An Introduction to Quantum Cosmology

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Abstract

We set out to provide an introduction to the area of quantum cosmology. We begin by introducing quantized general relativity or quantum geometrodynamics on which quantum cosmology is based, discussing issues in this construction. A wave function of the universe is constructed whose dynamics are governed by the Wheeler-DeWitt equation, the quantized Hamiltonian constraint of the system. It is found that, due to ambiguities arising from operator ordering issues in the Wheeler-DeWitt equation and issues in the path integral formulation of the wave function, it is often unreliable to work beyond the semiclassical approximation. In this approximation, the WKB wave function may employed to approximate the wave function.

We construct a probability measure valid in this règime with a view to making measurable predictions. In order to make such predictions, it is also found to be necessary to prescribe quantum mechanical boundary conditions on the wave function. There have been various proposals for making such prescriptions. These proposals must be viewed as, at best, being supplementary fundamental physical laws.

The 'problem of time' is analyzed for quantum cosmology or, more precisely, for reparametrization invariant systems. We outline three approaches to the problem: time before quantization, time after quantization and the timeless approach. We conclude that the most likely candidate is the timeless approach and focus on a particular evolving constants of motion form of this approach. This approach is motivated and analyzed. We find that a unique, with an additional physical argument, Hilbert space structure may be constructed using refined algebraic quantization here.

We introduce the two most prominent proposals for prescribing such boundary conditions: the no-boundary and tunneling wave functions. We give the definitions and interpretations of the quantum cosmological wave function satisfying these conditions.

Working in the semiclassical approximation, various predictions of quantum cosmology are studied. We particularly focus on inflation for the case of a closed Friedmann-Robertson-Walker model, finding

that both the no-boundary and tunneling wave functions are peaked about classical inflationary solutions. We then ask whether sufficient inflation is predicted by these wave functions, finding that on a history-by-history basis, with a physically motivated upper cut-off for the initial value of the scalar field, the tunneling wave function is found to predict sufficient inflation whereas the no-boundary wave function is not.

An argument is outlined for the inaccuracy of this result for the no-boundary wave function, proposing that it should be multiplied by a volume factor. The resulting volume weighted probability is found to predict sufficient inflation for both the tunneling and no-boundary wave functions.

We proceed to examine the probability in for the no-boundary universe in such a model to exhibit either an initial singularity or a bounce. Again a distinction is seen between the history-by-history probability, which is seen to predict a bounce, and the fully conditioned probability which is seen to predict an initial singularity.

Structure formation may be described in quantum cosmology by introducing quantum perturbations about a semiclassical spatially homogeneous and isotropic background. This provides perhaps the greatest potential in terms of falsifiable predictions. A spectrum for such anisotropies may be predicted for both boundary proposals. A vacuum state is also found to be selected in this analysis, the Bunch-Davies vacuum state. This is often assumed to be the vacuum state in cosmological calculations and the fact that this is selected by both boundary proposals is encouraging.

A non-physical analysis studying topology change in Friedmann-Robertson-Walker models with non-trivial topology is outlined. By non-physical, we mean that the boundary conditions were not chosen by any physical argument, rather for convenience. While the system is non-physical and the exact results are, in some senses, meaningless, a characteristic 'arrow of topology change' is observed two of the studied cases. This qualitative behaviour may well carry over to physical cases.

The final chapter focuses on the decoherent or consistent histories approach to quantum mechanics. We discuss some of the conceptual foundational issues arising for quantum cosmology. It is noted that the Copenhagen interpretation is incompatible with quantum cosmology. Alternatives are found in the form of generalized quantum mechanics.

We discuss how to formulate a well-defined probability measure for reparametrization invariant systems and find that, in the semiclassical limit, the probability measure that we have constructed indeed coincides with that found earlier in the thesis. The analysis of decoherence between WKB components is also studied. This is vital for the predictive power of quantum cosmology and, reassuringly, this components are found to decohere. Care was taken here as the most obvious candidates for class operators were seen to suffer from the Zeno effect.

We conclude by extracting predictions from this approach for an initial singularity or bounce in a flat Friedmann-Robertson-Walker model. There are concerns regarding the definition of the class operators here with regards to the Zeno effect but we ignore such concerns and proceed with the analysis. It is found that, for a general state, the probability for an initial singularity approaches unity.

We conclude by noting that although there are various fundamental issues in the construction of the quantum cosmological framework, the resulting science is seen to objectively predict much of the qualitative behaviour observed in the universe. The theory is falsifiable and may well provide a guide for other more fundamental theories.

Contents

Introduction

This thesis is intended to replicate a short lecture series providing an introduction to quantum cosmology for first year postgraduate students. Many such introductory articles have been written in the past and indeed we shall follow the basic structure of these articles, [29] [98] [60] [79] [78], for the first four chapters. In order for this thesis to begin at a suitable level for the aforementioned intended readers and also to include the more recent frontier research in the field, a balance was struck in terms of the level of detail. The first three chapters are intended to be as self-contained as possible for those unfamiliar with the field. The latter two chapters have more 'missing' steps yet the relevant literature is always referenced.

