Euclidean-signature semi-classical methods for quantum cosmology

Vincent Moncrief

ABSTRACT. We show how certain microlocal analysis methods, already well-developed for the study of conventional Schrödinger eigenvalue problems, can be extended to apply to the (mini-superspace) Wheeler-DeWitt equation for the quantized Bianchi type IX (or ‘Mixmaster’) cosmological model. We use the methods to construct smooth, globally defined expansions, for both ‘ground’ and ‘excited state’ wave functions, on the Mixmaster mini-superspace. We then review an expansive, ongoing program to further broaden the scope of such microlocal methods to encompass a class of interacting, bosonic quantum field theories and conclude with a discussion of the feasibility of applying this ‘Euclidean-signature semi-classical’ quantization program to the Einstein equations themselves — in the general, non-symmetric case — by exploiting certain established geometric results such as the positive action theorem.

1. Introduction

Einstein would almost surely never have approved of efforts to quantize his wondrous, geometric field equations. But the universal character of the gravitational interaction together with the undeniable necessity to quantize all other forms of matter and energy leads almost inexorably to the conclusion that the gravitational field itself should indeed be quantized. In addition to the natural demand for logical coherence in the formulation of fundamental physical laws as motivation for this pursuit there is the alluring potential benefit that quantum gravitational effects could ultimately furnish the agency needed to regularize not only the more troublesome, singular features of classical general relativity but perhaps also those of quantized matter systems as well. The fundamental nature of these challenging issues, together with the inconclusiveness of existing attempts at their resolution,

2010 Mathematics Subject Classification. 35A01, 83C05, 83C45, 83F05.

Key words and phrases. cosmological solutions, quantized cosmological model, mixmaster, Einstein equations, microlocal analysis.

© 2015 International Press
encourages one to search for new points of view towards the quantization problem.

Our aim herein is to explore the applicability of what we shall call ‘Euclidean-signature semi-classical’ analysis to the problem of solving, at least asymptotically, the Wheeler-DeWitt equation of canonical quantum gravity. Since this (functional differential) equation has, at present however, only a formal significance we shall begin by analyzing instead the mathematically well-defined model problem of constructing asymptotic solutions to the idealized Wheeler-DeWitt equation for spatially homogeneous, Bianchi type IX (or ‘Mixmaster’) universes. Though the (partial differential) Wheeler-DeWitt equation for this model problem was first formulated nearly a half century ago, techniques for solving it that bring to light the discrete, quantized character naturally to be expected for its solutions have, only recently, been developed. We shall show, in particular, how certain microlocal analytical methods, long since well-established for the study of conventional Schrödinger eigenvalue problems, can be modified in such a way as to apply to the (Mixmaster) Wheeler-DeWitt equation.

That some essential modification of the microlocal methods will be needed is evident from the fact that the Wheeler-DeWitt equation does not define an eigenvalue problem, in the conventional sense, at all. For closed universe models, such as those of Mixmaster type, all of the would-be eigenvalues of the Wheeler-DeWitt operator, whether for ‘ground’ or ‘excited’ quantum states, are required to vanish identically. But a crucial feature of standard microlocal methods, when applied to conventional Schrödinger eigenvalue problems, exploits the flexibility to adjust the eigenvalues being generated, order-by-order in an expansion in Planck’s constant, to ensure the smoothness of the eigenfunctions, being constructed in parallel, at the corresponding order. But if, as in the Wheeler-DeWitt problem, there are no eigenvalues to adjust, wherein lies the flexibility needed to ensure the required smoothness of the hypothetical eigenfunctions? And, by the same token, where are the ‘quantum numbers’ that one would normally expect to have at hand to label the distinct quantum states? The core of this paper is devoted to showing how the scope of microlocal methods can, in spite of this apparent impasse, be broadened to provide creditable, aesthetically appealing answers to such questions.

But the Mixmaster Wheeler-DeWitt equation is a quantum mechanical one whereas full Einstein gravity is a field theory. For reasons that we shall clarify later the microlocal methods alluded to above have, heretofore, been limited in applicability to Schrödinger operators defined on finite dimensional configuration spaces. The author, however, together with A. Marini and R. Maitra, has recently been engaged in further extending the scope of such methods to encompass certain (bosonic) relativistic field theories in a far-reaching program we refer to as ‘Euclidean-signature semi-classical’ analysis [1, 2, 3]. We shall review, in section 6 below, the current status of
this expansive, ongoing program, discussing in particular its applicability to self-interacting scalar and Yang-Mills fields on Minkowski spacetime.

With the backdrop of the aforementioned developments in mind it is natural to ask the question — could such (Euclidean-signature semi-classical) methods be applicable to the Wheeler-DeWitt equation of full canonical quantum gravity? Since research in this direction has only just begun we do not, by any means, have a conclusive answer to this overriding question. In the concluding section however we shall draw attention to several remarkably attractive features of such an approach and show, in particular, how it avoids some of the serious complications that obstructed progress on the, somewhat similar-in-spirit, Euclidean path integral approach to quantum gravity.

While Einstein most likely would not have approved of the ultimate aim of this research program he nevertheless himself initiated an elegant extension of the old Bohr quantization rules to classically integrable systems that has since, after subsequent refinements, come to be known as the Einstein-Brillouin-Keller (or EBK) approximation [4]. So perhaps he would have appreciated yet a different application of semi-classical methods to quantum systems — especially one that does not require classical integrability or even finite dimensionality for its implementation.

2. Mixmaster Spacetimes

The Bianchi IX, or ‘Mixmaster’ cosmological models are spatially homogeneous spacetimes defined on the manifold $S^3 \times \mathbb{R}$. Their metrics can be conveniently expressed in terms of a basis, $\{\sigma^i\}$, for the left-invariant one-forms of the Lie group $SU(2)$ which of course is diffeomorphic to the ‘spatial’ manifold under study. In a standard, Euler angle coordinate system for $S^3$ these basis one-forms can be written as:

\[
\begin{align*}
\sigma^1 &= \cos \psi d\theta + \sin \psi \sin \theta d\varphi, \\
\sigma^2 &= \sin \psi d\theta - \cos \psi \sin \theta d\varphi, \\
\sigma^3 &= d\psi + \cos \theta d\varphi
\end{align*}
\]

and satisfy

\[
(2.2) \quad d\sigma^i = \frac{1}{2} \epsilon_{ijk} \sigma^j \wedge \sigma^k
\]

where $\epsilon_{ijk}$ is completely anti-symmetric with $\epsilon_{123} = 1$.

In the absence of matter sources for the Einstein equations (i.e., in the so-called ‘vacuum’ case) it is well-known that the Mixmaster spacetime metric can always be put, after a suitable frame ‘rotation’, into diagonal form. Thus, without essential loss of generality, one can write the line element for
vacuum, Bianchi IX models in the form
\[ ds^2 = \gamma_{\mu\nu} dx^\mu dx^\nu \]
\[ = -N^2 dt^2 + \frac{L^2}{6\pi} e^{2\alpha} (e^{2\beta})_{ij} \sigma^i \sigma^j \]
where \( \{x^\mu\} = \{t, \theta, \varphi, \psi\} \) with \( t \in \mathbb{R}, e^{2\beta} \) is a diagonal, positive definite matrix of unit determinant and \( L \) is a positive constant with the dimensions of ‘length’.

In the notation introduced by Misner [5, 6] one writes
\[ (e^{2\beta}) = \begin{pmatrix} e^{2\beta_+ + 2\sqrt{3}\beta_-}, & e^{2\beta_+ - 2\sqrt{3}\beta_-}, & e^{-4\beta_+} \end{pmatrix} \]
and thereby expresses \( e^{2\beta} \) in terms of his (arbitrary, real-valued) anisotropy parameters \( \{\beta_+, \beta_-\} \). These measure the departure from ‘roundness’ of the homogenous, Riemannian metric on \( S^3 \) given by
\[ \gamma_{ij} dx^i \otimes dx^j := \frac{L^2}{6\pi} e^{2\alpha} (e^{2\beta})_{ij} \sigma^i \otimes \sigma^j \]
whereas the remaining (arbitrary, real-valued) parameter \( \alpha \) determines the sphere’s overall ‘size’ (in units of \( L \)).

To ensure spatial homogeneity the metric functions \( \{N, \alpha, \beta_+, \beta_-\} \) can only depend upon the time coordinate \( t \) which, for convenience, we take to be dimensionless. To ensure the uniform Lorentzian signature of the metric \( (4)g \) the ‘lapse’ function \( N \) must be non-vanishing (and, with our conventions, have the dimensions of length). Taken together the parameters \( \{\alpha, \beta_+, \beta_-\} \) coordinatize the associated ‘mini-superspace’ of spatially homogenous, diagonal Riemannian metrics on \( S^3 \). This minisuperspace is the natural configuration manifold for the Mixmaster dynamics.

In terms of Newton’s constant, \( G \), and the speed of light, \( c \), the Hilbert action functional is given by
\[ I_{\text{Hilbert}} := \frac{c^3}{16\pi G} \int_\Omega \sqrt{-\det (4)g} (4)R(4)g d^4x \]
where \((4)R(4)g\) is the scalar curvature of the metric \((4)g\) and \(\sqrt{-\det (4)g}\) its canonical 4-volume measure. When evaluated for metrics of the aforementioned, Bianchi IX, type on domains of the form \( \Omega \equiv S^3 \times I \), with \( I := [t_0, t_1] \subset \mathbb{R} \), the above integral specializes to
\[ I_{\text{Hilbert}} = \frac{c^3 L^3\pi}{G(6\pi)^{3/2}} \int_I dt \left\{ \frac{6e^{3\alpha}}{N} (-\dot{\alpha}^2 + \beta_+^2 + \beta_-^2) - \frac{6\pi Ne^{\alpha}}{2L^2} \left[ e^{-8\beta_+} - 4e^{-2\beta_+} \cosh (2\sqrt{3}\beta_-) + 2e^{4\beta_+} \left( \cosh (4\sqrt{3}\beta_-) - 1 \right) \right] + \frac{d}{dt} \left( \frac{6e^{3\alpha} \dot{\alpha}}{N} \right) \right\} \]
after the integration over the angular coordinates \( \{x^i\} = \{\theta, \varphi, \psi\} \) for \( S^3 \) has been carried out. Here \( \dot{\alpha} = \frac{d\alpha}{dt} \), etc., and the full set of Einstein equations
for these models results from independent variation of the metric functions \{N, \alpha, \beta_+, \beta_-\} subject to the requirement that their variations, together with that of \(\dot{\alpha}\), vanish at the boundary points of the interval \(I\) (i.e., at \(t = t_0\) and \(t = t_1\)). Under these constraints the final term in the integrand, \(\frac{d}{dt} \left( \frac{6e^{3\alpha}\dot{\alpha}}{N} \right)\), makes no contribution to the resulting equations of motion. Accordingly one is led to define the ADM (Arnowitt, Deser and Misner [7, 8]) action for Bianchi IX models by deleting it and setting

\[
I_{\text{ADM}} := \frac{c^3 L^3 \pi}{G(6\pi)^{3/2}} \int_I dt \left\{ \frac{6e^{3\alpha}}{N} (-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2) 
- \frac{(6\pi)Ne^\alpha}{2L^2} \left[ e^{-8\beta_+} - 4e^{-2\beta_+} \cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+}(\cosh(4\sqrt{3}\beta_-) - 1) \right] \right\}
\]

\[
:= \int_I L_{\text{ADM}} dt.
\]

The corresponding Hamiltonian formulation is arrived at via the Legendre transformation

\[
p_\alpha := \frac{\partial L_{\text{ADM}}}{\partial \dot{\alpha}} = -\frac{c^3 L^3 \pi}{G(6\pi)^{3/2}} \frac{12e^{3\alpha}\dot{\alpha}}{N}
\]

\[
p_+ := \frac{\partial L_{\text{ADM}}}{\partial \dot{\beta}_+} = \frac{c^3 L^3 \pi}{G(6\pi)^{3/2}} \frac{12e^{3\alpha}\dot{\beta}_+}{N}
\]

\[
p_- := \frac{\partial L_{\text{ADM}}}{\partial \dot{\beta}_-} = \frac{c^3 L^3 \pi}{G(6\pi)^{3/2}} \frac{12e^{3\alpha}\dot{\beta}_-}{N}.
\]

In terms of the canonical variables \(\{\alpha, \beta_+, \beta_-, p_\alpha, p_+, p_-\}\) the ADM action takes the form

\[
I_{\text{ADM}} = \int_I dt \left\{ p_\alpha \dot{\alpha} + p_+ \dot{\beta}_+ + p_- \dot{\beta}_- - N\mathcal{H}_\perp \right\}
\]

where

\[
\mathcal{H}_\perp := \frac{(6\pi)^{1/2}G}{4c^3 L^3 e^{3\alpha}} \left\{ (-p_\alpha^2 + p_+^2 + p_-^2) + \left( \frac{c^3}{G} \right) L^4 e^{4\alpha} \left[ \frac{e^{-8\beta_+}}{3} \right. 
- \frac{4e^{-2\beta_+}}{3} \cosh(2\sqrt{3}\beta_-) + \frac{2}{3} e^{4\beta_+}(\cosh(4\sqrt{3}\beta_-) - 1) \right] \right\}.
\]

Variation of the lapse function \(N\), which only appears now in ‘Lagrange multiplier’ form, leads to that Einstein equation known as the ‘Hamiltonian constraint’,

\[
\mathcal{H}_\perp(\alpha, \beta_+, \beta_-, p_\alpha, p_+, p_-) = 0,
\]
whereas variation of the canonical variables leads to the Hamiltonian evolution equations

\begin{align}
\dot{\alpha} &= \frac{\partial H_{\text{ADM}}}{\partial p_\alpha}, \\
\dot{\beta}_+ &= \frac{\partial H_{\text{ADM}}}{\partial p_+}, \\
\dot{\beta}_- &= \frac{\partial H_{\text{ADM}}}{\partial p_-} \\
\dot{p}_\alpha &= -\frac{\partial H_{\text{ADM}}}{\partial \alpha}, \\
\dot{p}_+ &= -\frac{\partial H_{\text{ADM}}}{\partial \beta_+}, \\
\dot{p}_- &= -\frac{\partial H_{\text{ADM}}}{\partial \beta_-}
\end{align}

with so-called super-Hamiltonian given by

\begin{equation}
H_{\text{ADM}} := NH_\perp.
\end{equation}

The choice of lapse function $N$ is essentially arbitrary but determines the coordinate ‘gauge’ by assigning a geometrical meaning to the time function $t$. For example the choice $N = L$ corresponds to taking $t = \frac{\tau}{L}$ where $\tau$ is ‘proper time’ normal to the hypersurfaces of spatial homogeneity. The Hamiltonian constraint, (2.12), is conserved in time by the evolution equations, (2.13, 2.14), independently of the choice of lapse.

