expansion formulae, the particular solution of the form (5.17) turns out to be (up to an \(\epsilon\)-dependent factor which is irrelevant)

\[ u = Bi(-x) - i \text{sgn}(\dot{h}) Ai(-x) \]  

with

\[ x = \frac{1 + 2\epsilon h}{(2\epsilon^2 |\dot{h}|)^{2/3}}. \]  

Hence, the proposed unique solution for \(H\) is given by

\[ \epsilon H + 1 = \frac{i \epsilon}{u} \frac{du}{dt} = i \text{sgn}(\dot{h}) \left( \frac{1 + 2\epsilon h}{x^{1/2}} \right)^{1/2} \frac{du}{dx}. \]  

34
This results into the corresponding expansion (5.4) in terms of $\epsilon$, the various $\text{sgn}(\dot{h})$ and $|\dot{h}|$ terms being properly absorbed into an expression analytic in $\dot{h}$ (which thus admits $\dot{h} = 0$ as a special case). An alternative way to expand $H$ is to keep the combination $1 + 2\epsilon h$ and treat only the $\epsilon$ in the denominator of (7.2) as expansion parameter. (This actually amounts to re-interpret the differential equation (5.3) by distinguishing the two $\epsilon$'s as two different parameters and expanding with respect to the second one). This type of expansion is given by

$$
\epsilon H = \left(\sqrt{1 + 2\epsilon h} - 1\right) - \frac{i}{2} \frac{\epsilon^2 \dot{h}}{1 + 2\epsilon h} + \frac{5}{8} \frac{(\epsilon^2 \dot{h})^2}{(1 + 2\epsilon h)^{5/2}} + O((\epsilon^2 \dot{h})^3), \quad (7.4)
$$

thus providing a generalization of (5.2). The factor $-\frac{i}{2}$ of the term linear in $\dot{h}$ may be checked against the second term of $H_1$ in the general expansion (5.7). The existence of this solution shows that the series (5.4), computed by means of the iteration (5.6) with $\ddot{h}$ and all higher derivatives neglected and operator ordering being ignored, is actually the power expansion of an analytic function.

This example provides an illustration that the form (5.17) is not intended to impose conditions on the asymptotic behaviour of $v$, because $u$ blows up exponentially in the domain $h \ll 0$ while it is bounded and oscillates for $h \gg 0$. Hence, the function $v$ is oscillating but has an exponential prefactor in the domain $\dot{ht} < 0$.

**Example 3:** $h = \text{polynomial in } t$ with commuting coefficients

This case seems to be untractable in general, but in principle works like the previous one when again use of the linear differential equation (5.16) is made. The case of $h$ being quadratic in $t$ leads to parabolic cylinder functions (Ref. [22], p. 685). In general, the power series of the proposed solution $H$ coincides with the result of the iteration procedure (5.6) when all derivatives of $h$ higher than the degree of the polynomial $P$ are dropped.

**Example 4:** $h = \alpha t^{-1}$

This case is distinguished by its scaling properties: a glance at the series (5.4) shows that $H$ is $\epsilon$ times a function of the ratio $t/\epsilon$. The linear differential equation (5.16) leads to a special case of confluent hypergeometric functions, the solution of the form (5.17) being (up to an irrelevant non-integer power of $\epsilon$)

$$
u = U(i\alpha, 0, z) e^{-it/\epsilon} \quad \text{with} \quad z = \frac{2i}{\epsilon} t. \quad (7.5)
$$

Here, $U$ is the second Kummer function (Ref. [22], p. 503)

$$
U(a, 0, z) = z^{-a} F(a, z) \quad \text{with} \quad F(a, z) = \sum_{q=0}^{\infty} \frac{(a)_q (a + 1)_q (-)^q}{q! z^q}, \quad (7.6)
$$