We shall be focusing particularly on the physical foundations of the theory rather than the predictions. A number of the predictions of the theory are outlined in *Chapter 4: The Predictions of Quantum Cosmology* as these predictions are what shall ultimately determine the validity of quantum cosmological theories. In many of these sections, the outline given is intended to provide a taste of the results rather than a rigourous analysis. As mentioned, we shall however always provide references for where a more extensive analysis is carried out.

The last chapter, *Chapter 5: A Consistent Histories Approach to Quantum Cosmology*, is the point at which this thesis diverges from the path of the previous articles. This is a more recent approach which can be used to consistently construct probability measures for closed quantum mechanical systems. We outline this formulation for reparametrization invariant systems and provide an example of a calculation for a cosmological model using this approach.

The concept of a quantum wave function of the universe may initially seem a paradox. One tends to think of quantum systems as 'small' systems, such as the atom. However, if the force(s) that govern the universe are fundamentally quantum mechanical then the universe must be a quantum mechanical system, albeit a macroscopic one. Indeed, if, as seems quite likely, when the evolution of the universe is tracked backwards a point is reached near the Planck scale, then a classical description of the universe will break down.

Quantum cosmology does not pertain to provide a complete, fundamental description of the universe, but rather provide a predictive guide for theories that do. It is a framework, based on quantized Einstein gravity or *quantum geometrodynamics*, in which the universe may be described as a closed quantum system. The validity of the approach is predicated on quantized Einstein gravity being a valid approximation to a full theory of quantum gravity at energies below the Planck scale.

Our first step will be to quantize general relativity. It is found that the concept of space-time is in contradiction with the uncertainty principle in the quantum règime. We therefore perform a $3+1$ 'split' of general relativity before quantization, obtaining the familiar Hamiltonian formalism from non-relativistic particle quantum mechanics. The four dimensional pseudo-Riemannian space-time manifold, $\mathcal{M}$, is *foliated* into a series of spacelike hypersurfaces, $\mathcal{M} = \mathbb{R} \times \Sigma$.

There are typically two approaches to quantization in quantum cosmology. The first of these is Dirac quantization. This involves the 'promotion' of the canonical variables and their conjugate momenta to operators. In the Hamiltonian formulation, we find, in particular, two secondary constraints: the Hamiltonian and momentum constraints. These constraints correspond to reparametrization invariance and diffeomorphism invariance on the three dimensional hypersurface, Σ, respectively. Reparametrization invariance is characterized here by the lack of explicit dependence on time. All time dependence is contained implicitly in the canonical variables. One may thus redefine time without changeing the dynamics of the system. These classical constraints of the system are also promoted to operators. The operators yielded from the Dirac quantization of the canonical coordinates and their conjugate momenta will form an algebra, $\mathcal{B}_{phys}$, on a physical Hilbert space, $\mathcal{H}_{phys}$.

We then require wave functionals, $\{\Psi\}$, to populate this Hilbert space. We show that the gravitational dependence of the wave function must be on the *intrinsic 3-metric* of the corresponding hypersurface, Σ. This wave functional[1], $\Psi[h_{ij}(\mathbf{x}), \Phi(\mathbf{x}), \Sigma]$, (first introduced by DeWitt [14]) is employed to describe the whole universe. It is not defined on space-time but rather is a wave function defined on 'superspace', an infinite-dimensional configuration space of Euclidean 3-metrics and matter field configurations. We discuss some of the properties of this space, in particular the its reduction to a finite-dimensional subspace of spatially homogeneous 3-metrics and matter fields, *minisuperspace*. Due to its finite-dimensionality, minisuperspace is far easier to work with; we shall exploit this in our derivations and calculations.

The dynamics of the wave function are governed by the *Wheeler-DeWitt equation*. This an analog of the functional Schrödinger equation in non-relativistic particle quantum mechanics, obtained from the Dirac quantization of the Hamiltonian constraint of geometrodynamics. This Hamiltonian constraint is in fact a property of all reparametrization invariant systems. As in the Klein-Gordon equation, there are factor ordering issues arising in this equation. We shall present two prominent choices of factor ordering. General consensus is yet to be reached on this issues.

The second method of quantization used is the path integral approach. This is used to find a quantum mechanical Hilbert space representation of the wave function. This approach was developed from that of quantum field theory in flat space-time and the quantum description of black holes. Here, however, the functional integrals over the '*histories*' of the Euclideanized 4-geometries and matter field configurations that satisfy yet to be specified boundary conditions. There are several fundamental issues in the definition of the gravitational path integral which we discuss.

These wave functionals require an inner product to form the Hilbert space, $\mathcal{H}_{phys}$. Defining a suitable inner product is not as straightforward as in non-relativistic particle mechanics, however. Quantum geometrodynamics is a reparametrization invariant system. This implies that there is no preferred external time parameter with which to describe the evolution of the system; a fundamental issue in any quantum theory of gravity, as this is seemingly incompatible with the standard quantum mechanical interpretation of time. We discuss some of the approaches to this problem with particular

[1] We shall henceforth use the term 'wave function' to describe this, as is the convention.

emphasis on the '*evolving constants of motion*' approach. This is a so-called 'timeless' approach and takes the view that time is not fundamental but rather an approximate notion of time is descibed by '*clock*' variables. Observables in this approach are constructed from operators commuting with the Hamiltonian constraint thereby preserving the reparametrization invariance of the system.