Though the general solution to the Mixmaster equations of motion is not known, much is known about the dynamical behavior and asymptotics of the resulting spacetimes. One can show for example that each such cosmological model expands from a ‘big bang’ singularity of vanishing spatial volume, $\alpha \to -\infty$, a finite proper time in the past, achieves a momentary maximal volume at some finite proper time from the big bang and then ‘recollapses’ to another vanishing-volume, ‘big crunch’ singularity a finite proper time in the future [9, 10, 11, 12]. For the generic solution spacetime curvature can be proven to blow up at these singular boundaries [13] but some exceptional cases, so-called Taub universes [14, 15], develop (compact, null hypersurface) Cauchy horizons $\approx S^3$ instead of curvature singular boundaries and are analytically extendable through these horizons to certain acausal NUT (Newman, Unti, Tamburino) spacetimes that admit closed timelike curves [16, 17]. The inextendability of the generic, vacuum Mixmaster spacetime is consistent with Penrose’s (strong) cosmic censorship conjecture according to which the maximal Cauchy developments of generic, globally hyperbolic solutions to the (vacuum) Einstein field equations should not allow such acausal extensions.

The dynamical behavior of the generic solution to equations (2.12–2.14), between its big bang and big crunch singular boundaries, entails an infinite sequence of intricate ‘bounces’ of the evolving system point in mini-superspace, $(\alpha(t), \beta_+(t), \beta_-(t))$, off of the ‘walls’ provided by the potential energy function

\begin{equation}
\mathcal{U}(\alpha, \beta_+, \beta_-) := \frac{c^3(6\pi)^{1/2}Le^\alpha}{4G} \left[ \frac{e^{-8\beta_+}}{3} - \frac{4}{3} e^{-2\beta_+} \cosh (2\sqrt{3}\beta_-) + \frac{2}{3} e^{4\beta_+} \left( \cosh (4\sqrt{3}\beta_-) - 1 \right) \right]
\end{equation}
appearing in the gravitational super-Hamiltonian $H_{\text{ADM}} = N \mathcal{H}_\perp$. This sequence of bounces has been extensively analyzed with various analytical and numerical approximation methods beginning with the fundamental investigations of Belinskiǐ, Khalanikov and Lifshitz (BKL) [18, 19] and Misner [20]. The insights gained therefrom led Belinskiǐ, et al to the bold conjecture that the Mixmaster dynamics provides a paradigm for the behavior of a generic, non-symmetric cosmological model at a spacelike singular boundary [21, 22]. The study of such BKL oscillations within models of increasing generality and complexity is a continuing, significant research area within mathematical cosmology [23, 24, 25]. Though Newtonian definitions of ‘chaos’ do not strictly apply to the Mixmaster dynamical system certain natural extensions of this concept have led to the conclusion that Mixmaster dynamics is indeed ‘chaotic’ in a measurably meaningful sense [26, 27].

At the same time it has long been suspected that quantum effects should dramatically modify the nature of the Mixmaster evolutions especially when the evolving universe models reach a size comparable to the so-called Planck length, i.e., when $L\varepsilon \alpha$ becomes comparable to $L_{\text{Planck}} \simeq 1.616 \times 10^{-33}$ cm. This suspicion led Misner to initiate the study of Mixmaster quantum cosmology [6], the subject to which we now turn.

3. The Wheeler-DeWitt Equation for Mixmaster Universes

One can formally quantize the Mixmaster dynamical system described above by working in the Schrödinger representation wherein quantum states are expressed as ‘wave’ functions of the canonical coordinates, $\Psi(\alpha, \beta_+, \beta_-)$, and the conjugate momenta to these variables are replaced by differential operators:

\[
p_\alpha \rightarrow \hat{p}_\alpha := \frac{\hbar}{i} \frac{\partial}{\partial \alpha},
\]

\[
p_+ \rightarrow \hat{p}_+ := \frac{\hbar}{i} \frac{\partial}{\partial \beta_+},
\]

\[
p_- \rightarrow \hat{p}_- := \frac{\hbar}{i} \frac{\partial}{\partial \beta_-}.
\]

(3.1)

Here $\hbar = \frac{h}{2\pi}$ where $h$ is Planck’s constant given by $h \simeq 6.62606957 \times 10^{-27}$ erg \cdot sec.

In this picture one converts, after making a suitable choice of operator ordering, the classical Hamiltonian constraint function $\mathcal{H}_\perp$ into a quantum operator $\hat{\mathcal{H}}_\perp$ and imposes it, à la Dirac, as a fundamental constraint on the allowed quantum states by setting

\[
\hat{\mathcal{H}}_\perp \Psi = 0.
\]

(3.2)

Since this equation is an idealized, finite dimensional model for the formal equation proposed by Wheeler and DeWitt for full, non-symmetric, canonical quantum gravity (formulated on the infinite dimensional ‘superspace’ of
Riemannian geometries [28, 29]) we shall refer to it as the Wheeler-DeWitt (WDW) equation for Mixmaster spacetimes.

For simplicity we shall limit our attention here to a particular one-parameter family of operator orderings for $\hat{H}_\perp$, first introduced by Hartle and Hawking [30], and characterized by the specific substitutions

$$-e^{-3\alpha} p_\alpha^2 \longrightarrow \frac{\hbar^2}{e^{(3-B)\alpha}} \frac{\partial}{\partial \alpha} \left( e^{-B\alpha} \frac{\partial}{\partial \alpha} \right),$$

$$e^{-3\alpha} p_+^2 \longrightarrow -\frac{\hbar^2}{e^{3\alpha}} \frac{\partial^2}{\partial \beta_+^2},$$

$$e^{-3\alpha} p_-^2 \longrightarrow -\frac{\hbar^2}{e^{3\alpha}} \frac{\partial^2}{\partial \beta_-^2},$$

for the ‘kinetic energy’ terms appearing in $\hat{H}_\perp$. Here $B$ is an arbitrary real parameter whose specification determines a particular ordering of the family. For any such ordering the WDW equation can be written as

$$\left( \frac{L_{\text{Planck}}}{L} \right)^3 \left\{ e^{-(3-B)\alpha} \frac{\partial}{\partial \alpha} \left( e^{-B\alpha} \frac{\partial \Psi}{\partial \alpha} \right) - e^{-3\alpha} \left( \frac{\partial^2 \Psi}{\partial \beta_+^2} + \frac{\partial^2 \Psi}{\partial \beta_-^2} \right) \right\}$$

$$+ \left( \frac{L}{L_{\text{Planck}}} \right) e^\alpha \left[ \frac{e^{-8\beta_+}}{3} - \frac{4}{3} e^{-2\beta_+} \cosh (2\sqrt{3}\beta_-) \right.$$

$$\left. + \frac{2}{3} e^{4\beta_+} \left( \cosh (4\sqrt{3}\beta_-) - 1 \right) \right] \Psi$$

$$= 0$$

where $L_{\text{Planck}}$ is the Planck length defined by

$$L_{\text{Planck}} = \left( \frac{G\hbar}{c^3} \right)^{1/2} \simeq 1.616199 \times 10^{-33} \text{ cm}.$$

Notice that the arbitrary ‘length’ constant $L$ always occurs in the combination $Le^\alpha$ so that a change of its value merely corresponds to a shift of $\alpha$ by an additive constant.

Notice in addition that when the WDW equation, $\hat{H}_\perp \Psi = 0$, is imposed to constrain the allowed, so-called ‘physical’, quantum states, then the conventional Schrödinger equation, which would be expected to have the form

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}_{\text{ADM}} \Psi = N\hat{H}_\perp \Psi,$$

reduces to the seemingly mysterious implication that physical states do not evolve in ‘time’, i.e., to the conclusion that $\frac{\partial \Psi}{\partial t} = 0$.

This result is a reflection of the conceptual ‘problem of time’ in canonical quantum cosmology for the case of (spatially) closed universes. It leads one inexorably to the conclusion that actual temporal evolution must be measured not with respect to some external, ‘absolute’ time, as in Newtonian or even special relativistic physics, but rather with respect to some internal ‘clock’ contained within the system itself. The most obvious such clock
variable for the Mixmaster models is the logarithmic scale parameter $\alpha$ whose value, classically, determines the instantaneous spatial ‘size’ of the model universe and which, again classically, evolves in an almost monotonic fashion. More precisely $\alpha$ increases monotonically during the epoch of cosmological expansion, stops for an instant at the moment of maximal volume and then decreases monotonically during the followup epoch of cosmological collapse until the final ‘big crunch’.

But, as Misner was the first to realize, the Wheeler-DeWitt equation for Mixmaster models does not have Schrödinger form and so many of the usual constructions, familiar from ordinary quantum mechanics, such as the eigenfunctions and eigenvalues of a self-adjoint Hamiltonian operator acting on a naturally associated Hilbert space of quantum states and the conservation, in ‘time’, of the Hilbert space norm of such evolving states, no longer seem to apply. The Wheeler-DeWitt equation is indeed a wave equation (though not one of Schrödinger type), but where is the discreteness, expected of a normal quantum system, to be found among its solutions?

In the sections to follow we shall bring certain microlocal analysis techniques, already well-developed for the study of conventional Schrödinger eigenvalue problems [31, 32, 33, 1], to bear on such questions and show how these techniques can indeed be extended to apply to the Mixmaster Wheeler-DeWitt equation.

At first sight though it is not apparent that such microlocal methods can be applied at all. In particular, for a conventional Schrödinger eigenvalue problem, they make crucial use of the freedom to adjust the eigenvalues under construction, order-by-order in an expansion in Planck’s constant, to ensure the global smoothness of the eigenfunctions being generated at the corresponding order. But for the Wheeler-DeWitt problem all eigenvalues of $\hat{\mathcal{H}}_{\perp}$, whether for ‘ground’ or ‘excited’ states (whatever those terms might ultimately be taken to mean) are required to vanish to all orders with no flexibility whatsoever. And if no meaningful eigenvalues can be defined wherein are the ‘quanta’ naturally demanded of a quantized system?

As we shall see however the special structure of the Wheeler-DeWitt operator, $\hat{\mathcal{H}}_{\perp}$, and the fact that it is not of Schrödinger type, comes to the rescue and allows one to generate smooth, globally defined expansions (to all orders in Planck’s constant) for both ground and excited states. These states are labeled by a pair of non-negative integers that can be naturally interpreted as graviton excitation numbers for the ultra-long-wavelength gravitational waves modes represented by the quantum dynamics of the anisotropy degrees of freedom, $\beta_+$ and $\beta_-$.

4. Microlocal Techniques for the Mixmaster Wheeler-DeWitt Equation

In view of the resemblance of $\hat{\mathcal{H}}_{\perp}$ to a conventional Schrödinger operator one is motivated to propose a ‘ground state’ wave function of real, nodeless
type and thus to introduce an ansatz of the form

\( (4.1) \quad \Psi_\hbar = e^{-S_\hbar / \hbar} \),

where \( S_\hbar = S_\hbar(\alpha, \beta_+, \beta_-) \) is a real-valued function on the Mixmaster mini-superspace having the dimensions of ‘action’. It will be convenient to define a dimensionless stand-in for \( S_\hbar \) by setting

\( (4.2) \quad S_\hbar := \frac{G}{c^3 L^2} S_\hbar \)

and to assume that \( S_\hbar \) admits a formal expansion in powers of the dimensionless ratio

\( (4.3) \quad X := \frac{L^2_{\text{Planck}}}{L^2} = \frac{G \hbar}{c^3 L^2} \)

given by

\( (4.4) \quad S_\hbar = S_{(0)} + X S_{(1)} + \frac{X^2}{2!} S_{(2)} + \cdots + \frac{X^k}{k!} S_{(k)} + \cdots \)

so that \( \Psi_\hbar \) now becomes

\( (4.5) \quad \Psi_\hbar = e^{-\frac{1}{X} S_{(0)} - S_{(1)} - \frac{X}{2} S_{(2)} - \cdots} \).

Substituting this ansatz into the Wheeler-DeWitt equation, \( \hat{H} \Psi_\hbar = 0 \), and requiring satisfaction, order-by-order in powers of \( X \) leads immediately to the sequence of equations:

\( (4.6) \quad \left( \frac{\partial S_{(0)}}{\partial \alpha} \right)^2 - \left( \frac{\partial S_{(0)}}{\partial \beta_+} \right)^2 - \left( \frac{\partial S_{(0)}}{\partial \beta_-} \right)^2 + e^{4\alpha} \left[ \frac{e^{-8\beta_+}}{3} - \frac{4}{3} e^{-2\beta_+} \cosh (2\sqrt{3}\beta_-) + \frac{2}{3} e^{4\beta_+} \left( \cosh (4\sqrt{3}\beta_-) - 1 \right) \right] = 0, \)

\( (4.7) \quad 2 \left[ \frac{\partial S_{(0)}}{\partial \alpha} \frac{\partial S_{(1)}}{\partial \alpha} - \frac{\partial S_{(0)}}{\partial \beta_+} \frac{\partial S_{(1)}}{\partial \beta_+} - \frac{\partial S_{(0)}}{\partial \beta_-} \frac{\partial S_{(1)}}{\partial \beta_-} \right] + B \frac{\partial S_{(0)}}{\partial \alpha} - \frac{\partial^2 S_{(0)}}{\partial \alpha^2} + \frac{\partial^2 S_{(0)}}{\partial \beta_+^2} + \frac{\partial^2 S_{(0)}}{\partial \beta_-^2} = 0, \)
and, for \( k \geq 2 \),

\[
2 \left[ \frac{\partial S_0}{\partial \alpha} \frac{\partial S_k}{\partial \alpha} - \frac{\partial S_0}{\partial \beta_+} \frac{\partial S_k}{\partial \beta_+} - \frac{\partial S_0}{\partial \beta_-} \frac{\partial S_k}{\partial \beta_-} \right] \\
+ k \left[ B \frac{\partial S_{k-1}}{\partial \alpha} - \frac{\partial^2 S_{k-1}}{\partial \alpha^2} + \frac{\partial^2 S_{k-1}}{\partial \beta_+^2} + \frac{\partial^2 S_{k-1}}{\partial \beta_-^2} \right] \\
+ \sum_{\ell=1}^{k-1} \frac{k!}{\ell!(k-\ell)!} \left( \frac{\partial S_\ell}{\partial \alpha} \frac{\partial S_{k-\ell}}{\partial \alpha} - \frac{\partial S_\ell}{\partial \beta_+} \frac{\partial S_{k-\ell}}{\partial \beta_+} - \frac{\partial S_\ell}{\partial \beta_-} \frac{\partial S_{k-\ell}}{\partial \beta_-} \right) = 0.
\]

One recognizes Eq. (4.6) as the Euclidean signature analogue of the Hamilton-Jacobi equation for Mixmaster spacetimes that results from making the canonical substitutions

\[
p_\alpha \rightarrow \frac{\partial S}{\partial \alpha} = \frac{c^3 L^2}{G} \frac{\partial S}{\partial \alpha}, \\
p_+ \rightarrow \frac{\partial S}{\partial \beta_+} = \frac{c^3 L^2}{G} \frac{\partial S}{\partial \beta_+}, \\
p_- \rightarrow \frac{\partial S}{\partial \beta_-} = \frac{c^3 L^2}{G} \frac{\partial S}{\partial \beta_-}
\]

for the momenta in the Euclidean signature Hamiltonian constant, \( \mathcal{H}_{\perp \text{Eucl}} = 0 \), where

\[
\mathcal{H}_{\perp \text{Eucl}} := \frac{(6\pi)^{1/2} G}{4c^3 L^3 e^{3\alpha}} \left\{ (p_\alpha - p_+^2 - p_-^2) \right. \\
+ \left. \left( \frac{c^3}{G} \right)^2 L^4 e^{4\alpha} \left[ \frac{e^{-8\beta_+}}{3} - \frac{4}{3} e^{-2\beta_+} \cosh (2\sqrt{3}\beta_-) \right] \right. \\
+ \left. \frac{2}{3} e^{4\beta_+} \left( \cosh (4\sqrt{3}\beta_-) - 1 \right) \right\}.
\]

This expression results from repeating the derivation of \( I_{\text{ADM}} \) given in Sect. 2, but now for a Euclidean signature Bianchi IX metric,

\[
(4) g_{\mu\nu}|_{\text{Eucl}} \, dx^\mu \otimes dx^\nu = N|_{\text{Eucl}}^2 \, dt \otimes dt + \frac{L^2}{6\pi} e^{2\alpha} (e^{2\beta})_{ij} \sigma^i \otimes \sigma^j,
\]

and differs from Eq. (2.11) only in the sign of the kinetic energy term.