where $(b)_0 = 1$, $(b)_q = b(b+1) \ldots (b+q-1)$ for any $b$. The proposed solution of (5.3) is given by $H = i\dot{u}u^{-1} - \epsilon^{-1} = i\dot{v}v^{-1}$ with $v$ — as defined in (5.17) — being proportional.
to $U(i\alpha,0,z)$. Using the form of $u$ as displayed above, we get $H = \frac{2}{t^2} - \frac{2}{t^2} F^{-1} \partial_\alpha F$ with $z = \frac{2i}{t} t$ inserted. Thus, $H$ is analytic in $\epsilon$ and in fact coincides with the series \ref{5.14} for $h = \alpha t^{-1}$. Denoting its functional dependence by $H(\alpha,\epsilon, t)$, we have the symmetries $H(\alpha, -\epsilon, -t) = -H(\alpha, \epsilon, t)$ and $H(\alpha, -\epsilon, t) = -H^*(\alpha, \epsilon, t)$ (all three variables are assumed to be real), hence $H(-\alpha, \epsilon, -t) = H^*(\alpha, \epsilon, t)$. For large $|t|$ the ratio $H/h$ approaches unity.

**Example 5:** $h = \beta t^{-2}$

This case is particularly important because it emerges in simple quantum cosmological minisuperspace models. In the spatially flat Friedmann-Robertson-Walker (FRW) universe with scale factor $a$ (being the only minisuperspace variable) and positive cosmological constant $\Lambda$, the DeWitt metric and the potential are given by $ds^2 = -da^2$ and $U = a^4 \Lambda$. The WKB-branch is specified by $S = -\frac{1}{3} a^3 \sqrt{\Lambda} = -t$ and $D = t^{-1/3}$ (it is unique up to $S \rightarrow \pm S + \text{const}$ and $D \rightarrow \text{const} D$), the range of the ”time” coordinate being $t > 0$. Equation \ref{3.10} gives (setting $H^\text{eff} = 0$) $h = \frac{1}{5} \beta t^{-2}$.

A slightly more sophisticated model is obtained by putting a massless scalar field $\phi$ into the FRW universe, thus $ds^2 = -da^2 + a^2 d\phi^2$ and $U = a^4 \Lambda$. The action is chosen as before $S = -\frac{1}{3} a^3 \sqrt{\Lambda} = -t$, whereas $D = t^{-1/2}$. The variable $\phi$ plays the role of the coordinates $\xi^A$, and applying \ref{3.10}–\ref{3.11} one easily finds $h = \frac{1}{2} t^{-2} (-\frac{1}{3} \partial_{\phi\phi} + \frac{1}{4})$. For any $t > 0$ this is a positive operator on the hypersurface $\Sigma_t$ (i.e. acting on functions $\chi(\phi)$). In more realistic models it is often extremely difficult to specify an exact solution of the Hamilton-Jacobi equation, but we can expect a $t^{-2}$ behaviour in $h$ to play a dominant role as well.

The general solution of the linear problem \ref{5.10} for $h = \beta t^{-2}$ may be expressed in terms of Bessel functions (Ref. \[22\], p. 358). Confining ourselves to the range $t > 0$ for the moment, the combination involving the second Hankel function

$$u = \sqrt{z} H^{(2)}_{\nu}(z) \equiv \sqrt{z} (J_{\nu}(z) - i Y_{\nu}(z))$$

with

$$z = \frac{t}{\epsilon} \quad \text{and} \quad \nu^2 = \frac{1}{4} - \frac{2\beta}{\epsilon}$$

is of the form \ref{5.17}, up to an irrelevant $\epsilon$-dependent factor. Expanding $u$ for small positive $\epsilon$ at constant $\nu$ and positive $t$ (i.e. using the asymptotic expansion of Bessel functions for $z \rightarrow \infty$) gives an expression of the structure $ce^{-it/\epsilon}$ where $c$ depends on $\nu$ and $\epsilon$ but not on $t$ (and is thus irrelevant for our purposes) and $v$ is a power series in $\epsilon$ that depends on $\nu$ only through $\nu^2$. Inserting the second equation of \ref{7.8} into $v$ yields a power series in $\epsilon$. Note that $\beta$ may be of either sign or zero, and $\nu$ will be real or imaginary, depending on the values of $\beta$ and $\epsilon$. The proposed solution for $H$ is given by $H = i \nu u^{-1} - \epsilon^{-1}$ or, likewise, by \ref{5.18}, its expansion in powers of $\epsilon$ reproducing the formal solution \ref{5.4} for $h = \beta t^{-2}$. In the closed expression for $H$, any of the two solutions for $\nu$ may be inserted because the ratio $H^{(2)}_{\nu}(z)^{-1} \partial_\nu H^{(2)}_{\nu}(z)$ is invariant under the substitution $\nu \rightarrow -\nu$. For fixed positive $\epsilon$, the ratio $H/h$ approaches unity in the limit $t \rightarrow \infty$. Due to singularities in
the Bessel functions, the closed expression is convenient only for positive $t$ and $\epsilon$. Nevertheless, the power series reveals that $H$ is analytic in $\beta$, $\epsilon$ and $t^{-1}$. Denoting this dependence by $H(\beta, \epsilon, t)$, the other ranges of variables are provided by the identities $H(\beta, \epsilon, -t) = H^*(\beta, \epsilon, t)$ and $H(\beta, -\epsilon, t) = -H^*(-\beta, \epsilon, t)$ where $\beta$, $\epsilon$ and $t$ are understood to be real. The simultaneous change of sign of these three variables changes the sign of $H$.