It has been argued that a well-defined Hibert space structure may still be defined despite these apparent obstacles. We will outline the *refined algebraic quantization* approach in *Refined Algebraic Quantization, Chapter 2*.

The aim of any theory must be to provide measurable predictions. In order to do so, a well-defined conserved probability measure is required. Due to ambiguities arising in the formulation of the theory, it is often unreliable to work beyond the semiclassical approximation. The wave function in this approximation is provided by the WKB wave function, Ψ_{WKB}. This wave function is a sum over 4-geometries corresponding to *saddle-points* of the original wave function or *instantons*. We will substitute this wave function into the Wheeler-DeWitt equation under the condition for classicality at late times, examining the properties of the solutions picked out. From these properties we shall attempt to construct a WKB probability measure.

There is a fundamental difference between quantum cosmological probabilities and the quantum mechanical probabilities which we are used to. In standard non-relativistic quantum mechanics, experiments are typically repeated multiple times with the free parameters varied. In cosmology, the lifetime of the universe is the length of the experiment, we have no control over the parameters and neither may it be repeated. Thus, it may be argued that a new type of probability is required. Hawking *et al.* have posited *top-down* probabilities pertaining to this. For quantum cosmological models we are also necessarily restricted to *conditional probabilities*, as we shall discuss.

For a specific solution it is necessary to impose boundary conditions on the wave function. The boundary conditions corresponding to the hypersurface, Σ, at the present universe are naturally constrained by observations. Unlike many other quantum systems though, for quantum cosmology the remaining boundary conditions for this wave function are not selected naturally from symmetries of the system. It was initially hoped, however, that the boundary conditions would be selected by mathematical consistency alone. This, unfortunately, proved unfounded and the choice of boundary conditions became an area of much research and debate. Indeed, these boundary conditions must be regarded, at best, as being supplementary fundamental physical laws.

Various proposals have been made regarding the appropriate choice of boundary conditions (e.g. [14] [38] [93] [68] [9] [84]). The foremost are the no-boundary and tunneling proposals. The no-boundary proposal considers the universe as having only a boundary at the present universe and can be considered as 'smoothing off' any initial boundary with imaginary time. The tunneling proposal suggests that the universe essentiall tunneled 'out of nothing' in analogy with the tunneling process in quantum mechanics.

In the classical description of the universe, initial conditions must be selected such that the homogeneity, isotropy and flatness that we observe in the present universe are predicted. The initial conditions are chosen such that *inflation* occurs. This is a rather unsatisfactory case of the 'the ends justifying the means' in that there is no physical reasoning in this choice, other than the fact that we will get an accurate description of the late universe as we evolve the model forward in time.

It may seem as if, in describing the universe as a quantum mechanical wave, $\Psi[h_{ij}(\mathbf{x}), \Phi(\mathbf{x}), \Sigma_t]$, we are simply replacing the problem of initial conditions with that of finding suitable boundary conditions for the wave function. However, as we have mentioned already, it is likely that the universe originated in a quantum phase. It may then be argued that the problem of boundary conditions is more fundamental than that of initial conditions. We may also propose boundary conditions on other grounds, such as a geometric argument. It is then hoped that, with the wave function selected by these means, the universe universe that we observe today will be selected by the wave function.

We proceed to examine some of the predictions of both the no-boundary and tunneling wave functions. We compare the probabilities for the amount of inflation predicted by the two; asking in particular whether sufficient inflation is predicted. A measure of the 'amount' of inflation is provided by the number of *efolds* of inflation. Around sixty five efolds of inflation are required to solve the horizon and flatness problems as well as to give the homogeneity and isotropy which we observe in the universe today.

Other predictions discussed include predictions for either an initial singularity or a classical bounce, structure formation, the arrow of time and topology change. Quantum cosmology aims to provide measurable predictions and the evolution of inhomogeneous perturbations predicted in the CMB by quantum cosmology may be measured by the MAP and PLANCK satellites in forthcoming years. Topology change is forbidden in classical cosmology, however the transition to the quantum règime opens up the probability for such changes. We shall examine some non-physical cases in the hope that these may provide an indication of some of the qualitative features in physical cases which may be examined in the future.

Quantum cosmology may also be thought of more simply as a quantum mechanical description of a closed gravitational system. Perhaps the most compelling argument for the study of quantum cosmology comes from this description. It is known that macroscopic quantum systems exhibit a strong coupling or *entanglement* to their environment. As a result, it effectively becomes impossible to talk about an isolated quantum system, unless we talk about the universe as a whole which, by definition, has no environment to couple to. Thus, if one wished to talk about a closed quantum system, the universe is the only relevant system.