The remaining equations (4.7, 4.8) are linear ‘transport’ equations to be integrated along the flow generated by a solution for \( S_0 \) to sequentially determine the quantum corrections \( \{ S_k, k = 1, 2, \ldots \} \) in the formal expansion (4.4) for \( S_0 \).

There are two known, globally defined, smooth solutions to Eq. (4.6) that share the rotational symmetry of the Wheeler-DeWitt operator under rotations by \( \pm \frac{2\pi}{3} \) in the \( \beta \)-plane. By virtue of the geometrical characters
of the Euclidean signature ‘spacetimes’ they respectively generate they are sometimes referred to as the ‘wormhole’ solution,

\[(4.12) \quad S_{(0)}^{\text{wh}} := \frac{1}{6} e^{2\alpha} \left( e^{-4\beta_+} + 2e^{2\beta_+} \cosh (2\sqrt{3}\beta_-) \right), \]

and the ‘no boundary’ solution

\[(4.13) \quad S_{(0)}^{\text{nb}} := \frac{1}{6} e^{2\alpha} \left[ \left( e^{-4\beta_+} + 2e^{2\beta_+} \cosh (2\sqrt{3}\beta_-) \right) \right. \]
\[\left. -2 \left( e^{2\beta_+} + 2e^{-\beta_+} \cosh (\sqrt{3}\beta_-) \right) \right]. \]

The first of these was discovered in the present context by Ryan and the author in [34] and independently, in a somewhat related, but supersymmetric setting by Graham in [35] who then, together with Bene, proceeded to construct the second solution [36, 37]. An additional, non-symmetric solution, together with its (geometrically equivalent) images under \( \pm \frac{2\pi}{3} \) rotations in the \( \beta \)-plane, was later uncovered by Barbero and Ryan in a systematic, further search [38].

On the other hand the Euclidean signature Mixmaster ‘spacetimes’ generated by these various solutions, together with a characterization of their global geometric properties, were actually known much earlier, having been discovered through extensive searches for self-dual-curvature solutions to the field equations by Gibbons and Pope in [39] and by Belinski\’\i et al. in [40]. With respect to a certain time function \( \eta \), which corresponds to our choice

\[(4.14) \quad N|_{\text{Eucl}} = \frac{Le^{3\alpha}}{(6\pi)^{1/2}} \]

for the Euclidean signature lapse, these authors found that the metric functions

\[(4.15) \quad \omega_1 := e^{2\alpha - \beta_+ - \sqrt{3}\beta_-} \]
\[\omega_2 := e^{2\alpha - \beta_+ + \sqrt{3}\beta_-} \]
\[\omega_3 := e^{2\alpha + 2\beta_+} \]

satisfied the evolution equations

\[(4.16) \quad \frac{d\omega_1}{d\eta} = \omega_2\omega_3, \]
\[\frac{d\omega_2}{d\eta} = \omega_1\omega_3, \]
\[\frac{d\omega_3}{d\eta} = \omega_1\omega_2 \]
for the ‘wormhole’ family and
\[
\begin{align*}
\frac{d\omega_1}{d\eta} &= \omega_2\omega_3 - \omega_1(\omega_2 + \omega_3), \\
\frac{d\omega_2}{d\eta} &= \omega_1\omega_3 - \omega_2(\omega_1 + \omega_3), \\
\frac{d\omega_3}{d\eta} &= \omega_1\omega_2 - \omega_3(\omega_1 + \omega_2)
\end{align*}
\]
(4.17)
for the ‘no boundary’ family. One can easily recover these flow equations from our Hamilton-Jacobi formalism by making the substitutions (4.9) and (4.14) for \(\{p_\alpha, p_+, p_\}\) and \(N|_{\text{Eucl}}\) in the Euclidean signature Hamilton equations
\[
\begin{align*}
\dot{\alpha} &= \frac{(6\pi)^{1/2}G}{2c^3L^3e^{3\alpha}}N|_{\text{Eucl}} p_\alpha \\
\dot{\beta}_+ &= -\frac{(6\pi)^{1/2}G}{2c^3L^3e^{3\alpha}}N|_{\text{Eucl}} p_+ \\
\dot{\beta}_- &= -\frac{(6\pi)^{1/2}G}{2c^3L^3e^{3\alpha}}N|_{\text{Eucl}} p_-
\end{align*}
\]
(4.18) - (4.20)
and choosing \(S = S_{\text{wh}}^{(0)}\) or \(S = S_{\text{nb}}^{(0)}\) accordingly.

Because of its remarkable correspondence to the Euler equations for an asymmetric top [41] the ‘Euler’ system (4.16) was integrated long ago by Abel and Jacobi in terms of elliptic functions [39, 42, 43]. But system (4.17) also long predated general relativity having been discovered by Darboux in connection with a pure geometry problem [44]. This ‘Darboux’ system was subsequently integrated by Halphen [45] and later Bureau [46] in terms of Hermite modular elliptic functions. Both systems also occur as reductions of the self-dual Yang-Mills equations [42, 43].

Since the asymptotically Euclidean behavior of the wormhole ‘space-times’, as elucidated by Belinskiê, et al. in [40] and by Gibbons and Pope in [39], fits most naturally with our current perspective on appropriate boundary conditions for a ground state wave function \(\Psi_h\) we shall focus exclusively on the ‘wormhole’ solution, \(S_{\text{wh}}^{(0)}\), and its associated ‘flow’, in the analysis to follow. It is worth remarking however that the same (microlocal) methods could also be brought to bear on the ‘no boundary’ solution, \(S_{\text{nb}}^{(0)}\), and its ‘flow’.

Though the classical solution to the Euler system (4.16) entails elliptic functions [39, 40], J. Bae was recently able, using a choice for the Euclidean signature lapse proposed by the author, to reintegrate this system purely in terms of elementary functions and thus to simplify some of the subsequent analysis [47]. With the lapse function taken to be
\[
N|_{\text{Eucl}} = \frac{-Le^{\alpha-2\beta_+}}{(2\pi)^{1/2}}
\]
(4.21)
the wormhole flow equations become

\[
\begin{align*}
\frac{d\beta_-}{dt} &= \sinh (2\sqrt{3}\beta_-), \\
\frac{d\beta_+}{dt} &= -\frac{1}{\sqrt{3}} \left( e^{-6\beta_+} - \cosh (2\sqrt{3}\beta_-) \right), \\
\frac{d\alpha}{dt} &= -\frac{1}{2\sqrt{3}} \left( e^{-6\beta_+} + 2 \cosh (2\sqrt{3}\beta_-) \right)
\end{align*}
\]

and can be readily integrated in the order given.\(^1\)

In terms of initial values \(\{\alpha_0, \beta_{+0}, \beta_{-0}\}\) prescribed at \(t = 0\) Bae’s solution is expressible as

\[
\begin{align*}
e^{12\alpha(t)} &= e^{12\alpha_0 - 6\beta_{+0}} H_+ (h_+ h_-)^2, \\
e^{6\beta_+(t)} &= \frac{H_+}{h_+ h_-}, \\
e^{2\sqrt{3}\beta_-(t)} &= \frac{h_+}{h_-}
\end{align*}
\]

where

\[
\begin{align*}
H_+ &= e^{6\beta_{+0}} - \cosh (2\sqrt{3}\beta_{-0}) + \frac{1}{2}(h_+^2 + h_-^2) \\
&= e^{6\beta_{+0}} + (h_\pm)^2 - (h_{\mp0})^2, \\
h_+ &= e^{-\sqrt{3}t} \cosh (\sqrt{3}\beta_{-0}) + e^{\sqrt{3}t} \sinh (\sqrt{3}\beta_{-0}), \\
h_- &= e^{-\sqrt{3}t} \cosh (\sqrt{3}\beta_{-0}) - e^{\sqrt{3}t} \sinh (\sqrt{3}\beta_{-0}).
\end{align*}
\]

Several useful identities that follow from these formulas are given by

\[
\begin{align*}
\cosh (2\sqrt{3}\beta_-(t)) &= \frac{h_+^2 + h_-^2}{2h_+ h_-}, \\
e^{2\alpha(t)+2\beta_+(t)} &= e^{2\alpha_0 - 2\beta_{+0}} \sqrt{H_+}, \\
e^{4\alpha(t)-2\beta_+(t)} &= e^{4\alpha_0 - 2\beta_{+0}} h_+ h_-.
\end{align*}
\]

It is not difficult to verify that every solution is globally, smoothly defined on a maximal interval of the form \((-\infty, t_*)\) where \(t_*>0\) so that, in particular, every solution curve is well-defined on the sub-interval \((-\infty, 0]\). Furthermore \(\beta_+(t)\) and \(\beta_-(t)\) each decay exponentially rapidly to zero as \(t \to -\infty\) with

\[
\beta_\pm(t) \sim \text{const}_\pm e^{2\sqrt{3}t}
\]

while \(\alpha\) diverges, asymptotically linearly,

\[
\alpha(t) \sim -\frac{\sqrt{3}}{2} t + \text{const}
\]

\(^1\)Since the chosen lapse (4.21) does not share the triangular symmetry of \(S^{(0)}_{n0}\) in the \(\beta\)-plane, geometrically equivalent solutions to the flow equations (4.22–4.24) will often be parametrized differently.
in this limit. This behavior of the solution curves will play a crucial role in the integration of the transport equations (4.7, 4.8).

It is worth noting that one can linearize the β-plane flow equations (4.22–4.23) through an explicit transformation to ‘Sternberg coordinates’ \( \{y_+, y_-\} \) in terms of which these equations reduce to

\[
\frac{dy_+}{dt} = 2\sqrt{3}y_+, \quad \frac{dy_-}{dt} = 2\sqrt{3}y_-.
\]

These Sternberg coordinates are defined by

\[
y_+ = \frac{1}{6} \left( \frac{e^{6\beta} - \cosh(2\sqrt{3}\beta_-)}{\cosh^2(\sqrt{3}\beta_-)} \right),
\]

\[
y_- = \frac{1}{\sqrt{3}} \frac{\sinh(\sqrt{3}\beta_-)}{\cosh(\sqrt{3}\beta_-)}.
\]

which has the explicit inverse

\[
e^{6\beta} = 3y_+ + (3y_+ + 1) \left( \frac{1 + 3y_+^2}{1 - 3y_+^2} \right),
\]

\[
e^{2\sqrt{3}\beta_-} = \frac{1 + \sqrt{3}y_-}{1 - \sqrt{3}y_-}
\]

and maps the β-plane diffeomorphically onto the ‘strip’ given by

\[
\frac{-1}{\sqrt{3}} < y_- < \frac{1}{\sqrt{3}},
\]

\[
y_+ > -\frac{1}{6}(1 + y_-^2).
\]

Taking \( S_{(0)} = S_{(0)}^{wh} \) Bae found a particular solution to the first transport equation (4.7) given by

\[
S_{(1)} = -\frac{1}{2}(B + 6)\alpha.
\]

Though one would be free to add an arbitrary solution to the corresponding homogeneous equation we shall reserve such flexibility for the subsequent construction of excited states, retaining Bae’s particular solution as the natural choice to make for a ground state.

The ensuing transport equations (4.8) can now be solved inductively by making the ansatz

\[
S_{(k)}^{wh} = 6e^{-2(k-1)\alpha}\Sigma_{(k)}^{wh}(\beta_+, \beta_-)
\]

for \( k = 2, 3, \ldots \) and, for convenience, defining

\[
\Sigma_{(0)}^{wh} = e^{-4\beta_+} + 2e^{2\beta_+} \cosh(2\sqrt{3}\beta_-)
\]

so that

\[
S_{(0)}^{wh} = \frac{e^{2\alpha}}{6}\Sigma_{(0)}^{wh}(\beta_+, \beta_-).
\]
The resulting transport equations for the $\Sigma_{(k)}^{\text{wh}}$'s now take the form

\begin{equation}
\frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} + \frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_-} + 4 \Sigma_{(0)}^{\text{wh}} \Sigma_{(2)}^{\text{wh}} = \left(9 - \frac{B^2}{4}\right),
\end{equation}

\begin{equation}
\frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} + \frac{\partial \Sigma_{(3)}^{\text{wh}}}{\partial \beta_-} + 8 \Sigma_{(0)}^{\text{wh}} \Sigma_{(3)}^{\text{wh}} = 9 \left[\frac{\partial^2 \Sigma_{(2)}^{\text{wh}}}{\partial \beta^2_+} + \frac{\partial^2 \Sigma_{(2)}^{\text{wh}}}{\partial \beta^2_-} + 8 \Sigma_{(2)}^{\text{wh}}\right],
\end{equation}

and, for all $k \geq 4$:

\begin{equation}
\frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} + \frac{\partial \Sigma_{(k)}^{\text{wh}}}{\partial \beta_-} + 4(k - 1) \Sigma_{(0)}^{\text{wh}} \Sigma_{(k)}^{\text{wh}} = 3k \left[\frac{\partial^2 \Sigma_{(k-1)}^{\text{wh}}}{\partial \beta^2_+} + \frac{\partial^2 \Sigma_{(k-1)}^{\text{wh}}}{\partial \beta^2_-} - (k - 2)(4(k - 2) - 12) \Sigma_{(k-1)}^{\text{wh}}\right]
\end{equation}

\begin{equation}
+ \sum_{\ell=2}^{k-2} \frac{18k!}{\ell!(k - \ell)!} \left[4(\ell - 1)(k - \ell - 1) \Sigma_{(\ell)}^{\text{wh}} \Sigma_{(k-\ell)}^{\text{wh}} - \left(\frac{\partial \Sigma_{(\ell)}^{\text{wh}}}{\partial \beta_+} \frac{\partial \Sigma_{(k-\ell)}^{\text{wh}}}{\partial \beta_-} + \frac{\partial \Sigma_{(\ell)}^{\text{wh}}}{\partial \beta_-} \frac{\partial \Sigma_{(k-\ell)}^{\text{wh}}}{\partial \beta_+}\right)\right].
\end{equation}