Example 6: $h = k + \beta t^{-2}$

This case may be treated in complete analogy to the previous one. The relevant solution of (5.16) is given by

$$u = \sqrt{t} H^{(2)}(ct) \quad \text{with} \quad c = \frac{1}{\epsilon \sqrt{1 + 2\epsilon k}} \quad (7.9)$$

and $\nu$ as before. The preferred decomposition is therefore defined by $H = iuu^{-1} - \epsilon^{-1}$. The factor $c$ replacing $\epsilon^{-1}$ in the argument of the Hankel function has the effect already encountered in the first example that the ratio $H/h$ does not approach unity but $(\epsilon k)^{-1}(\sqrt{1 + 2\epsilon k} - 1)$ for large $t$.

A further possible generalization is $h = k + \alpha t^{-1} + \beta t^{-2}$ which leads to Whittaker functions (Ref. [22], p. 505).

Example 7: $h$ being asymptotically constant in two regions

Here we would like to discuss an argument that might be raised against the existence of a preferred decomposition. Suppose $h$ is a c-number function of $t$ converging to a constant $h_\infty$ as $|t| \to \infty$ but undergoing some non-trivial smooth change at finite times. For simplicity we assume $h_\infty = 0$ and set $D = 1$. Naively, one would expect the form of the series (5.4) to indicate that $H$ vanishes asymptotically for large $|t|$. If this were true, the proposed decomposition could be thought of agreeing with the standard asymptotic flat space-type decomposition into positive and negative frequencies ($\psi^\pm \sim e^{\mp it}$) in the ”far past” region $t \to -\infty$ and at the same time it would agree with the according frequency decomposition (again $\psi^\pm \sim e^{\mp it}$) in the ”far future” region $t \to \infty$. However, we know that in case of a nontrivial time-dependence of $h$ in some intermediate region, these two frequency decompositions are different. This is because a wave function starting with, say, positive frequency in the far past ($\psi \sim e^{-it}$) will ”feel” the time-dependence of $h$ and in general evolve into a linear combination of both frequencies $e^{\pm it}$ at late times. (In terms of the physics of a scalar field, this indicates the production of particles by the time-dependent background. In terms of mathematics, it is represented by a Bogoljubov transformation). Thus, the argument states that the proposed preferred decomposition coincides with the two asymptotic ones which are however different: this is obviously a contradiction. The answer is presumably that the expectation $H \to 0$ in the asymptotic regions is in general not justified. In the Examples 4, 5 and 6 treated above, $h$ vanishes for large $|t|$ but has a singularity at $t = 0$, so that these cases are no good illustrations for the issue under consideration here.
A better example would be $h = \beta(1 + t^2/a^2)^{-1}$. In this case either $H$ does not exist (its formal series (5.4) diverging for all $\epsilon \neq 0$ and for all $t$) or does not vanish asymptotically. In any case, the non-local character of the principle specifying $H$ is clear. Although having no explicit example at hand, these considerations should illustrate how our proposal might be capable to transcent the point of view that a preferred decomposition necessarily relies on local geometric structures. In view of the speculations made in Section 6, the preferred decomposition — in case it exists — might turn out to be an average over the asymptotic frequency decompositions.

8 Relation to refined algebraic quantization?

The results achieved in this paper have been of a rather formal nature, and the precise condition under which they materialize into well-defined mathematical objects is not known (apart from the speculation that it refers to the global structure of minisuperspace and possibly has something to do with analyticity). This makes it difficult to re-express our findings in terms of an underlying structure or object for which the equations we wrote down are just representations with respect to local WKB-branches.