Treating the universe as a quantum system, there can be no external classical observers. Thus, the Copenhagen interpretation of quantum mechanics can no longer apply. If one treats observers quantum mechanically in a *generalized quantum theory*, it is found that the wave collapse mechanism can be 'replaced' by the *decoherence mechanism.* In the final chapter, we will deal with the application of generalized quantum theory which may provide a consistent description of closed quantum mechanical systems to quantum cosmology. We focus specifically on the *decoherent or consistent histories* approach. In particular, we will look at the decoherence of WKB solutions in this framework which is vital for the predictive power of quantum cosmology. We also follow an analysis of the probability for an initial singularity or bounce in the early universe for a flat Friedmann-Robertson-Walker model.

Chapter 1

Hamiltonian Formulation of General Relativity

At the large scale interactions of cosmology, the dominant interactions are those of gravity. Thus, any quantum theory of cosmology must be built upon a quantum theory of gravity.

Indeed, the Hawking-Penrose singularity theorems [48] indicate that general relativity itself cannot provide a fundamental description of gravity in the universe. They show that the occurrence of singularities in general relativity is an inevitability under reasonable physical assumptions, yet there is no given prescription for how matter behaves at these singularity. It is hoped that a quantum theory of gravity would provide such a fundamental description.

As there is presently not a full theory of quantum gravity, we will concern ourselves with energy scales below the Planck scale. At these energies, quantized general relativity or *quantum geometrodynamics*, as proposed by [3], should provide an "effective" low energy approximation. Essentially, the space-time manifold, $\mathcal{M}$, from relativity is split into spacelike hypersurfaces labeled by a timelike coordinate, t, and a Hamiltonian formalism adopted, in analogy with non-relativistic quantum mechanics. Quantization is then carried out in the familiar way [15] promoting canonical variables and momenta to operators as will be described in Chapter 2. A detailed and insightful account of this approach is given in [76].

The Decomposition of Lorentzian Space-Time

Indeed, directly quantizing space-time would contradict the uncertainty principle. Suppose one knows the precise 3-geometry at an instant; if one then also knows the time rate of change of that 3-geometry at that instant, then the precise evolution of that 3-geometry is known. One therefore must set about decomposing our space-time into a form consistent with the quantum principle.

Penrose conjectured [86] that all physically reasonable space-times are globally hyperbolic (*see Appendix*). We shall follow this conjecture and restrict ourselves to the case of globally hyperbolic Lorentzian space-times $\{(\mathcal{M}, g)\}$. These space-times possess a number of important properties,

- The occurrence of naked singularities is prohibited in such space-times [86].
- A Cauchy surface Σ may be defined in the space-time such that it uniquely determines the while space-time once initial data is specified on it (in fact, this is the definition of a globally hyperbolic manifold used by Wald [96]).
- It has been proven [51] that, for such space-times, a global 'time' function, f, may always be found such that each spacelike hypersurface on which $f = constant$ is a Cauchy surface.

Using this third property, one may now proceed to *foliate* the Lorentzian space-time $(\mathcal{M}, g)$ into a set of 3-dimensional spacelike hypersurfaces, $\{\Sigma_t\}$, labeled by some global time function, t. One thus finds,

$$\mathcal{M} \cong \mathbb{R} \times \Sigma \tag{1.1}$$

It is clear that the topology of the space-time is now fixed. In the classical theory, changes in topology for a time orientable manifold with a Lorentzian metric are necessarily associated with singularities or closed timelike curves [20]. These are prohibited for globally hyperbolic space-times and our restriction is hence motivated. However, some have argued that this restriction is a flaw in the canonical approach to quantum gravity. In the path integral approach[1], topology change may

[1]See *Path Integral Quantization, Chapter 2.*

be consistently accommodated. We shall discuss the possibility of topology change within quantum cosmology in *Topology Change, Chapter 4*.

Consider an initial hypersurface Σ in $(\mathcal{M}, g)$; using the second property above, this may be chosen such that it is a Cauchy surface. Suppose one is given initial date $h_{ij}(\mathbf{x}), \Phi(\mathbf{x})$, where $\mathbf{x}$ are the coordinates of a chart, U, on Σ, h is the *intrinsic 3-metric* induced by g on the initial hypersurface and Φ is a single matter scalar field. The hypersurfaces, Σ_t, may then be 'stitched' back together using *Cauchy development* to recover the original manifold, $\mathcal{M}$.

Explicitly, there exists an embedding, $\epsilon_t : \Sigma \to \mathcal{M}$ for each t where $\Sigma_t \equiv \epsilon_t(\Sigma)$ is a spacelike submanifold of $\mathcal{M}$. Each Σ_t is endowed with an *intrinsic* 3-metric given by,

$$h_t \equiv \epsilon_t^\star g \tag{1.2}$$

where $\epsilon_t^\star : \mathcal{M} \to \Sigma$ is the pull-back by ϵ_t. (1.2) is unique for a given t; thus, for compact Σ_t, the 3-metric uniquely fixes the position of the embedding in the enveloping 4-geometry. Indeed the 3-curvature, ${}^{(3)}R$, of the hypersurface is the 'carrier of information on physical time' [4].