Noting that

\begin{equation}
\frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} = -4e^{-4\beta_+} + 4e^{2\beta_+} \cosh (2\sqrt{3}\beta_-)
\end{equation}

and

\begin{equation}
\frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_-} = 4\sqrt{3}e^{2\beta_+} \sinh (2\sqrt{3}\beta_-)
\end{equation}

both vanish at the origin whereas

\begin{equation}
\Sigma_{(0)}^{\text{wh}}(0,0) = 3
\end{equation}

it follows from equations (4.47–4.49) that any set of smooth solutions would have to satisfy

\begin{equation}
\Sigma_{(2)}^{\text{wh}}(0,0) = \frac{1}{12} \left(9 - \frac{B^2}{4}\right),
\end{equation}

\begin{equation}
\Sigma_{(3)}^{\text{wh}}(0,0) = \frac{3}{8} \left[\frac{\partial^2 \Sigma_{(2)}^{\text{wh}}}{\partial \beta^2_+} + \frac{\partial^2 \Sigma_{(2)}^{\text{wh}}}{\partial \beta^2_-} + 8 \Sigma_{(2)}^{\text{wh}}\right](0,0),
\end{equation}
and

\[ \Sigma^{\text{wh}}_{(k)}(0, 0) = \left\{ \begin{array}{l}
\frac{k}{4(k-1)} \left[ \frac{\partial^2 \Sigma^{\text{wh}}_{(k-1)}}{\partial \beta_+^2} + \frac{\partial^2 \Sigma^{\text{wh}}_{(k-1)}}{\partial \beta_-^2} - (k - 2) (4(k - 2) - 12) \Sigma^{\text{wh}}_{(k-1)} \right] \\
+ \frac{3}{2(k-1)} \sum_{\ell=2}^{k-2} \frac{k!}{\ell!(k-\ell)!} \left[ 4(\ell - 1)(k - \ell - 1) \Sigma^{\text{wh}}_{(\ell)} \right] \left[ \frac{\partial \Sigma^{\text{wh}}_{(k-\ell)}}{\partial \beta_+} + \frac{\partial \Sigma^{\text{wh}}_{(k-\ell)}}{\partial \beta_-} \right]
\end{array} \right\} (0, 0) \] (4.55)

\[ \forall k \geq 4. \]

From equations (4.22–4.23, 4.50–4.51) one easily verifies that

\[ 1 = \frac{1}{4\sqrt{3}} e^{-2\beta_+} \left( \frac{\partial \Sigma^{\text{wh}}_{(0)}}{\partial \beta_+} + \frac{\partial \Sigma^{\text{wh}}_{(0)}}{\partial \beta_-} \right) = \frac{d\Sigma^{\text{wh}}_{(k)}}{dt} \] (4.56)

along the flow generated by \( \mathcal{S}^{\text{wh}}_{(0)} \). Thus multiplying each of equations (4.47, 4.48, 4.49) by \( \frac{1}{4\sqrt{3}} e^{-2\beta_+} \) and exploiting equation (4.24) to reexpress a term on the left hand side converts it to the first order, linear ‘transport’ form

\[ \frac{d\Sigma^{\text{wh}}_{(k)}}{dt} + 4(k - 1) \Sigma^{\text{wh}}_{(k)} \frac{1}{4\sqrt{3}} \left( e^{-6\beta_+} + 2 \cosh (2\sqrt{3}\beta_-) \right) \] (4.57)

where \( \Lambda_{(k)} \) denotes the right hand side of the original equation multiplied by \( \frac{1}{4\sqrt{3}} e^{-2\beta_+} \). This ‘source’ term for \( \Sigma^{\text{wh}}_{(k)} \) will be smooth provided that \( \left\{ \Sigma^{\text{wh}}_{(2)}, \ldots, \Sigma^{\text{wh}}_{(k-1)} \right\} \) are each globally smooth.

An integrating factor for equation (4.57) is now easily seen to be

\[ \mu_{(k)}(t) = \frac{e^{-2(k-1)\alpha(t)}}{e^{-2(k-1)\alpha(0)}} \] (4.58)

and has the important property of vanishing exponentially rapidly in \( t \) as \( t \searrow -\infty \) along an arbitrary solution curve of the flow equations (4.22–4.24).

The strategy for computing \( \Sigma^{\text{wh}}_{(k)} \) at an arbitrary point \((\beta_+, \beta_-)\) in the \( \beta \)-plane is now as follows: integrate equation (4.57) along the solution curve ‘beginning’ at \((\beta_+, \beta_-)\) at \( t = 0 \) and adjust the ‘initial value’, \( \Sigma^{\text{wh}}_{(k)}(\beta_+, \beta_-) \), of this function in such a way as to ensure that its asymptotically attained limit has the pre-determined value given for it in equations (4.53–4.55) above, i.e., that

\[ \Sigma^{\text{wh}}_{(k)}(0, 0) = \lim_{t \searrow -\infty} \Sigma^{\text{wh}}_{(k)}(\beta_+(t), \beta_-(t)). \] (4.59)
Finally, verify the smoothness of the function so constructed and proceed, inductively, to the subsequent order.

Applying the technique first to $\Sigma^{\text{wh}}_{(2)}$ one finds that

\begin{equation}
\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0) = \left\{ \frac{\left( \frac{9-B^2}{4} \right)}{4\sqrt{3}} \int_{-\infty}^{0} ds \ e^{-2(\alpha(s)-\alpha(0))-2\beta+0(s)} \right\}
\end{equation}

$\forall \ t \leq 0$. In view of the asymptotic vanishing of the denominator as $t \searrow -\infty$ there is only one choice for $\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0)$ that can yield a finite value for $\Sigma^{\text{wh}}_{(2)}(0,0)$ in this limit, namely:

\begin{equation}
\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0) = \frac{\left( \frac{9-B^2}{4} \right)}{4\sqrt{3}} \int_{-\infty}^{t} ds \ e^{-2(\alpha(s)-\alpha(0))-2\beta+0(s)}.
\end{equation}

This integral converges for any $(\beta+0, \beta-0)$ by virtue of the exponential decay of the integrating factor along the corresponding solution curve. With the choice (4.61) for ‘initial condition’ the formula for $\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0)$ simplifies to

\begin{equation}
\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0) = \left\{ \frac{\left( \frac{9-B^2}{4} \right)}{4\sqrt{3}} \int_{-\infty}^{t} ds \ e^{-2(\alpha(s)-\alpha(0))-2\beta+0(s)} \right\}
\end{equation}

and a straightforward application of L’Hôpital’s rule shows that this solution has the desired limit (4.53) as $t \searrow -\infty$.

Substituting the explicit expressions (4.25–4.30) for the solution curves into (4.61) one arrives at the formula

\begin{equation}
\Sigma^{\text{wh}}_{(2)}(\beta+0, \beta-0) = \left\{ \frac{\left( \frac{9-B^2}{4} \right)}{4\sqrt{3}} \int_{-\infty}^{t} ds \ e^{-2(\alpha(s)-\alpha(0))-2\beta+0(s)} \right\}
\end{equation}

from which it is easily seen that one can differentiate arbitrarily many times with respect to $\beta+0$ and $\beta-0$ without disturbing the convergence of the resulting integral. Thus $\Sigma^{\text{wh}}_{(2)}$ is globally smooth on the $\beta$-plane and one can proceed to the calculation of $\Sigma^{\text{wh}}_{(3)}$. 
Assuming that \( \{\Sigma^{wh}_{(2)}, \ldots, \Sigma^{wh}_{(k-1)}\} \), for \( k \geq 2 \), have all been shown to be globally smooth one integrates equation (4.57) to find that (4.64)

\[
\Sigma^{wh}_{(k)}(\beta_+(t), \beta_-(t)) = \left\{ \Sigma^{wh}_{(k)}(\beta_0^+, \beta_0^-) - \int_{-\infty}^t ds \frac{e^{-2(k-1)(\alpha(s) - \alpha(0))} \Lambda_{(k)}(s)}{e^{-2(k-1)(\alpha(t) - \alpha(0))}} \right\},
\]

\( \forall t \leq 0 \). Again there is only one choice possible for \( \Sigma^{wh}_{(k)}(\beta_0^+, \beta_0^-) \) that can yield a finite value for \( \Sigma^{wh}_{(k)}(0,0) \) in the limit as \( t \downarrow -\infty \), namely

(4.65) \[
\Sigma^{wh}_{(k)}(\beta_0^+, \beta_0^-) = \int_{-\infty}^0 ds \frac{e^{-2(k-1)(\alpha(s) - \alpha(0))} \Lambda_{(k)}(s)}{e^{-2(k-1)(\alpha(t) - \alpha(0))}}.
\]

The integral converges for any smooth function \( \Lambda_{(k)}(\beta_+, \beta_-) \) and for any choice of \( (\beta_0^+, \beta_0^-) \) by virtue of the exponential decay of the integrating factor along the solution curve that interpolates between \( (\beta_0^+, \beta_0^-) \) and the origin. Making this choice for \( \Sigma^{wh}_{(k)}(\beta_0^+, \beta_0^-) \) one can simplify equation (4.64) to

(4.66) \[
\Sigma^{wh}_{(k)}(\beta_+(t), \beta_-(t)) = \frac{\int_{-\infty}^t ds \frac{e^{-2(k-1)(\alpha(s) - \alpha(0))} \Lambda_{(k)}(s)}{e^{-2(k-1)(\alpha(t) - \alpha(0))}}}{e^{-2(k-1)(\alpha(t) - \alpha(0))}}.
\]

and verify, again via L'Hôpital's rule, that the function so constructed has the desired limit (4.55) as \( t \downarrow -\infty \).

By differentiating the explicit formulas (4.25–4.30) for \( \{\alpha(t) - \alpha(0), \beta_+(t), \beta_-(t)\} \) with respect to the ‘initial’ data \( (\beta_0^+, \beta_0^-) \) it is now straightforward to verify that, for any smooth function \( \Lambda_{(k)}(\beta_+, \beta_-) \), the defining expression (4.65) for \( \Sigma^{wh}_{(k)}(\beta_0^+, \beta_0^-) \) is globally smooth on the \( (\beta_0^+, \beta_0^-) \)-plane. A key element in this argument is the resulting exponential decay, as \( t \longrightarrow -\infty \), of the derivatives of \( (\beta_+(t), \beta_-(t)) \) with respect to \( (\beta_0^+, \beta_0^-) \) to arbitrarily high order. This completes the proof by induction that the quantum corrections \( \{\mathcal{S}^{wh}_{(k)}(\alpha, \beta_+, \beta_-)\} \) to the logarithm of the ground state wave function are globally defined smooth functions on the Mixmaster minisuperspace for all \( k \geq 1 \).

One can now begin to resolve the ‘paradox’ alluded to at the end of Section 3 concerning how microlocal methods could possibly be used to generate smooth quantum corrections to candidate ‘eigenfunctions’ when there are no corresponding ‘eigenvalues’ available to adjust. In a conventional Schrödinger eigenvalue problem [1] the values, \( \{\mathcal{S}_{(k)}(0, \ldots, 0)\} \), of the functions under construction \( \{\mathcal{S}_{(k)}(x^1, \ldots, x^n)\} \) are, at the minimum of the potential energy (taken here to be the origin), arbitrary constants of integration that can be lumped into an overall normalization constant for the ground state wave function. Thus these adjustable constants play no role in guaranteeing the smoothness of the \( \{\mathcal{S}_{(k)}\} \). On the other hand the freedom
to adjust the coefficients \( \{ (0) E_{E_k} \} \) in an expansion for the ground state energy eigenvalue, \( (0) E \), precisely allows one to ensure the needed smoothness while, at the same time, uniquely determining the \( \{ (0) E_{E_k} \} \) to all orders. Here however the functions being computed by the analogous ‘transport’ analysis are the \( \{ \Sigma^{wh}_{E_k}(\beta_+, \beta_-) \} \). But, because they multiply correspondingly different powers of \( e^\alpha \) in the ansatz (4.44) for \( S^{wh}_{E_k} \), their values at the classical equilibrium (i.e., at the origin in \((\beta_+, \beta_-)-space\)) are not arbitrary (c.f., Eqs. (4.53)–(4.55)) but instead provide precisely the flexibility needed, in the absence of eigenvalue coefficients, to ensure the smoothness of the functions \( \{ \Sigma^{wh}_{E_k}(\beta_+, \beta_-) \} \) and hence also that of the \( \{ S^{wh}_{E_k}(\alpha, \beta_+, \beta_-) \} \). In the section below we shall encounter an analogous phenomenon occurring in the construction of excited states.

5. Conserved Quantities and Excited States

To generate ‘excited state’ solutions to the Wheeler-DeWitt equation we begin by making the ansatz

\[
(5.1) \quad \Psi_h = \phi_h e^{-S_h/h}
\]

where \( S_h = \frac{c^3 L^2}{G} S_h = \frac{c^3 L^2}{G} \left( S_{(0)} + X S_{(1)} + \frac{X^2}{2!} S_{(2)} + \cdots \right) \) is the same formal expansion derived in the preceding section for the ground state solution and where the new factor \( \phi_h \) is assumed to admit an expansion of similar type,

\[
(5.2) \quad \phi_h = \phi_{(0)} + X \phi_{(1)} + X^2 \phi_{(2)} + \cdots + \frac{X^k}{k!} \phi_{(k)} + \cdots,
\]

with \( X = \frac{L^2_{\text{Planck}}}{L^2} = \frac{Gc^6}{\hbar} \) as before. Substituting this ansatz into the Mixmaster Wheeler-DeWitt equation and demanding satisfaction, order-by-order in \( X \), one arrives at the sequence of equations

\[
(5.3) \quad -\frac{\partial \phi_{(0)}}{\partial \alpha} \frac{\partial S_{(0)}}{\partial \alpha} + \frac{\partial \phi_{(0)}}{\partial \beta_+} \frac{\partial S_{(0)}}{\partial \beta_+} + \frac{\partial \phi_{(0)}}{\partial \beta_-} \frac{\partial S_{(0)}}{\partial \beta_-} = 0,
\]

\[
(5.4) \quad + \left( -\frac{\partial \phi_{(0)}}{\partial \alpha} \frac{\partial S_{(1)}}{\partial \alpha} + \frac{\partial \phi_{(0)}}{\partial \beta_+} \frac{\partial S_{(1)}}{\partial \beta_+} + \frac{\partial \phi_{(0)}}{\partial \beta_-} \frac{\partial S_{(1)}}{\partial \beta_-} \right)
+ \frac{1}{2} \left( -B \frac{\partial \phi_{(0)}}{\partial \alpha} + \frac{\partial^2 \phi_{(0)}}{\partial \alpha^2} - \frac{\partial^2 \phi_{(0)}}{\partial \beta_+^2} - \frac{\partial^2 \phi_{(0)}}{\partial \beta_-^2} \right) = 0,
\]
and, for $k \geq 2$

\begin{equation}
(5.5) \quad - \frac{\partial \phi_{(k)}^{(*)}}{\partial \alpha} \frac{\partial S_{(0)}}{\partial \alpha} + \frac{\partial \phi_{(k)}^{(*)}}{\partial \beta_+} \frac{\partial S_{(0)}}{\partial \beta_+} + \frac{\partial \phi_{(k)}^{(*)}}{\partial \beta_-} \frac{\partial S_{(0)}}{\partial \beta_-} + k \left( - \frac{\partial \phi_{(k-1)}^{(*)}}{\partial \alpha} \frac{\partial S_{(1)}}{\partial \alpha} + \frac{\partial \phi_{(k-1)}^{(*)}}{\partial \beta_+} \frac{\partial S_{(1)}}{\partial \beta_+} + \frac{\partial \phi_{(k-1)}^{(*)}}{\partial \beta_-} \frac{\partial S_{(1)}}{\partial \beta_-} \right) \\
+ \frac{k}{2} \left( - B \frac{\partial \phi_{(k-1)}^{(*)}}{\partial \alpha} + \frac{\partial^2 \phi_{(k-1)}^{(*)}}{\partial \alpha^2} - \frac{\partial^2 \phi_{(k-1)}^{(*)}}{\partial \beta_+^2} - \frac{\partial^2 \phi_{(k-1)}^{(*)}}{\partial \beta_-^2} \right) \\
+ \sum_{\ell=2}^{k} \frac{k!}{\ell!(k-\ell)!} \left( - \frac{\partial \phi_{(k-\ell)}^{(*)}}{\partial \alpha} \frac{\partial S_{(\ell)}}{\partial \alpha} + \frac{\partial \phi_{(k-\ell)}^{(*)}}{\partial \beta_+} \frac{\partial S_{(\ell)}}{\partial \beta_+} + \frac{\partial \phi_{(k-\ell)}^{(*)}}{\partial \beta_-} \frac{\partial S_{(\ell)}}{\partial \beta_-} \right) = 0.
\end{equation}