Nevertheless, in pursuing the subject, one might gain some unified view of what happens when different quantization and interpretation schemes are applied. As already mentioned in Section 2, the interpretational framework associated with the wave equation (2.2) can be based either on the $L^2$-scalar product $q$ from (2.7) or on the Klein-Gordon type scalar product $Q$ from (2.8), the latter being particularly appropriate for the scalar particle quantization picture. Our approach is in some sense a mixture between the use of $Q$ (which admits the notion of causal propagation on the manifold $\mathcal{M}$) and a proposal for solving the decomposition problem that is motivated by quantum cosmology and transcends the notion of causality.

This opens perspectives for a deeper understanding of the relation between various structures associated with the wave equation (2.2). With regards to our proposal for fixing a decomposition $I\mathcal{H} = I\mathcal{H}^+ \oplus I\mathcal{H}^-$, the most natural question seems to be whether the space $(I\mathcal{H}, Q_{\text{phys}}) \equiv (I\mathcal{H}^+, Q) \oplus (I\mathcal{H}^-, -Q)$ is closely related (or even identical to) the Hilbert space of physical states $(\mathcal{H}_{\text{phys}}, \langle | \rangle_{\text{phys}})$ as constructed by the refined algebraic quantization approach, i.e. to what extent the results achieved for the flat Klein-Gordon equation [3, 6, 7], as mentioned in Section 2, carry over to more general models. In the positive case, our approach seems to provide a piece of information that does not show up explicitly in the refined algebraic scheme, namely the decomposition, i.e. the natural appearance of two orthogonal subspaces $I\mathcal{H}^\pm$ spanning the whole of $I\mathcal{H}$. Even if the answer to this question is more complicated, one can reasonably expect to learn more about the relation between $Q$, $q$ and $\langle | \rangle_{\text{phys}}$. Eventually, one might be able to reconcile the different approaches in terms of a single, unified understanding of quantization.
Although we have not entered into the formalism of the refined algebraic quantization, there is a heuristic argument relating the inner (positive definite) product $\langle | \rangle_{\text{phys}}$ to the (indefinite) Klein-Gordon type scalar product $Q$. (A construction of the type we will now describe seems to have been written down first in the context of de Sitter space by Nachtmann long ago [11]. In a more general context a similar reasoning appears in the work of Rumpf and Urbantke [12]). Although the Hilbert space $\mathcal{H}_{\text{phys}}$ of physical states emerging in this quantization scheme is constructed in a rather abstract way, it seems likely [23] that it can be represented as a set of solutions to the wave equation (2.2) — modulo the issue of completion —, i.e. that it essentially agrees with $\mathcal{H}$. The space $\mathcal{H}$ thus carries two scalar products, $\langle | \rangle_{\text{phys}}$ and $Q$. We may find some basis $\{\Xi_r\}$ of wave functions which are orthonormal with respect to the former scalar product, i.e. $\langle \Xi_r | \Xi_s \rangle_{\text{phys}} = \delta_{rs}$. Generic states may be expanded as $\psi = \sum_r \psi_r \Xi_r$. The matrix $K_{rs} = Q(\Xi_r, \Xi_s)$ defines a linear operator $K$ by $(K\psi)_r = \sum_s K_{rs} \psi_s$ which relates the two scalar products by