A diffeomorphism may be constructed using this embedding which identifies the hypersurfaces. Firstly, define a vector field on $\mathcal{M}$, $\frac{\partial}{\partial t}$, via,

$$\left.\frac{\partial}{\partial t}\right|_{\epsilon_t(p)} \equiv \frac{d}{dt}\epsilon_t(p) \tag{1.3}$$

where p is a point on Σ_t. The diffeomorphisms generated by this vector field may be used to identify the hypersurfaces, $\{\Sigma_t\}$ [23]. The vector field can be decomposed into components normal and tangential (with respect to g) to the leaves Σ_t respectively,

$$\left(\frac{\partial}{\partial t}\right)^i = \mathcal{N} n_t^i + \mathcal{N}^i \tag{1.4}$$

where $\mathbf{n}_t$ is the unit vector field normal at Σ_t.

The normal component, $\mathcal{N}$, or lapse function, generates diffeomorphisms that identify one leaf Σ_t

with the next. Thus, it can be understood as describing the temporal evolution of the hypersurface, Σ_t. More precisely, it measures the difference between the coordinate time, t, and the proper time, τ along curves normal to our hypersurfaces.

The tangential component or shift vector-field, $\mathcal{N}^i$, generates diffeomorphisms on each Σ_t. This measures the spatial evolution of the hypersurface. Suppose one has a point $\mathbf{p}$ on a hypersurface, Σ_t. Let the coordinates of this point on this hypersurface be given by $\mathbf{x}$. Let $\mathbf{n}_t$ be the normal vector field at this point. Now consider the hypersurface Σ_{t+dt}. There will be a point on this hypersurface with coordinates $\mathbf{x}$. The shift vector field provides a measure of the separation between this point and the point of intersection between the integral curve generated by $\mathbf{n}_t$. The lapse and shift are illustrated in *Figure 1.*

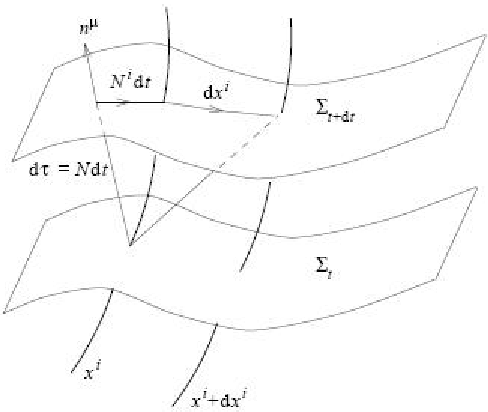

Figure 1: (Taken from [98]) *The lapse function, $\mathcal{N}$, provides a relation between the coordinate time, t, of each leaf, Σ_t, and the proper time, τ. The shift vector field relates the position on Σ_{t+dt} obtained by following the normal vector field, $\mathbf{n}$, with respect to Σ_t at a point, $\mathbf{p}$, with the point on Σ_{t+dt} with the same coordinates in a chart U (defined on both Σ_t and Σ_{t+dt}) as $\mathbf{p}$ in U.*

Formally, they can both be considered as arbitrary (gauge) functions, reflecting the freedom in foliating $\mathcal{M}$ by Σ. Indeed, although the general covariance of general relativity is no longer apparent, it is preserved through the freedom in the choice of foliation.

Assuming that $\mathcal{M}$ is globally hyperbolic, the 4-metric can be decomposed in terms of the lapse and shift as,

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = -\omega^0 \otimes \omega^0 + h_{ij}\omega^i \otimes \omega^j \tag{1.5}$$

where a basis has been chosen such that $\omega^0 = \mathcal{N}dt$ and $\omega^i = dx^i + \mathcal{N}^i dt$.

Given a spatial hypersurface, Σ_t, we not only wish to know the geometry of the hypersurface itself, which is given by the 3-metric, h_{ij}, and the intrinsic curvature tensor, ${}^{(3)}R^i{}_{jkl}(h)$, but also how the 3-geometry is embedded in the enveloping 4-geometry. This is described by the extrinsic curvature tensor (or second fundamental form)[2][3],

$$K_{\mu\nu} \equiv -\frac{1}{2}\mathcal{L}_{\mathbf{n}_t} h_{\mu\nu} \tag{1.6}$$

where $\mathcal{L}_{\mathbf{n}_t}$ is the Lie derivative with respect to the normal vector field $\mathbf{n}_t$ and $h_{\mu\nu}$ is the intrinsic 4-metric of the spatial hypersurface (also the first fundamental form in this case). The intrinsic 3-metric is extended to a four dimensional object by,

$$h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu \tag{1.7}$$

where n_μ are the components of $\mathbf{n}_t$ above, where we have dropped the "t" subscript (note that $n_\mu n^\mu = -1$). From (1.6), it is clear that the extrinsic curvature may be interpreted as the rate of change of the intrinsic metric as one travels along the normal vector field.