The first of these is easily seen to be the requirement that $\phi_{(0)}^{(*)}$ be constant along the flow in mini-superspace generated by $S_{(0)}$, the chosen solution to the Euclidean-signature Hamilton-Jacobi equation (4.6). For the case of most interest here, $S_{(0)} \to S_{(0)}^{\text{wh}}$, Bae discovered two such conserved quantities through direct inspection of his solution (4.25–4.30) of the corresponding flow equations, namely

\begin{equation}
(5.6) \quad C_{(0)} := \frac{1}{6} e^{4\alpha - 2\beta_+} \left( e^{6\beta_+} - \cosh(2\sqrt{3}\beta_-) \right)
\end{equation}

and

\begin{equation}
(5.7) \quad S_{(0)} := \frac{1}{2\sqrt{3}} e^{4\alpha - 2\beta_+} \sinh(2\sqrt{3}\beta_-)
\end{equation}

[47]. By reexpressing these in terms of the functions $\{\omega_1, \omega_2, \omega_3\}$ defined previously, one arrives at the alternative forms

\begin{equation}
(5.8) \quad C_{(0)} = \frac{1}{12} (2\omega_3^2 - \omega_1^2 - \omega_2^2)
\end{equation}

\begin{equation}
(5.9) \quad S_{(0)} = \frac{1}{4\sqrt{3}} (\omega_2^2 - \omega_1^2)
\end{equation}

and can recognize them in terms of the well-known, conserved kinetic energy and squared angular momentum of the asymmetric top [41, 43].

Of course any differentiable function of $C_{(0)}$ and $S_{(0)}$ would be equally conserved but the Taylor expansions of these in particular,

\begin{equation}
(5.10) \quad C_{(0)} \simeq e^{4\alpha} \left( \beta_+ + \beta_+^2 - \beta_-^2 + O(\beta^3) \right),
\end{equation}

\begin{equation}
(5.11) \quad S_{(0)} \simeq e^{4\alpha} \left( \beta_- - 2\beta_+\beta_- + O(\beta^3) \right),
\end{equation}
reveal their preferred features of behaving linearly in $\beta_+$ and $\beta_-$ (respectively) near the origin in $\beta$-space. It therefore seems natural to seek to construct a ‘basis’ of excited states by taking

$$
\phi(0) \rightarrow \phi(0) := C_{(0)}^{m_1} S_{(0)}^{m_2} \approx e^{A(m_1+m_2)\alpha} \beta_+^{m_1} \beta_-^{m_2} + \cdots
$$

as seeds for the computation of higher order quantum corrections. Here $\mathbf{m} = (m_1, m_2)$ is a pair of non-negative integers that can be plausibly interpreted as graviton excitation numbers for the ultralong wavelength gravitational wave modes embodied in the $\beta_+$ and $\beta_-$ degrees of freedom.

To see this more concretely note that, to leading order in $X$ and near the origin in $\beta$-space, one then gets

$$
\Psi_{\mathbf{n}} \approx e^{A(m_1+m_2)\alpha} \beta_+^{m_1} \beta_-^{m_2} e^{-\frac{2\alpha}{\Lambda} (\frac{1}{2} + 2(\beta_1^2 + \beta_2^2) + \cdots)}
$$

which, for any fixed $\alpha$, has the form of the top order term in the product of Hermite polynomials multiplied by a gaussian that one would expect to see for an actual, harmonic oscillator wave function.

One wishes, however, to construct wave functions that share the invariance of the Wheeler-DeWitt operator under rotations by $\pm \frac{2\pi}{3}$ in the $\beta$-plane since these correspond to residual gauge transformations. The functions $\{S_{(k)}\}$ constructed in the preceding section have this property automatically by virtue of the rotational invariance of the flow generated by the chosen $S_{(0)} = S_{(0)}^{\text{wh}}$ and the corresponding invariance of the technique employed for generating initial conditions for the $\{S_{(k)}, k = 1, 2, \cdots \}$. On the other hand the functions $\phi_{(0)} := C_{(0)}^{m_1} S_{(0)}^{m_2}$ are not, in general, invariant but can be modified to become so by the straightforward technique of averaging over the group of rotations in question: $\{I, \pm \frac{2\pi}{3}\}$. Some elegant graphical depictions of the lowest few such invariant states (to leading order in $X$) have been given by Bae in [47]. The linearity of equations (5.3, 5.4, 5.5) in the $\{\phi_{(k)}\}$ and the rotational invariance of the operators therein acting upon these functions will allow one to construct rotationally invariant quantum corrections to all orders, either by starting with an invariant ‘seed’ of the type described above or, alternatively, carrying out the group averaging at the end of the sequence of calculations. We shall follow the latter approach here.

We begin by setting

$$
\phi_{(0)} \rightarrow C_{(0)}^{m_1} S_{(0)}^{m_2} := e^{A|m| \alpha}\chi_{(0)}(\beta_+, \beta_-)
$$

where $|m| := m_1 + m_2$ and proceed by making the ansatz

$$
\phi_{(k)} = e^{A|m|-2k\alpha}\chi_{(k)}(\beta_+, \beta_-)
$$
∀ \( k \geq 1 \). Recalling the definitions of the functions \( \{ \Sigma_{(k)}^{\text{wh}}(\beta_+, \beta_-) \} \) given by (4.44–4.46) we now find that equations (5.4–5.5) can be reexpressed as flow equations in the \( \beta \)-plane for the unknowns \( \{ \chi_{(k)}(\beta_+, \beta_-); \ k = 1, 2, \ldots \} \):

\[
\frac{\partial \chi_{(1)}(m)}{\partial \beta_+} \frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} + \frac{\partial \chi_{(1)}(m)}{\partial \beta_-} \frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_-} - 2 \chi_{(1)}(m) (4|m| - 2) \Sigma_{(0)}^{\text{wh}}
\]

(5.16)

\[
+ 3 \left[ (16|m|^2 + 24|m|) \chi_{(0)}(m) - \frac{\partial^2 \chi_{(0)}(m)}{\partial \beta_+^2} - \frac{\partial^2 \chi_{(0)}(m)}{\partial \beta_-^2} \right] = 0,
\]

and, for \( k \geq 2 \),

\[
\frac{\partial \chi_{(k)}(m)}{\partial \beta_+} \frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_+} + \frac{\partial \chi_{(k)}(m)}{\partial \beta_-} \frac{\partial \Sigma_{(0)}^{\text{wh}}}{\partial \beta_-} - 2 \chi_{(k)}(m) (4|m| - 2k) \Sigma_{(0)}^{\text{wh}}
\]

(5.17)

\[
+ 3k \left\{ [4|m| - 2(k - 1)]^2 + 6 (4|m| - 2(k - 1)) \chi_{(k-1)}(m) - \frac{\partial^2 \chi_{(k-1)}(m)}{\partial \beta_+^2} \right\}
\]

\[
+ 3k \left\{ \frac{k!}{(k - \ell)!} \left( 2(\ell - 1)(4|m| - 2(k - \ell)) \chi_{(k-\ell)}(m) \Sigma_{(\ell)}^{\text{wh}} \right) \right\}
\]

As for the ground state problem our aim is to solve these transport equations sequentially and thereby to establish, for any given \( m = (m_1, m_2) \), the existence of smooth, globally defined functions \( \{ \chi_{(k)}(\beta_+, \beta_-); k = 1, 2, \ldots \} \) on the \( \beta \)-plane. When \( k > 2|m| \) the relevant transport operator is of the same type dealt with in the previous section and the corresponding equation can be solved, for an arbitrary smooth ‘source’ inhomogeneity, by the same methods exploited therein. When \( k \leq 2|m| \) however the associated integrating factor,

\[
\mu_{(k)}(t) = \frac{e^{(4|m|-2k)\alpha(t)}}{e^{(4|m|-2k)\alpha(0)}}
\]

(5.18)

is either constant or blows up at \( t \downarrow -\infty \) and a different approach is needed. Fortunately there is a well-developed microlocal technique for handling such problems that can be sketched as follows [1, 31, 32, 33]:
Assuming, inductively, that smooth solutions up to order \( k - 1 \), for \( k \geq 1 \), have already been constructed, derive a formal power series for the subsequent unknown \( \chi^{(m)}_{(k)}(\beta_+, \beta_-) \),

(ii) apply a standard method to generate a globally smooth function, \( \nu^{(m)}_{(k)}(\beta_+, \beta_-) \), that has the same Taylor expansion about the origin in the \( \beta \)-plane as that determined in step (i) [48],

(iii) solve an associated transport equation for the ‘correction’,

\[
\eta^{(m)}_{(k)} = \chi^{(m)}_{(k)} - \nu^{(m)}_{(k)},
\]

and show that \( \eta^{(m)}_{(k)} \) is smooth, globally defined and vanishes to infinite order at the origin (i.e., has identically vanishing Taylor expansion).

Setting \( \chi^{(m)}_{(k)} = \eta^{(m)}_{(k)} + \nu^{(m)}_{(k)} \) provides a (not necessarily unique, as we shall see) solution to the relevant transport equation and allows one to proceed to the construction of \( \chi^{(m)}_{(k+1)} \).

In the last step one exploits the fact that the integrating factor, (5.18), for the \( \eta^{(m)}_{(k)} \) transport equation, though it remains constant or blows up as \( t \searrow -\infty \), is now being integrated against a ‘source’ that vanishes to infinite order [1, 31, 32, 33]. Since steps (ii) and (iii) are routine (c.f., [48] and [1, 31, 32, 33] respectively) we shall focus here on step (i) which entails a certain subtlety for the present problem.

The technique for carrying out step (i) developed in [31, 32, 33] involves first splitting the transport operator

\[
\mathcal{L}^{(m)}_{(k)} := \frac{\partial \Sigma^{wh}_{(0)}}{\partial \beta_+} \frac{\partial}{\partial \beta_+} + \frac{\partial \Sigma^{wh}_{(0)}}{\partial \beta_-} \frac{\partial}{\partial \beta_-} - 2(4|m| - 2k)\Sigma^{wh}_{(0)}
\]

into linear and higher order terms

\[
\mathcal{L}^{(m)}_{(k)} = \mathcal{L}^{(m)}_{(k)0} + \mathcal{L}^{(m)}_{(k)R}
\]

with

\[
\mathcal{L}^{(m)}_{(k)0} := 24 \left( \beta_+ \frac{\partial}{\partial \beta_+} + \beta_- \frac{\partial}{\partial \beta_-} \right) - 6(4|m| - 2k).
\]

One would like to apply the arguments given in the foregoing references to generate the formal Taylor expansion for \( \chi^{(m)}_{(k)} \) needed for step (i) and, when \( 1 \leq k \leq 2|m| \) and \( k \) is odd, this is straightforward to carry out.

The basic reason for this is that, when \( k \) is odd, \( \mathcal{L}^{(m)}_{(k)0} \) is a bijection on the space, \( \mathcal{P}^\ell_{\text{hom}} \), of polynomials in \( \beta_+ \) and \( \beta_- \) which are homogeneous of
degree $\ell \in \mathbb{N}$ and the monomials $\beta_+^{\ell_1} \beta_-^{\ell_2}$, with $|\ell| = \ell_1 + \ell_2$, constitute a basis of eigenvectors of the restriction of $(m) L_{(k)0}$ to $\mathcal{P}_{\text{hom}}^\ell$ with eigenvalues $24 (|\ell| - |m| + \frac{k}{2}) \neq 0$. Though the choice of $(m) \nu_{(k)}$ for step (ii) is not unique it is nevertheless straightforward to show, in these odd $k$ cases, that the resulting solution for $(m) \chi_{(k)}$ is unique. The reason is that the difference of any two such solutions would necessarily be a ‘flat’ function (i.e., one with identically vanishing Taylor expansion) that satisfies the homogeneous form of the original transport equation for $(m) \chi_{(k)}$. But using the integrating factor for this equation it is easy to show that any flat, globally smooth solution must in fact vanish identically.

When $k$ is even, on the other hand, $(m) L_{(k)0}$ has a nontrivial kernel, $\mathcal{P}_{\text{hom}}^{[m]-\frac{k}{2}}$, spanned by the monomials $\beta_+^{\ell_1} \beta_-^{\ell_2}$, with $|\ell| = \ell_1 + \ell_2 = |m| - \frac{k}{2}$. $(m) L_{(k)0}$ is still a bijection on $\mathcal{P}_{\text{hom}}^\ell$ for all $\ell \neq |m| - \frac{k}{2}$ but since $\mathcal{P}_{\text{hom}}^{[m]-\frac{k}{2}}$ does not lie in this operator’s range we must arrange to cancel any elements of $\mathcal{P}_{\text{hom}}^{[m]-\frac{k}{2}}$ that occur in the ‘source’ inhomogeneity for this operator. For $k = 2$ the flexibility to accomplish this cancellation arises through the freedom to replace the ‘seed’ $(m) \chi_{(0)}$ by an arbitrary linear combination

$$\chi_{(0)} \rightarrow \sum_{m_1,m_2} c_{m_1,m_2} \chi_{(0)}$$

and adjust the choice of the $|m| + 1$ independent coefficients $\{c_{m_1,m_2}\}$ until the $|m|$ coefficients of the monomials $\beta_+^{\ell_1} \beta_-^{\ell_2}$, with $|\ell| := \ell_1 + \ell_2 = |m| - 1$, all vanish.

For higher, even values of $k$ it is straightforward to verify that the functions

$$\chi_{(k)} := \sum_{\ell_1,\ell_2} c^{(k)}_{\ell_1,\ell_2} \chi_{(0)}$$

with $(\ell) := (\ell_1,\ell_2)$ and $|\ell| := \ell_1 + \ell_2 = |m| - \frac{k}{2}$, satisfy the exact, homogeneous transport equation

$$L_{(k)}^{(m)} \chi_{(k)} = 0$$

for arbitrarily chosen values of the $|\ell| + 1$ coefficients $\{c^{(k)}_{\ell_1,\ell_2}\}$. These coefficients are thus available to ensure the integrability of the transport equation for $(m) \chi_{(k+2)}$. Some additional work would be needed to precisely enumerate the independent solutions obtainable by this analysis — in particular those remaining after the averaging over the $\pm 2\pi/3$ rotations in the $\beta$-plane has been carried out.
6. Euclidean-Signature Semi-Classical Methods for Bosonic Field Theories

One would like to think that the foregoing results could serve as a prototype for the application of microlocal methods to the quantization of Einstein’s equations more generally. But general relativity is a field theory and, so far as the author knows, such microlocal methods have heretofore been confined to quantum mechanical applications. There is a good reason for this.