$$Q(\psi, \phi) = \langle \psi | K \phi \rangle_{\text{phys}}. \quad (8.1)$$

The properties of $Q$ imply that the matrix $K_{rs}$ (and hence the operator $K$) is hermitean with respect to $\langle | \rangle_{\text{phys}}$ and invertible. (Actually $K$ is invertible if $Q$ is non-degenerate, i.e. if $Q(\psi, \phi) = 0$ for all $\psi$ implies $\phi = 0$. There are situations $(ds^2, U)$ in which this is not true, i.e. in which harmless initial data $(\psi|_\Sigma, n^a \nabla_a \psi|_\Sigma)$ may lead to an exponential blow-up with time and thus have to be excluded from $\mathcal{H}$. Accordingly, $Q(\psi, \phi) = 0$ for all $\psi \in \mathcal{H}$ with $\phi \neq 0$ becomes possible [14]. Although this is not likely to happen in reasonable quantum cosmological models, it restricts the number of mathematically admissible models for which our argument applies. Hence, we assume the model under consideration to be such that $Q$ is non-degenerate). If an operator $K$ defined by (8.1), it is unique because $\langle \psi | K \phi \rangle_{\text{phys}}$ is known for all $\psi$ and $\phi$, and its matrix elements with respect to the basis $\{\Xi_r\}$ are just $K_{rs}$. Since $K$ is invertible, its spectrum decays into a positive and a negative part. (Thereby we actually assume that $K$ is self-adjoint with respect to $\langle | \rangle_{\text{phys}}$, a point that should be made more rigorous in a deeper investigation). The space $\mathcal{H}$ may thus be expected to decompose into two subspaces $\mathcal{H}^\pm$, associated with the positive and negative part of the spectrum, respectively. In other words, $\mathcal{H}^\pm$ is spanned by the (generalized) eigenvectors of $K$ to positive/negative (generalized) eigenvalues (the latter appearing in pairs $(\lambda, -\lambda)$). In addition, there are good chances for the spectrum of $K$ to be bounded off zero. (For the flat Klein-Gordon equation only one pair $(\lambda, -\lambda)$ with $\lambda \neq 0$ occurs). The two subspaces $\mathcal{H}^\pm$ are orthogonal to each other with respect to $\langle | \rangle_{\text{phys}}$ and hence, using (8.1), also with respect to $Q$. Moreover, it is clear that if this construction can be made rigorous, complex conjugation maps $\mathcal{H}^+$ onto $\mathcal{H}^-$ and vice versa in a bijective way. This argument shows that the inner product $\langle | \rangle_{\text{phys}}$ is likely to serve as a structure in addition to the local geometry of minisuperspace and to single out a preferred decomposition. Since the procedure leading to $\langle | \rangle_{\text{phys}}$ in the refined algebraic quantization scheme is essentially unique, the decomposition derived from (8.1) should be unique as well.
Hence, it should rely on the "geometry" of minisuperspace in some \textit{global} sense. It is however unclear whether this decomposition coincides with the one proposed in Section 5, i.e. the one based on the formal solution \eqref{eq:5.4} for $H$.

This point — at least as a theoretical possibility — seems to have escaped the attention of several authors that have contributed to the development of the refined algebraic quantization approach. For example, Higuchi \cite{6} quotes Kuchař’s discussion \cite{8, 17} that the absence of symmetries of the Wheeler-DeWitt equation does not allow a unique separation of positive- and negative-frequency solutions and simply states that his method (which is essentially the refined algebraic approach) "does not require such a separation". Also, Ashtekar \textit{et al.} \cite{3} remark that the construction of $\mathcal{H}_\text{phys}$ (in the context of the Klein-Gordon equation on a curved background space-time) "may come as a surprise to some readers, as it seems to violate the accepted idea that there is no well-defined notion of a single particle in a non-stationary space-time". Their resolution of this paradox is that the new quantum theory "contains no notion of a conserved probability associated with Cauchy surfaces, as our particle appears to 'scatter backwards in time' when it encounters a lump of space-time curvature". However, when the heuristic argument given above holds, this situation is actually reversed: The mere co-existence of $Q$ and $\langle \, | \, \rangle_\text{phys}$ implies the existence of a unique preferred decomposition, and there \textbf{is} a well-defined notion of a conserved (not necessarily positive) probability-type density, provided by the scalar product $Q$ (namely the integrand of \eqref{eq:2.8}). What is missing in this framework is of course the notion of causality underlying the decomposition. Maybe one could say that the group average applied in this quantization procedure has singled out a decomposition by some kind of average of global type.