Assuming that the normal vector field is geodesic everywhere (i.e. $n^\nu \nabla_\nu n^\mu = 0$ with ∇ being the covariant derivative with respect to g), the extrinsic curvature takes on the form,

$$K_{\mu\nu} = -\nabla_\mu n_\nu \tag{1.8}$$

Written in terms of the lapse and shift, this becomes (*see Appendix*),

$$K_{ij} = \frac{1}{2\mathcal{N}}(D_i\mathcal{N}_j + D_j\mathcal{N}_i - \dot{h}_{ij}) \tag{1.9}$$

[2] For more on fundamental forms, see [7]

[3] This is often defined with opposite sign; this is purely conventional.

where D denotes the covariant derivative with respect to h_{ij} and the dot denotes differentiation with respect to t.

Gaussian normal coordinates[4] are coordinates that can be chosen on a manifold (or part of the manifold) which prove extremely useful. In these coordinates the shift vector and hence the time-space cross terms in the metric vanish. Thus, a spatially homogeneous ($\mathcal{N} = \mathcal{N}(t)$) and isotropic metric will take the form,

$$ds^2 = -\mathcal{N}(t)^2 dt^2 + h_{ij} dx^i dx^j \tag{1.10}$$

Using these coordinates will vastly simplify any derivations and we shall employ them henceforth.

The Action and its Classical Constraints

We shall now perform a 3+1 decomposition and derive the constraints for the Einstein-Hilbert action,

$$S_{EH} = \frac{1}{4\kappa^2} \int_{\mathcal{M}} d^4x \sqrt{-g} ({}^{(4)}R - 2\Lambda) + \frac{1}{2\kappa^2} \int_{\partial\mathcal{M}} d^3x \sqrt{h} K \tag{1.11}$$

where $\kappa^2 = 4\pi G$, ${}^{(4)}R$ is the Ricci scalar, Λ is the cosmological constant, g is the determinant of the 4-metric, h is the determinant of the 3-metric, $K \equiv K^i{}_i$ is the spatial trace of the extrinsic curvature, Λ is the cosmological constant and integration is carried out over all space-time. The second term is a surface term which vanishes under the classical field equations. In the quantum theory, we will also be considering 'off-shell' situations in which the classical field equations do not hold and, in this case, there will be contributions from this term.

We introduce the matter action,

$$S_{matter} = \int_{\mathcal{M}} d^4x \sqrt{-g} (-\frac{1}{2} g^{\mu\nu} \partial_\mu \Phi \partial_\nu \Phi - \mathcal{V}(\Phi)) \tag{1.12}$$

where Φ is a single scalar field with potential $\mathcal{V}(\Phi)$. There are many other possible ways to incorporate

[4]See [7] for further details

the matter sector into the theory, but we shall consider just this case. One may express these actions in terms of the $3+1$ formalism of the previous section to find a total action (*see Appendix*),

$$S \equiv \int dtL = \frac{1}{4\kappa^2} \int dtd^3x\mathcal{N}\sqrt{h}(K_{ij}K^{ij} - K^2 +^{(3)} R - 2\Lambda) + S_{matter} \tag{1.13}$$

Recall that we wish to find the Hamiltonian of this action before quantization. One proceeds in the manner introduced by Dirac [15]. It is found that the conjugate momenta for the lapse function and shift vector vanish, imposing primary constraints,

$$\pi^0 \equiv \frac{\delta L}{\delta \dot{\mathcal{N}}} = 0 \tag{1.14}$$

$$\pi^i \equiv \frac{\delta L}{\delta \dot{\mathcal{N}}_i} = 0 \tag{1.15}$$

The canonical momenta are given by (*see Appendix*),

$$\pi^{ij} \equiv \frac{\delta L}{\delta \dot{h}_{ij}} = -\frac{\sqrt{h}}{4\kappa^2}(K^{ij} - h^{ij}K) \tag{1.16}$$

$$\pi_\Phi \equiv \frac{\delta L}{\delta \dot{\Phi}} = \frac{\sqrt{h}}{\mathcal{N}}\left(\dot{\Phi} - \mathcal{N}^i\Phi_{,i}\right) \tag{1.17}$$

where "$_{,i}$" denotes partial differentiation with respect to the spatial coordinates $\{x^i\}$ in a chart, U. Using these definitions, one obtains a Hamiltonian (*see Appendix*),

$$H = \int d^3x(\pi^0\dot{\mathcal{N}} + \pi^i\dot{\mathcal{N}}_i + \mathcal{N}\mathcal{H} + \mathcal{N}_i\mathcal{H}^i) \tag{1.18}$$

leading to the Hamiltonian form of the action,

$$S = \int dtd^3x(\pi^0\dot{\mathcal{N}} + \pi^i\dot{\mathcal{N}}_i - \mathcal{N}\mathcal{H} - \mathcal{N}_i\mathcal{H}^i) \tag{1.19}$$