When ansätze of the form (4.1) and (5.1) are applied to a conventional Schrödinger eigenvalue problem they lead, at lowest order, to the necessity to solve the Hamilton-Jacobi equation for an inverted-potential-energy mechanics problem. This is the analogue of the ‘Euclidean-signature’ Hamilton-Jacobi equation (4.6) that arose for the Mixmaster system considered above. For the Schrödinger problem microlocal analysts solve this HJ equation, locally near an equilibrium, by assembling several dynamical systems results such as the stable manifold theorem for hyperbolic fixed points and the existence, uniqueness and smoothness properties for the associated Hamiltonian flow \(1, 31, 32, 33\).

But even when such theorems can be generalized to apply to suitable classes of infinite dimensional dynamical systems they are nevertheless totally inadequate for solving the Hamilton-Jacobi equation that arises when one is attempting to quantize a relativistic field theory. The reason for this is that the Hamilton-Jacobi equation for such problems is that for the Euclidean signature analogue of the original, Lorentzian-signature field equations that one is intending to quantize. But such Euclidean-signature field equations are not a dynamical system at all. They correspond instead to an elliptic problem that admits no well-posed, Cauchy evolutionary formulation.

For this reason the author, together with A. Marini and R. Maitra, has recently been developing an alternative program for solving these fundamental Hamilton-Jacobi problems by exploiting the direct method of the calculus of variations \(1, 2, 3\). This strategy has the decisive advantage of being naturally applicable to the elliptic problems that arise for relativistic field theories with this approach and, even for finite-dimensional quantum mechanical problems, succeeds to unify and globalize the essential microlocal results, for a large and interesting class of potential energy functions, in an aesthetically appealing way.

To see these methods in action, first in the technically simpler setting of ordinary quantum mechanics, consider Schrödinger operators of the (‘nonlinear oscillatory’) type

\[
\hat{H} = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m \sum_{i=1}^{n} \omega_i^2 (x^i)^2 + A(x)
\]
where \( x = (x^1, \ldots, x^n) \), \( \Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x^i \partial x^i} \) is the ordinary Laplacian on \( \mathbb{R}^n \) and \( A : \mathbb{R}^n \rightarrow \mathbb{R} \) is a smooth function whose Taylor expansion about the origin begins at third order so that

\[
A(0, \ldots, 0) = \frac{\partial A(0, \ldots, 0)}{\partial x^i} = \frac{\partial^2 A(0, \ldots, 0)}{\partial x^i \partial x^j} = 0.
\]

If the \( A \) term is dropped then \( \hat{H} \) reduces to the Schrödinger operator for an ordinary harmonic oscillator in \( n \) dimensions having mass \( m > 0 \) and oscillation frequencies \( \{\omega_i\} \), each assumed \( > 0 \), along the corresponding Cartesian coordinate axes. When \( A \) is reinstated the oscillator becomes nonlinear or ‘anharmonic’. Such oscillators are rudimentary models for the field theoretic systems that we shall turn to later.

To simplify the analysis assume the total potential energy function \( V : \mathbb{R}^n \rightarrow \mathbb{R} \), given by

\[
V(x) = \frac{1}{2} m \sum_{i=1}^{n} \omega_i^2 (x^i)^2 + A(x),
\]

to be convex and to have its (unique, isolated) global minimum at the origin so that

\[
V(x^1, \ldots, x^n) > V(0, \ldots, 0) = 0 \quad \forall (x^1, \ldots, x^n) \in \mathbb{R}^n \setminus (0, \ldots, 0).
\]

In the event that \( A \) has indefinite sign we shall also impose a certain coercivity condition to bound its behavior from below [49]. Finally we shall require that the frequencies \( \{\omega_i\} \), characterizing the (non-dengenerate) quadratic term in the potential energy satisfy a convenient (but not strictly essential [50]) ‘non-resonance’ condition that is designed to simplify the analysis of quantum excited states.

We begin by attempting to construct a ground state wave function of the form

\[
\psi_{\hbar}^{(0)}(x) = N_{\hbar} e^{-S_{\hbar}(x)/\hbar}
\]

wherein \( S_{\hbar} \) is real-valued and assumed to admit a formal series expansion in \( \hbar \) that we write as

\[
S_{\hbar}(x) \simeq S_{(0)}^{(0)}(x) + \hbar S_{(1)}^{(0)}(x) + \frac{\hbar^2}{2!} S_{(2)}^{(0)}(x) + \cdots + \frac{\hbar^n}{n!} S_{(n)}^{(0)}(x) + \cdots
\]

and where \( N_{\hbar} \) is a normalization constant. We expand the corresponding ground state energy eigenvalue \( E_{\hbar}^{(0)} \) in the analogous way, writing

\[
E_{\hbar}^{(0)} : = \hbar E_{\hbar} \simeq \hbar \left( E_{(0)}^{(0)} + \hbar E_{(1)}^{(0)} + \frac{\hbar^2}{2!} E_{(2)}^{(0)} + \cdots + \frac{\hbar^n}{n!} E_{(n)}^{(0)} + \cdots \right)
\]

and substitute these ansätze into the time-independent Schrödinger equation,

\[
\hat{H} \psi_{\hbar}^{(0)} = E_{\hbar}^{(0)} \psi_{\hbar}^{(0)}.
\]
requiring the latter to hold, order by order, in powers of Planck’s constant.

At leading order this procedure immediately generates the ‘inverted potential-vanishing-energy’ Hamilton-Jacobi equation,

\[
\frac{1}{2m} \nabla S_{(0)} \cdot \nabla S_{(0)} - V = 0,
\]

that is intended to determine the function \( S_{(0)} \). Under the convexity and coercivity hypotheses alluded to above we proved the existence and smoothness of a globally defined ‘fundamental solution’ to Eq. (6.9) using methods drawn from the calculus of variations \([1]\). The higher order ‘quantum corrections’ to \( S_{(0)} \) (i.e., the functions \( S_{(k)} \) for \( k = 1, 2, \ldots \)) can then be computed through the systematic integration of a sequence of (first order, linear) ‘transport equations’, derived from Schrödinger’s equation, along the integral curves of the gradient (semi-) flow generated by \( S_{(0)} \) \([1]\). The natural demand for global smoothness of these quantum corrections forces the (heretofore, undetermined) energy coefficients \( \{ E_{(0)}, E_{(1)}, E_{(2)}, \ldots \} \) all to take on specific, computable values.

Excited states were then studied by substituting the ansatz

\[
\psi_{(\star)}^h(x) = \phi_{(\star)}^h(x)e^{-S_{(\star)}^h(x)/h}
\]

into the Schrödinger equation

\[
\hat{H}\psi_{(\star)}^h = E_{(\star)}^h \psi_{(\star)}^h
\]

and formally expanding the unknown wave functions, \( \phi_{(\star)}^h \), and energy eigenvalues \( E_{(\star)}^h \), in powers of \( h \) as before,

\[
\phi_{(\star)}^h \simeq \phi_{(0)} + h\phi_{(1)} + \frac{h^2}{2!}\phi_{(2)} + \ldots
\]

\[
E_{(\star)}^h := h E_{(\star)} \simeq h \left( E_{(0)} + h E_{(1)} + \frac{h^2}{2!} E_{(2)} + \ldots \right),
\]

while retaining the ‘universal’ factor, \( e^{-S_{(\star)}^h(x)/h} \), determined by the ground state calculations.

From the leading order analysis one finds that these excited state expansions naturally allow themselves to be labelled by an \( n \)-tuple \( m = (m_1, m_2, \ldots, m_n) \) of non-negative integer ‘quantum numbers’, \( m_i \), so that the foregoing notation can be refined to

\[
\psi_{(m)}^h(x) = \phi_{(m)}^h(x)e^{-S_{(m)}^h(x)/h}
\]

and

\[
E_{(m)}^h = h E_{(m)}
\]
with \( \phi_h \) and \( E_h \) expanded as before. Since all the coefficients \( \{ \phi^{(k)}, E^{(k)} \} \) for \( k = 0, 1, 2, \ldots \) are, however, computable through the solution of linear, first order transport equations, integrated along the semi-flow generated by \( S_{(0)} \), using methods that are already well-known from the microlocal literature [1, 31, 32, 33] we shall focus here on the fundamental way in which our approach differs from the microlocal one — namely in the solution of the basic Hamilton-Jacobi equation (6.9) by means of the direct method of the calculus of variations.

A natural approach for generating solutions to the inverted potential \((ip)\) dynamics problem formulated above is to establish the existence of minimizers for the \((ip)\) action functional

\[
I_{ip}[\gamma] = \int_{-\infty}^0 L_{ip}(x^1(t), \ldots, x^n(t), \dot{x}^1(t), \ldots, \dot{x}^n(t)) \, dt
\]

within the affine space of curves

\[
D_x := \{ \gamma \in H^1(I, \mathbb{R}^n) | I = (-\infty, 0], \gamma(t) = (x^1(t), \ldots x^n(t)), \lim_{t \to 0} \gamma(t) = x, x = (x^1, \ldots, x^n) \in \mathbb{R}^n \}.
\]

Here \( H^1(I, \mathbb{R}^n) \) is the Sobolov space of (distributional) curves on \( \mathbb{R}^n \) equipped with the norm

\[
\| \gamma(\cdot) \|_{H^1(I, \mathbb{R}^n)} := \left\{ \int_{-\infty}^0 \sum_{i=1}^n \left[ (\dot{x}^i(t))^2 + \omega_i^2 (x^i(t))^2 \right] dt \right\}^{1/2}
\]

and \( x = (x^1, \ldots, x^n) \) is an arbitrary, but fixed, right endpoint lying in \( \mathbb{R}^n \). From the Sobolov embedding theorem for \( H^s \)-maps [51, 52] one has that \( H^1(I, \mathbb{R}^n) \) is continuously embedded in

\[
C^0_b(I, \mathbb{R}^n) := \left\{ \gamma \in C^0(I, \mathbb{R}^n) \right\}
\]

and

\[
\| \gamma(\cdot) \|_{L^\infty(I, \mathbb{R}^n)} := \sup_{t \in I} \sqrt{\sum_{i=1}^n (x^i(t))^2} < \infty
\]

where \( C^0(I, \mathbb{R}^n) \) is the space of continuous curves in \( I \), and furthermore that these curves automatically (as a consequence of having finite \( H^1 \)-norm)
‘vanish at infinity’ in the sense that

\[(6.21) \lim_{t \searrow -\infty} |\gamma(t)| = \lim_{t \searrow -\infty} \sqrt{\sum_{i=1}^{n} \left( x^i(t) \right)^2} = 0. \]

Thus the curves in \( D_\mathbf{x} \) have their (asymptotically attained) left endpoints at the origin in \( \mathbb{R}^n \) which, in our formulation, coincides with the unique, global maximum of the inverted potential energy function

\[(6.22) V_{ip}(x^1, \ldots, x^n) := -V(x^1, \ldots, x^n). \]

Strictly speaking, though the ‘curves’ in \( H^1(I, \mathbb{R}^n) \) are distributional, the Sobolev embedding theorem referenced above allows one to represent each such distribution by a continuous curve which (by a slight abuse of notation) we also write as \( \gamma : I \rightarrow \mathbb{R}^n \). For this reason one can meaningfully speak of the values of \( \gamma \) (as points in \( \mathbb{R}^n \)) for any \( t \in I = (-\infty, 0] \) and thus, in particular, impose the right endpoint boundary condition,

\[(6.23) \lim_{t \nearrow 0} \gamma(t) = \mathbf{x} = (x^1, \ldots, x^n) \in \mathbb{R}^n \]

that was included in the definition of \( D_\mathbf{x} \).

When the convexity and coercivity hypotheses for \( V \) alluded to above are taken into account one can show that the functional \( I_{ip}[\gamma] \) is globally defined on \( D_\mathbf{x} \) for any \( \mathbf{x} \in \mathbb{R}^n \). For each such \( \mathbf{x} \) one can proceed to prove that \( I_{ip}[\gamma] \) has a unique minimizer \( \gamma_{\mathbf{x}} \in D_\mathbf{x} \), that this minimizer is actually smooth (i.e., that \( \gamma_{\mathbf{x}} \in C^\infty(I, \mathbb{R}^n) \)), satisfies the ip Euler-Lagrange equations,

\[(6.24) m \frac{d^2 x^i(t)}{dt^2} = -\frac{\partial V_{ip}(\mathbf{x}(t))}{\partial x^i} = \frac{\partial V(\mathbf{x}(t))}{\partial x^i}, \quad i = 1, \ldots, n, \]

for all \( t \in I \) and has vanishing ip energy,

\[(6.25) E_{ip}(\mathbf{x}(t), \dot{\mathbf{x}}(t)) := \frac{m}{2} \sum_{i=1}^{n} \left( \dot{x}^i(t) \right)^2 + V_{ip}(\mathbf{x}(t)) = \frac{m}{2} \sum_{i=1}^{n} \left( \dot{x}(t) \right)^2 - V(\mathbf{x}(t)) = 0 \]

on this interval \([53]\).

Setting, for each such minimizer,

\[(6.26) S_{(0)}(\mathbf{x}) = I_{ip}[\gamma_{\mathbf{x}}] \]

one can further prove, using the Banach space version of the implicit function theorem, that the function \( S_{(0)} : \mathbb{R}^n \rightarrow \mathbb{R} \), so defined, is globally smooth, satisfies the ‘inverted-potential-vanishing-energy’ Hamilton-Jacobi equation,

\[(6.27) \frac{1}{2m} \nabla S_{(0)} \cdot \nabla S_{(0)} - V = 0 \]
on $\mathbb{R}^n$ and regenerates the minimizers as the integral solution curves of its gradient semi-flow [54] defined via

$$\frac{d\gamma^i(t)}{dt} = \frac{1}{m} \frac{\partial S_0}{\partial x^i}, \quad i = 1, \ldots, n.$$  

These are the essential features required of $S_0$ in order to be able to compute, via linear transport analysis, its quantum corrections and corresponding excited states to all orders in Planck’s constant [1].