In the case of the flat Klein-Gordon equation we actually know the above argument to hold, and in addition we know that $K^2$ is a multiple of the identity operator ($\langle \, | \, \rangle_\text{phys}$ therefore being normalized such that $K^2 = 1$). This implies that $\langle \, | \, \rangle_\text{phys}$, when restricted to $\mathcal{H}^\pm$, is just $\pm Q$. We do not know whether this feature carries over to more general cases. In general, we can only give a symbolic expression for $K$. As already mentioned in Section 2, physical states are represented as $\psi_\text{phys} = \delta(C)\psi$ with $C$ the wave operator in \eqref{eq:2.2} and $\psi$ a more or less arbitrary function (not satisfying the wave equation). Defining an auxiliary operator $\tilde{K}$ by $(K\psi)_\text{phys} = \delta(C)\tilde{K}\psi$, one finds

$$\tilde{K} = -\frac{i}{2} \left\{ \delta_\Sigma, n^\alpha \nabla_\alpha \right\} \delta(C), \quad (8.2)$$

where $\Sigma$ is a hypersurface on which $Q$ is computed, $\delta_\Sigma(y)$ the $\delta$-function on $\Sigma$, such that $\int_\mathcal{M} d\mu \delta_\Sigma \varphi = \int_\Sigma d\Sigma \varphi$ for any (test)function $\varphi$ on $\mathcal{M}$, and $d\Sigma$ the scalar hypersurface element on $\Sigma$. The unit normal to $\Sigma$ is $n^\alpha$, so that $d\Sigma^\alpha = d\Sigma n^\alpha$ is the hypersurface element as used in \eqref{eq:2.8}. The expression \eqref{eq:8.2} — when treated rigorously — should be independent of $\Sigma$. In flat space, its Fourier transform may be written down explicitly, exhibiting the expression $\delta(k^\mu k_\mu + m^2)$. This is identical to $\frac{1}{2} k^\alpha k_\alpha (\delta(k_\alpha - \omega k_z) - \delta(k_\alpha + \omega k_z))$ with $\omega = (k^2 + m^2)^{1/2}$. This illustrates the origin of the change of sign in the negative frequency sector.
As stated above, it is unclear how our heuristic argument leading to $K$ relates to the formalism proposed in the main part of this paper, and how an *analyticity* condition might appear. The main condition for the refined algebraic quantization scheme to work is the self-adjointness of the wave operator $C$ with respect to the scalar product $(2.7)$, and this is essentially a condition on the metric and the potential, without any obvious relation to analyticity issues.

9 Outlook

There is another important issue that seems worth being pursued. In this paper we have confined ourselves to the case that the potential $U$ is positive everywhere in minisuperspace. As a consequence, the classical trajectories (whose tangent vector squared has the opposite sign as $U$) were always timelike, and we could clearly distinguish between incoming and outgoing modes at the classical level. Technically, we have used $\sqrt{U}$ in various expressions. However, in most realistic models the potential may take both signs. It is thus desirable to know how far the findings of this paper may be generalized for these models. One might still have a classically well-defined notion of outgoing and incoming trajectories (as long as $\mathcal{M}$ is foliated by spacelike hypersurfaces), but the classical trajectories would be spacelike in the $U < 0$ domains (which are sometimes called "Euclidean"). Thus, a classical trajectory could start with outgoing orientation, dive into a Euclidean domain and re-enter the $U > 0$ domain with incoming orientation. This might be a hint for the breakdown of the framework developed in this paper. In particular, evolution equations like $(3.23)$ would not easily be defined, and one might have to invoke the mathematics of signature changing metrics. Also, one could try to save the notion of decomposition by making it a local concept. On the other hand, the hints at analyticity playing a deep role in our framework open another possibility. Since analytic functions exist "as a whole", one could think of applying our formalism to the $U > 0$ region and look whether it naturally "extends" to the whole of $\mathcal{M}$ (maybe in some complexified sense). Note that, for example, by describing a hypersurface $\Sigma_t$ in terms of some (real) analytic function in the domain $U > 0$, a (complex) global behaviour is fixed at the same time. This might help clarifying the role of Euclidean domains and the complexified concepts (like Euclidean trajectories and Euclidean action) that are sometimes used in this field.

As a last issue we mention that the most ambitious goal would of course be to carry over our proposal to the framework of the Wheeler-DeWitt equation in full (rather than mini-) superspace. In the metric representation [24], one would have to deal with functional differential equations, and the analogues of evolution equations like $(3.23)$ and $(3.38)$ would be of the Schwinger-Tomonaga rather than the Schrödinger type, i.e. involve the feature of many-fingered time. Also, regularization issues are likely do make this a very hard job. As an alternative, one could try to work in the connection representation [25] and ask whether the notions of Klein-
Gordon type scalar product and decomposition can be given any sense therein.

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