where,

$$\mathcal{H}^i = -2D_j\pi^{ij} + \mathcal{H}_{matter} \tag{1.20}$$

$$\mathcal{H} = 4\kappa^2\mathcal{G}_{ijkl}\pi^{ij}\pi^{kl} - \frac{\sqrt{h}}{4\kappa^2}({}^{(3)}R - 2\Lambda) + \mathcal{H}_{matter} \tag{1.21}$$

and

$$\mathcal{G}_{ijkl} = \frac{1}{2\sqrt{h}}(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}) \tag{1.22}$$

is the DeWitt metric [14] and we have not concerned ourselves with the matter sector, $\mathcal{H}_{matter}$, of $\mathcal{H}$. With $\mathcal{N}$ and $\mathcal{N}^i$ as Lagrange multipliers, the Hamiltonian constraint,

$$\mathcal{H} \simeq 0 \tag{1.23}$$

is found from the variation of the Hamiltonian with respect to $\mathcal{N}$. The equivalence relation here is such that we may only set $\mathcal{H}$ to zero once all Poisson brackets have been evaluated. Similarly, from the variation with respect to $\mathcal{N}^i$, the momentum constraint,

$$\mathcal{H}^i \simeq 0 \tag{1.24}$$

is obtained. These are the secondary constraints of the system which correspond to the (00) and $(0i)$ components of the Einstein equations respectively.

The Hamiltonian, H, is purely a sum of constraints; a property of all reparametrization invariant systems. We stated earlier that the hypersurfaces may be stitched back together by Cauchy development to construct the four dimensional space-time. These constraints must first be solved to determine the Cauchy development of the spacelike hypersurface, Σ. Only after this has been done may a space-time be constructed, i.e. if h and K satisfy these constraints then the space-time $(\mathcal{M}, g)$ will be a solution to Einstein's equation.

Algebra of the Constraints

Hojman *et al.* demonstrated [55] that geometrodynamics is constructed from the algebra of the generators of surface deformations assuming the principle of path independence and that the sole canonical gravitational variables on the hypersurfaces are given by the intrinsic 3-metric, $h_{ij}(\mathbf{x})$, and its conjugate momentum, $\pi^{ij}(\mathbf{x})$.

They began by assuming that the Hamiltonian and momentum constraints may be treated as the generators of surface deformations. They did not assume that they were constrained to vanish, rather they derived this, hence recovering geometrodynamics. By this they proved that the in geometrodynamics, the gravitational dependence on the hypersurfaces must be on the canonical variable, h_{ij}, and its conjugate momentum, π^{ij}. We shall follow this derivation.

We saw that the Hamiltonian may be expressed as,

$$H = \int d^3x(\mathcal{N}\mathcal{H} + \mathcal{N}^i\mathcal{H}_i) \tag{1.25}$$

where $\mathcal{H}$ and $\mathcal{H}_i$ are the Hamiltonian and momentum constraints respectively. The dynamics of the system will be preserved only if the algebra of constraints is closed, i.e. the Poisson brackets of two constraints is another constraint. We are assuming that the algebra of the constraints is that of the generators of surface deformations for three dimensional hypersurfaces embedded in a pseudo-Riemannian manifold. We identify the Hamiltonian constraint with the generators of normal surface deformations and the momentum constraints with the generators of tangential surface deformations. It is found [64] that the algebra is given by,

$$\{\mathcal{H}(\mathbf{x}), \mathcal{H}(\mathbf{y})\} = -\delta_{,i}(\mathbf{x}, \mathbf{y})(h^{ij}(\mathbf{x})\mathcal{H}_j(\mathbf{x}) + h^{ij}(\mathbf{y})\mathcal{H}_j(\mathbf{y}) \tag{1.26}$$

$$\{\mathcal{H}_i(\mathbf{x}), \mathcal{H}(\mathbf{y})\} = \mathcal{H}\delta_{,i}(\mathbf{x}, \mathbf{y}) \tag{1.27}$$

$$\{\mathcal{H}_i(\mathbf{x}), \mathcal{H}_j(\mathbf{y})\} = \mathcal{H}_j(\mathbf{x})\delta_{,i}(\mathbf{x}, \mathbf{y}) + \mathcal{H}_i(\mathbf{y})\delta_{,j}(\mathbf{x}, \mathbf{y}) \tag{1.28}$$

where "$_{,i}$" denotes differentiation with respect to the coordinates $\{x^i\}$ on the spatial hypersurface Σ.

The starting assumption for this construction is the principle of path independence. Consider the evolution of an arbitrary function(al), $F(h_{ij}(x), \pi^{kl}(x))$. Given the form of the Hamiltonian, it is found that this is described by,

$$F(h_{ij}, \pi^{kl}) = \int dx' \left(\{F, \mathcal{H}(x')\}\mathcal{N}(x') + \{F, \mathcal{H}_j(x')\}\mathcal{N}^i(x')\right) \tag{1.29}$$

Now consider the evolution of this function via two different paths, path I and path II, from the same initial hypersurface to the same final hypersurface. It is found that,

$$\delta F = -\int dx' dx'' \{\{\mathcal{H}(x'), \mathcal{H}(x'')\}, F\}\delta\mathcal{N}_I(x'')\delta\mathcal{N}_{II}(x') \tag{1.30}$$