For a first glimpse at how these techniques can be applied to relativistic quantum field theories consider the formal Schrödinger operator for the massive, quartically self-interacting scalar field on $(3 + 1$ dimensional) Minkowski spacetime given by

$$\hat{H} = \int_{\mathbb{R}^3} \left\{ -\frac{\hbar^2}{2} \frac{\delta^2}{\delta \phi^2} + \frac{1}{2} \nabla \phi \cdot \nabla \phi(x) + \frac{m^2}{2} \phi^2(x) + \lambda \phi^4(x) \right\} d^3x$$

where $m$ and $\lambda$ are constants $> 0$. Though the functional Laplacian term requires regularization to be well-defined, the influence of this regularization will only be felt at the level of quantum corrections and not for the (so-called ‘tree level’) determination of a fundamental solution, $S_0[\phi(\cdot)]$, to the ‘vanishing-energy-Euclidean-signature’ functional Hamilton-Jacobi equation given by

$$\int_{\mathbb{R}^3} \left\{ \frac{1}{2} \frac{\delta S_0}{\delta \phi(x)} \frac{\delta S_0}{\delta \phi(x)} - \frac{1}{2} \nabla \phi \cdot \nabla \phi(x) - \frac{m^2}{2} \phi^2(x) - \lambda \phi^4(x) \right\} d^3x = 0.$$

As in the quantum mechanical examples discussed above this equation arises, at leading order, from substituting the (Euclidean-signature) ground state wave functional ansatz

$$\psi_0[\phi(\cdot)] = N_0 e^{-S_0[\phi(\cdot)]}/\hbar$$

into the time-independent Schrödinger equation,

$$\hat{H} \psi_0 = E_0 \psi_0,$$

and demanding satisfaction, order-by-order in powers of $\hbar$, relative to the formal expansions

$$S_0[\phi(\cdot)] \simeq S_0[\phi(\cdot)] + \hbar S_1[\phi(\cdot)] + \frac{\hbar^2}{2!} S_2[\phi(\cdot)] + \ldots$$

and

$$E_0 \simeq \hbar \left\{ E_0(0) + \hbar E_1(0) + \frac{\hbar^2}{2!} E_2(0) + \ldots \right\}.$$

In the foregoing formulas $\phi(\cdot)$ symbolizes a real-valued distribution on $\mathbb{R}^3$ belonging to a certain Sobolov ‘trace’ space that we shall characterize more precisely below. In accordance with our strategy for solving the functional
Hamilton-Jacobi equation (6.30) each such \( \phi(\cdot) \) will be taken to represent boundary data, induced on the \( t = 0 \) hypersurface of (Euclidean)

\[
\mathbb{R}^4 = \{(t,x)| t \in \mathbb{R}, x \in \mathbb{R}^3\},
\]
for a real (distributional) scalar field \( \Phi \) defined on the half-space

\[
\mathbb{R}^4^- := (-\infty,0] \times \mathbb{R}^3.
\]

Here \( \Phi \) plays the role of the curve \( \gamma : (-\infty,0] \rightarrow \mathbb{R}^n \) in the quantum mechanics problem and \( \phi(\cdot) \) the role of its right endpoint \( (x^1, \ldots, x^n) \).

By generalizing the technique sketched above for the quantum mechanics problem the author, together with Marini and Maitra, has proven the existence of a ‘fundamental solution’, \( S_{(0)}[\phi(\cdot)] \), to Eq. (6.30) by first establishing the existence of unique minimizers, \( \Phi_\phi \), for the Euclidean-signature action functional

\[
I_{es}[\Phi] := \int_{\mathbb{R}^3} \int_{-\infty}^0 \left\{ \frac{1}{2} \dot{\Phi}^2 + \frac{1}{2} \nabla \Phi \cdot \nabla \Phi + \frac{1}{2} m^2 \Phi^2 + \lambda \Phi^4 \right\} dt \, d^3x
\]

for ‘arbitrary’ boundary data \( \phi(\cdot) \), prescribed at \( t = 0 \) and then setting

\[
S_{(0)}[\phi(\cdot)] = I_{es}[\Phi_\phi].
\]

This was accomplished by defining the action functional \( I_{es}[\Phi] \) on the Sobolov space \( H^1(\mathbb{R}^4^-, \mathbb{R}) \), with boundary data naturally induced on the corresponding trace space, and proving that this functional is coercive, weakly (sequentially) lower semi-continuous and convex. Through an application of the (Banach space) implicit function theorem one then proved that the functional \( S_{(0)}[\phi(\cdot)] \) so-defined is Fréchet smooth throughout its (Sobolev trace space) domain of definition and that it indeed satisfies the (Euclidean-signature-vanishing-energy) functional Hamilton-Jacobi equation,

\[
\frac{1}{2} \int_{\mathbb{R}^3} \left| \frac{\delta S_{(0)}[\phi(\cdot)]}{\delta \phi(x)} \right|^2 d^3x = \int_{\mathbb{R}^3} \left\{ \frac{1}{2} \nabla \phi \cdot \nabla \phi(x) + \frac{1}{2} m^2 \phi^2(x) + \lambda \phi^4(x) \right\} d^3x,
\]

and thus provides the fundamental solution that one needs for the computation of all higher order quantum corrections [2]. These analytical methods were shown to work equally well in lower spatial dimensions for certain higher-order nonlinearities, allowing, for example, \( \Phi^6 \) in (Euclidean) \( \mathbb{R}^{3^-} \) and \( \Phi^p \) for any even \( p > 2 \) in \( \mathbb{R}^{2^-} \), and also for more general convex polynomial interaction potentials \( \mathcal{P}(\Phi) \), allowing terms of intermediate degrees, replacing the \( \frac{1}{2} m^2 \Phi^2 + \lambda \Phi^4 \) of the example above. These correspond precisely to the usual ‘renormalizable’ cases when treated by more conventional quantization methods.

To proceed with the calculation of higher-order quantum corrections one will need to \textit{regularize} the formal functional Laplacians that arise in the associated linear transport equations and allow the various ‘constants’ that appear in the Hamiltonian (e.g., \( m \) and \( \lambda \) in the above example) to ‘run’ with the cutoff introduced thereby, as part of the procedure of \textit{renormalization}. 
The details of this renormalization program, well-known within the standard perturbation formalism, are currently under development within the framework of the present setup. A main motivation for pursuing it though is the expectation that the Euclidean-signature semi-classical approach will ultimately lead to much more accurate approximations for wave functionals and their associated, non-gaussian integration measures than those generated by conventional (Rayleigh/Schrödinger) perturbation theory.

In continuing research the authors of Refs. [1] and [2] are currently applying these (Euclidean-signature, semi-classical) ideas to the quantization of Yang-Mills fields [3]. While the methods in question apply equally well to both 3 and 4 dimensional gauge theories, we shall focus here on the physically most interesting case of Yang-Mills fields in 4 spacetime dimensions. The formal Schrödinger operator for this problem is expressible as

$$\hat{H}_{YM} := \int_{\mathbb{R}^3} \sum_i \left\{ \frac{-\hbar^2}{2} \sum_{i=1}^{3} \frac{\delta}{\delta A^I_i(x)} \frac{\delta}{\delta A^I_i(x)} + \frac{1}{4} \sum_{j,k=1}^{3} F^I_{jk} F^I_{jk} \right\} d^3x$$

where the index $I$ labels a basis for the Lie algebra of the gauge structure group, $A^I_k$ is the spatial connection field with curvature

$$F^I_{jk} = \partial_j A^I_k - \partial_k A^I_j + g [A_j, A_k]^I$$

and $g$ is the gauge coupling constant.

As in the case of scalar field theory the functional Laplacian requires regularization to be well-defined even when acting on smooth functionals but, since the influence of this regularization will not be felt until higher order quantum ‘loop’ corrections are computed, we can temporarily ignore this refinement here and attempt first to construct a (gauge invariant) fundamental solution, $S(0)[A(\cdot)]$, to the Euclidean-signature-vanishing-energy Hamilton-Jacobi equation

$$\int_{\mathbb{R}^3} \sum_i \left\{ \frac{1}{2} \sum_{i=1}^{3} \frac{\delta S(0)}{\delta A^I_i(x)} \frac{\delta S(0)}{\delta A^I_i(x)} - \frac{1}{4} \sum_{j,k=1}^{3} F^I_{jk} F^I_{jk} \right\} d^3x = 0$$

by seeking minimizers of the corresponding Euclidean-signature action functional in the form of connections defined in $\mathbb{R}^{4-} = (-\infty, 0) \times \mathbb{R}^3$ with boundary data prescribed at $t = 0$.

Using the techniques developed in [55, 56, 57, 58, 59] and [60] one can indeed establish the existence of such minimizers for ‘arbitrary’ boundary data lying in an appropriate trace Sobolev space but, since a full verification of the properties expected for the functional $S(0)[A(\cdot)]$ has not yet been completed we shall postpone giving a more precise characterization of our (anticipated) analytical results until a later time.

The self-interactions of ‘gluons’ (the quanta of the Yang-Mills field) are closely connected to the non-abelian character of the associated gauge group. Thus a conventional perturbative approach to quantization, which disregards these interactions at lowest order, necessarily ‘approximates’ the
gauge group as well, replacing it with the abelian structure group of the associated free field theory (i.e., several copies of the Maxwell field labelled by the index $I$), and then attempts to reinstate both the interactions and the non-commutative character of the actual gauge group gradually, through the development of series expansions in the Yang-Mills coupling constant. By contrast the Euclidean-signature-semi-classical program that we are advocating for the Yang-Mills problem has the advantage of maintaining full, non-abelian gauge invariance at every order of the calculation and of generating globally defined (approximate) wave functionals on the naturally associated Yang-Mills configuration manifold.

Though much remains to be done to complete the program sketched above the initial results are sufficiently promising that one is highly motivated to look ahead and ask — could the same ideas be applied to Einstein gravity?

7. Euclidean-Signature Asymptotic Methods and the Wheeler-DeWitt Equation

Globally hyperbolic spacetimes, $\{(^{(4)}V, ^{(4)}g)\}$, are definable over manifolds with the product structure, $^{(4)}V \approx M \times \mathbb{R}$. We shall focus here on the ‘cosmological’ case for which the spatial factor $M$ is a compact, connected, orientable 3-manifold without boundary. The Lorentzian metric, $^{(4)}g$, of such a spacetime is expressible, relative to a time function $x^0 = t$, in the 3+1-dimensional form

$$^{(4)}g = ^{(4)}g_{\mu\nu} \, dx^\mu \otimes dx^\nu$$

$$= -N^2 dt \otimes dt + \gamma_{ij}(dx^i + Y^i dt) \otimes (dx^j + Y^j dt)$$

wherein, for each fixed $t$, the Riemannian metric

$$\gamma = \gamma_{ij} dx^i \otimes dx^j$$

is the first fundamental form induced by $^{(4)}g$ on the corresponding $t =$ constant, spacelike hypersurface. The unit, future pointing, timelike normal field to the chosen slicing (defined by the level surfaces of $t$) is expressible in terms of the (strictly positive) ‘lapse’ function $N$ and ‘shift vector’ field $Y^i \frac{\partial}{\partial x^i}$ as

$$^{(4)}n = ^{(4)}n^\alpha \frac{\partial}{\partial x^\alpha} = \frac{1}{N} \frac{\partial}{\partial t} - \frac{Y^i}{N} \frac{\partial}{\partial x^i}$$

or, in covariant form, as

$$^{(4)}n = ^{(4)}n_\alpha dx^\alpha = -N \, dt.$$

The canonical spacetime volume element of $^{(4)}g$, $\mu_{^{(4)}g} := \sqrt{-\det ^{(4)}g}$, takes the 3+1-dimensional form

$$\mu_{^{(4)}g} = N \mu_\gamma$$

where $\mu_\gamma := \sqrt{\det \gamma}$ is the volume element of $\gamma$. 
In view of the compactness of $M$ the Hilbert and ADM action functionals, evaluated on domains of the product form, $\Omega = M \times I$, with $I = [t_0, t_1] \subset \mathbb{R}$, simplify somewhat to

\[
I_{\text{Hilbert}} := \frac{c^3}{16\pi G} \int_{\Omega} \sqrt{-\det (4)g} (4)R^{(4)}g \, d^4x \\
= \frac{c^3}{16\pi G} \int_{\Omega} \left\{ N\mu_\gamma \left( K^{ij}K_{ij} - (tr_\gamma K)^2 \right) + N\mu_\gamma^{(3)}R(\gamma) \right\} d^4x \\
+ \frac{c^3}{16\pi G} \int_{M} (-2\mu_\gamma tr_\gamma K) d^3x \bigg|_{t_0}^{t_1} \\
:= I_{\text{ADM}} + \frac{c^3}{16\pi G} \int_{M} (-2\mu_\gamma tr_\gamma K) d^3x \bigg|_{t_0}^{t_1}
\] (7.6)

wherein $(4)R^{(4)}g$ and $(3)R(\gamma)$ are the scalar curvatures of $(4)g$ and $\gamma$ and where

\[
(7.7) \quad K_{ij} := \frac{1}{2N} \left( -\gamma_{ij,t} + Y_{i|j} + Y_{j|i} \right)
\]

and

\[
(7.8) \quad tr_\gamma K := \gamma^{ij}K_{ij}
\]
designate the second fundamental form and mean curvature induced by $(4)g$ on the constant $t$ slices. In these formulas spatial coordinate indices, $i, j, k, \ldots$, are raised and lowered with $\gamma$ and the vertical bar, $'|'$, signifies covariant differentiation with respect to this metric so that, for example, $Y_{i|j} = \nabla_j(\gamma)\gamma_{i\ell}Y^\ell$. When the variations of $(4)g$ are appropriately restricted, the boundary term distinguishing $I_{\text{Hilbert}}$ from $I_{\text{ADM}}$ makes no contribution to the field equations and so can be discarded.

Writing

\[
(7.9) \quad I_{\text{ADM}} := \int_{\Omega} \mathcal{L}_{\text{ADM}} d^4x,
\]

with Lagrangian density

\[
(7.10) \quad \mathcal{L}_{\text{ADM}} := \frac{c^3}{16\pi G} \left\{ N\mu_\gamma \left( K^{ij}K_{ij} - (tr_\gamma K)^2 \right) + N\mu_\gamma^{(3)}R(\gamma) \right\},
\]

one defines the momentum conjugate to $\gamma$ via the Legendre transformation

\[
(7.11) \quad p^{ij} := \frac{\partial \mathcal{L}_{\text{ADM}}}{\partial \gamma_{ij,t}} = \frac{c^3}{16\pi G} \mu_\gamma \left( -K^{ij} + \gamma^{ij}tr_\gamma K \right)
\]

so that $p = p^{ij} \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j}$ is a symmetric tensor density induced on each $t = \text{constant slice}$.

In terms of the variables $\{\gamma_{ij}, p^{ij}, N, Y^i\}$ the ADM action takes the Hamiltonian form

\[
(7.12) \quad I_{\text{ADM}} = \int_{\Omega} \left\{ p^{ij} \gamma_{ij,t} - N\mathcal{H}_\perp(\gamma, p) - Y^i\mathcal{J}_i(\gamma, p) \right\} d^4x
\]
where
\begin{equation}
(7.13) \quad \mathcal{H}_\perp(\gamma, p) := \left(\frac{16\pi G}{c^3}\right) \left(\frac{p^{ij}p_{ij} - \frac{1}{2}(p^m_m)^2}{\mu_\gamma}\right) - \left(\frac{c^3}{16\pi G}\right) \mu_\gamma (3) R(\gamma)
\end{equation}
and
\begin{equation}
(7.14) \quad J_i(\gamma, p) := -2 p^j_{\ |j}. \tag{7.14}
\end{equation}

Variation of \( I_{ADM} \) with respect to \( N \) and \( Y^i \) leads to the Einstein (‘Hamiltonian’ and ‘momentum’) constraint equations
\begin{equation}
(7.15) \quad \mathcal{H}_\perp(\gamma, p) = 0, \quad J_i(\gamma, p) = 0,
\end{equation}
whereas variation with respect to the canonical variables, \( \{\gamma_{ij}, p^{ij}\} \), gives rise to the complementary Einstein evolution equations in Hamiltonian form,
\begin{equation}
(7.16) \quad \gamma_{ij,t} = \frac{\delta H_{ADM}}{\delta p^{ij}}, \quad p^{ij}_{\ |t} = -\frac{\delta H_{ADM}}{\delta \gamma_{ij}}
\end{equation}
where \( H_{ADM} \) is the ‘super’ Hamiltonian defined by
\begin{equation}
(7.17) \quad H_{ADM} := \int_M \left(N \mathcal{H}_\perp(\gamma, p) + Y^i J_i(\gamma, p)\right) d^3x.
\end{equation}

The first of equations (7.16) regenerates (7.7) when the latter is reexpressed in terms of \( p \) via (7.11). Note that, as a linear form in the constraints, the super Hamiltonian vanishes when evaluated on any solution to the field equations. There are neither constraints nor evolution equations for the lapse and shift fields which are only determined upon making, either explicitly or implicitly, a choice of spacetime coordinate gauge. Bianchi identities function to ensure that the constraints are preserved by the evolution equations and thus need only be imposed ‘initially’ on an arbitrary Cauchy hypersurface. Well-posedness theorems for the corresponding Cauchy problem exist for a variety of spacetime gauge conditions \([61, 62]\).

A formal ‘canonical’ quantization of this system begins with the substitutions
\begin{equation}
(7.18) \quad p^{ij} \rightarrow \hbar \frac{\delta}{\delta \gamma_{ij}},
\end{equation}

\begin{equation}
\text{together with a choice of operator ordering, to define quantum analogues} \quad \hat{\mathcal{H}}_\perp(\gamma, \frac{\hbar}{i} \frac{\delta}{\delta \gamma}) \text{ and } \hat{J}_i(\gamma, \frac{\hbar}{i} \frac{\delta}{\delta \gamma}) \text{ of the Hamiltonian and momentum constraints. These are then to be imposed, à la Dirac, as restrictions upon the allowed quantum states, regarded as functionals, } \Psi[\gamma], \text{ of the spatial metric, by setting}
\end{equation}
\begin{equation}
(7.19) \quad \hat{\mathcal{H}}_\perp \left(\gamma, \frac{\hbar}{i} \frac{\delta}{\delta \gamma}\right) \Psi[\gamma] = 0,
\end{equation}
and
\begin{equation}
(7.20) \quad \hat{J}_i \left(\gamma, \frac{\hbar}{i} \frac{\delta}{\delta \gamma}\right) \Psi[\gamma] = 0.
\end{equation}
The choice of ordering in the definition of the quantum constraints \( \{ \hat{H}_\perp, \hat{J}_i \} \) is highly restricted by the demand that the commutators of these operators should ‘close’ in a natural way without generating ‘anomalous’ new constraints upon the quantum states.

While a complete solution to this ordering problem does not currently seem to be known it has long been realized that the operator, \( \hat{J}_i(\gamma, \hbar \ddelta \delta \gamma) \), can be consistently defined so that the quantum constraint equation (7.20), has the natural geometric interpretation of demanding that the wave functional, \( \Psi[\gamma] \), be invariant with respect to the action (by pullback of metrics on \( M \)) of Diff\(^0\)(\( M \)), the connected component of the identity of the group, Diff\(^+\)(\( M \)), of orientation preserving diffeomorphisms of \( M \), on the space, \( \mathcal{M}(M) \), of Riemannian metrics on \( M \). In other words the quantized momentum constraint (7.20) implies, precisely, that

\[
\Psi[\varphi^* \gamma] = \Psi[\gamma]
\]

\( \forall \varphi \in \text{Diff}^0(M) \) and \( \forall \gamma \in \mathcal{M}(M) \). In terminology due to Wheeler wave functionals can thus be regarded as passing naturally to the quotient ‘superspace’ of Riemannian 3-geometries \([28, 29, 63]\) on \( M \),

\[
\mathcal{S}(M) := \frac{\mathcal{M}(M)}{\text{Diff}^0(M)}.
\]

Insofar as a consistent factor ordering for the Hamiltonian constraint operator, \( \hat{H}_\perp(\gamma, \hbar \ddelta \delta \gamma) \), also exists, one will be motivated to propose the (Euclidean-signature, semi-classical) ansatz

\[
\Psi_0[\gamma] = e^{-S_0[\gamma]\hbar}\]

for a ‘ground state’ wave functional \( \Psi_0[\gamma] \). In parallel with our earlier examples, the functional \( S_0[\gamma] \) is assumed to admit a formal expansion in powers of \( \hbar \) so that one has

\[
S_0[\gamma] = S_{(0)}[\gamma] + \hbar S_{(1)}[\gamma] + \frac{\hbar^2}{2!} S_{(2)}[\gamma] + \cdots + \frac{\hbar^k}{k!} S_{(k)}[\gamma] + \cdots.
\]

Imposing the momentum constraint (7.20) to all orders in \( \hbar \) leads to the conclusion that each of the functionals, \( \{ S_{(k)}[\gamma]; k = 0, 1, 2, \ldots \} \), should be invariant with respect to the aforementioned action of Diff\(^0\)(\( M \)) on \( \mathcal{M}(M) \), ie, that

\[
S_{(k)}[\varphi^* \gamma] = S_{(k)}[\gamma], \quad k = 0, 1, 2, \ldots
\]

\( \forall \varphi \in \text{Diff}^0(M) \) and \( \forall \gamma \in \mathcal{M}(M) \).

Independently of the precise form finally chosen for \( \hat{H}_\perp(\gamma, \hbar \ddelta \delta \gamma) \), the leading order approximation to the Wheeler-DeWitt equation,

\[
\hat{H}_\perp \left( \gamma, \frac{\hbar \ddelta \delta \gamma}{i} \right) e^{-S_{(0)}[\gamma]/\hbar - S_{(1)}[\gamma] - \cdots} = 0,
\]
for the ground state wave functional will, inevitably, reduce to the Euclidean-signature Hamilton-Jacobi equation

$$ \left( \frac{16\pi G}{c^3} \right)^2 \left( \gamma_{ik} \gamma_{jl} - \frac{1}{2} \gamma_{ij} \gamma_{kl} \right) \frac{\delta S(0)}{\delta \gamma_{ij}} \frac{\delta S(0)}{\delta \gamma_{kl}} + \mu_\gamma (3) R(\gamma) = 0. $$

This equation coincides with that obtained from making the canonical substitution,

$$ p^{ij} \rightarrow \delta S(0)[\gamma] \frac{\delta S(0)}{\delta \gamma_{ij}}, $$

in the Euclidean-signature version of the Hamiltonian constraint,

$$ H_{\perp \text{Eucl}} := - \left( \frac{16\pi G}{c^3} \right) \left( (p^{ij} p_{ij} - \frac{1}{2} (p^m_m)^2) - \left( \frac{c^3}{16\pi G} \right) \mu_\gamma (3) R(\gamma) \right) = 0, $$

that, in turn, results from repeating the derivation sketched above for $I_{\text{ADM}}$ but now for the Riemannian metric form

$$ (4) g_{\mid \text{Eucl}} = (4) g_{\mu\nu} \bigg|_{\text{Eucl}} dx^\mu \otimes dx^\nu = N \bigg|_{\text{Eucl}}^2 dt \otimes dt + \gamma_{ij} (dx^i + Y^i dt) \otimes (dx^j + Y^j dt) $$

in place of (7.1). The resulting functional $I_{\text{ADM Eucl}}$ differs from $I_{\text{ADM}}$ only in the replacements $H_{\perp (\gamma, p)} \rightarrow H_{\perp \text{Eucl}}(\gamma, p)$ and $N \rightarrow N \bigg|_{\text{Eucl}}$.

The essential question that now comes to light is thus the following:

Is there a well-defined mathematical method for establishing the existence of a $\text{Diff}^0(M)$-invariant, fundamental solution to the Euclidean-signature functional differential Hamilton-Jacobi equation (7.27)?

In view of the field theoretic examples discussed in Section 6 one’s first thought might be to seek to minimize an appropriate Euclidean-signature action functional subject to suitable boundary and asymptotic conditions. But, as is well-known from the Euclidean-signature path integral program [64], the natural functional to use for this purpose is unbounded from below within any given conformal class — one can make the functional arbitrarily large and negative by deforming any metric $(4) g_{\mid \text{Eucl}}$ with a suitable conformal factor [39, 64].

But the real point of the constructions of Section 6 was not to minimize action functionals but rather to generate certain ‘fundamental sets’ of solutions to the associated Euler-Lagrange equations upon which the relevant action functionals could then be evaluated. But the Einstein equations, in vacuum or even allowing for the coupling to conformally invariant matter sources, encompass, as a special case, the vanishing of the 4-dimensional scalar curvature, $(4) R^{(4) g_{\mid \text{Eucl}}}$. Thus there is no essential loss in generality, and indeed a partial simplification of the task at hand to be
gained, by first restricting the relevant, Euclidean-signature action functional to the ‘manifold’ of Riemannian metrics satisfying (in the vacuum case) \( (4) R((4) g)_{\text{Eucl}} = 0 \) and then seeking to carry out a constrained minimization of this functional.

Setting \( (4) R((4) g)_{\text{Eucl}} = 0 \) freezes out the conformal degree of freedom that caused such consternation for the Euclidean path integral program \([39, 64]\), wherein one felt obligated to integrate over all possible Riemannian metrics having the prescribed boundary behavior, but is perfectly natural in the present context and opens the door to appealing to the positive action theorem which asserts that the relevant functional is indeed positive when evaluated on arbitrary, asymptotically Euclidean metrics that satisfy \( (4) R((4) g)_{\text{Eucl}} \geq 0 \) \([65, 66, 67, 68]\).

Another complication of the Euclidean path integral program was the apparent necessity to invert, by some still obscure means, something in the nature of a ‘Wick rotation’ that had presumably been exploited to justify integrating over Riemannian, as opposed to Lorentzian-signature, metrics. Without this last step the formal ‘propagator’ being constructed would presumably be that for the Euclidean-signature variant of the Wheeler-DeWitt equation and not the actual Lorentzian-signature version that one wishes to solve. In ordinary quantum mechanics the corresponding, well-understood step is needed to convert the Feynman-Kac propagator, derivable by rigorous path-integral methods, back to one for the actual Schrödinger equation.

But in the present setting no such hypothetical ‘Wick rotation’ would ever have been performed in the first place so there is none to invert. Our focus throughout is on constructing asymptotic solutions to the original, Lorentz-signature Wheeler-DeWitt equation and not to its Euclidean-signature counterpart. That a Euclidean-signature Einstein-Hamilton-Jacobi equation emerges in this approach has the very distinct advantage of leading one to specific problems in Riemannian geometry that may well be resolvable by established mathematical methods. By contrast, path integral methods, even for the significantly more accessible gauge theories discussed in Section 6, would seem to require innovative new advances in measure theory for their rigorous implementation. Even the simpler scalar field theories, when formulated in the most interesting case of four spacetime dimensions, seem still to defy realization by path integral means. It is conceivable, as was suggested in the concluding section of [1], that focusing predominantly on path integral methods to provide a ‘royal road’ to quantization may, inadvertently, render some problems more difficult to solve rather than actually facilitating their resolution.

The well-known ‘instanton’ solutions to the Euclidean-signature Yang-Mills equations present a certain complication for the semi-classical program that we are advocating in that they allow one to establish the
existence of non-unique minimizers for the Yang-Mills action functional for certain special choices of boundary data [3]. This in turn can obstruct the global smoothness of the corresponding solution to the Euclidean-signature Hamilton-Jacobi equation. While it is conceivable that the resulting, apparent need to repair the associated ‘scars’ in the semi-classical wave functionals may have non-perturbative implications for the Yang-Mills energy spectrum — of potential relevance to the ‘mass-gap’ problem — no such corrections to the spectrum are expected or desired for the gravitational case. Thus it is reassuring to note that analogous ‘gravitational instanton’ solutions to the Euclidean-signature Einstein equations have been proven not to exist [39].

We conclude by noting that other interesting, generally covariant systems of field equations exist to which our (‘Euclidean-signature semi-classical’) quantization methods could also be applied. Classical relativistic ‘membranes’, for example, can be viewed as the evolutions of certain embedded submanifolds in an ambient spacetime — their field equations determined by variation of the volume functional of the timelike ‘worldsheets’ being thereby swept out. The corresponding Hamiltonian configuration space for such a system is comprised of the set of spacelike embeddings of a fixed $n - 1$ dimensional manifold $M$ into the ambient $n + k$ dimensional spacetime, each embedding representing a possible spacelike slice through some $n$-dimensional membrane worldsheet. Upon canonical quantization wave functionals are constrained (by the associated, quantized momentum constraint equation) to be invariant with respect to the induced action of $\text{Diff}^0(M)$ on this configuration space of embeddings. The corresponding quantized Hamiltonian constraint, imposed à la Dirac, provides the natural analogue of the Wheeler-DeWitt equation for this problem.

A solution to the operator ordering problem for these quantized constraints, when the ambient spacetime is Minkowskian, was proposed by the author in [69]. For the compact, codimension one case (i.e., when $M$ is compact and $k = 1$) it is not difficult to show that the relevant Euclidean-signature Hamilton-Jacobi equation has a fundamental solution given by the volume functional of the maximal, spacelike hypersurface that uniquely spans, à la Plateau, the arbitrarily chosen embedding [70]. It would be especially interesting to see whether higher-order quantum corrections and excited state wave functionals can be computed for this system in a way that realizes a quantum analogue of general covariance.

Acknowledgments

The author is grateful to the Albert Einstein Institute in Golm, Germany for hospitality and support during the course of his work on this article. This research was supported in part by National Science Foundation grant PHY-1305766 to Yale University.
References


[41] Wherein, however, one needs to take particular, complex moments of inertia, namely the cube roots of unity to make the correspondence (Thibault Damour, private communication). See also the comment in [40].


[48] See, for example the article, A Brief Introduction to Singularity Theory by A. O. Remizov (Trieste, 2010). Lemma 2 of Section 1.3 gives the relevant construction; http://sissa.it/fa/download/publications/remizov.pdf.

[49] c.f., eq. (3.20) of [1].

[50] See the discussion in section IIB of [1].

[52] G. Buttazzo, M. Giaquinta, and S. Hildebrandt. One-Dimensional Variational Problems — An Introduction. Clarendon, Oxford, 2005. Chapter 2 develops, in detail, Sobolev spaces on open intervals of the real line but includes a discussion (cf., p. 61) of the existence of well-defined “traces” for such distributions at (finite) endpoints. This result together with their Theorem 2.5 implies that the distributions in $H^1(I, \mathbb{R}^n)$, where $I = (-\infty, 0]$, have meaningful endpoint values at $t = 0$ and vanish at $t \downarrow -\infty$. For a different discussion of “vanishing-at-infinity” results for Sobolev spaces see Chapter 5 of R. Richtmeyer, Principles of Advanced Mathematical Physics (Springer-Verlag, Berlin Heidelberg, 1978), Vol. I.

[53] See section IIA of [1].

[54] See section IIB of [1].


[63] c.f., chapter 43 of [8].


[70] V. Moncrief. Unpublished. This extends a result contained in [69] to the case of curved, maximal hypersurfaces spanning an arbitrary, spacelike embedding.