Using the Jacobi identity and the arbitrariness of $\delta\mathcal{N}_I$ and $\delta\mathcal{N}_{II}$ it is found,

$$\{F, \{\mathcal{H}(x'), \mathcal{H}(x'')\}\} = \delta_{,j}(x', x'')h^{ij}(x')\{F, \mathcal{H}_i(x'')\} - \delta_{,j}(x'', x')h^{ij}(x')\{F, \mathcal{H}_i(x'')\} \tag{1.31}$$

We now insert (1.26) into the left hand side of this equation to find,

$$\delta_{,j}(x', x'')\left(\mathcal{H}_i(x')\{F, h^{ij}(x')\} + \mathcal{H}_i(x'')\{F, h^{ij}(x'')\right) = 0 \tag{1.32}$$

As F is an arbitrary function, we find that,

$$\mathcal{H}_i \simeq 0 \tag{1.33}$$

i.e. we have derived the momentum constraint. This result depends inherently on the explicit dependence on h_{ij} in (1.26). This is due to our assumption of h_{ij} as the sole canonical gravitational variable on the hypersurfaces. We now see that this is a requirement in geometrodynamics. From (1.27), it is seen that the Hamiltonian constraint is must also weakly vanish, i.e.

$$\mathcal{H} \simeq 0 \tag{1.34}$$

We have derived the constraints characterizing geometrodynamics from the classical Poisson bracket algebra of surface deformations plus our assumptions.

Chapter 2

Quantization

We now wish to quantize this reparametrization invariant system to obtain *quantum geometrodynamics*. We shall quantize the canonical variables and their conjugate momenta by Dirac quantization [15] and we shall formulate a wave function, defined on $\mathcal{S}(\Sigma)$ by path integral quantization [77]. We have seen that the classical constraints form the Poisson bracket algebra of surface deformations of the hypersurfaces. The quantized algebra will form an algebra $\mathcal{B}_{phys}$ acting on a Hilbert space $\mathcal{H}_{phys}$. This Hilbert space is populated by the wave functions $\{\Psi\}$ and its operation defined by an inner product operation. We shall demonstrate how to construct such a Hilbert space in *Refined Algebraic Quantization*.

Superspace and Minisuperspace

Superspace (unrelated to that of supersymmetry) is the infinite dimensional configuration space of 3-geometries, $h_{ij}(\mathbf{x})$, and matter field configurations, $\Phi(\mathbf{x})$ on a spatial hypersurface, Σ. It is on superspace that the wave function of the universe is defined. The *supermetric*, an extension of the DeWitt metric introduced in the previous section, is the metric on this manifold.

More formally, superspace can be identified as,

$$\mathcal{S}(\Sigma) \equiv \frac{Riem(\Sigma)}{Diff_0(\Sigma)} \tag{2.1}$$

where Σ is a three dimensional spatial hypersurface, $Riem(\Sigma)$ is the space of all Riemannian 3-metrics and matter configurations on the spatial hypersurfaces,

$$Riem(\Sigma) \equiv \{h_{ij}(\mathbf{x}), \Phi(\mathbf{x}) | \mathbf{x} \in \Sigma\} \tag{2.2}$$

and $Diff(\Sigma)$ is the space of diffeomorphisms from Σ to itself. The zero subscript indicates that only diffeomorphisms that are connected to the identity are considered. These are the 'redundancy' diffeomorphisms; those without physical significance. More specifically they are the transformations leading to the same intrinsic geometry. The remaining diffeomorphisms in the quotient space correspond to physical significant 'symmetries' and are not factored out.

The DeWitt metric may be written as,

$$\mathcal{G}_{AB}(\mathbf{x}) \equiv \mathcal{G}_{(ij)(kl)}(\mathbf{x}) \tag{2.3}$$

with A and B running over the six independent components of h_{ij}. It can be considered as a 6×6 matrix defined at each space point, $\mathbf{x}$, with signature $(- + + + ++)$ (unrelated to the Lorentzian signature of space-time). This can be extended, by allowing the indices A and B to run over the matter degrees of freedom, to provide the metric on $Riem(\Sigma)$ and hence superspace. This is then the superspace metric or *supermetric* with indefinite signature $(- + + + ...)$.

Due to its infinite dimensionality, superspace is extremely difficult to work with; the formulations of quantum cosmology that we describe will take place in *minisuperspace* (unless otherwise stated). This is superspace with a number of its degrees of freedom "frozen". This is typically done such that only configurations corresponding to homogeneous, isotropic universes or small perturbations about these are considered. Once this restriction is imposed, the space becomes finite-dimensional and is described quantum mechanically rather than by quantum field theory. This has some physical justification as the universe is known to be approximately homogeneous and isotropic. However, setting these field modes and their corresponding momenta identically to zero is in clear violatation of the uncertainty principle. Once restricted to minisuperspace, the DeWitt metric can be described by a finite number of functions of t, e.g. $q^\alpha(t)$ with $\alpha = 0, 1, ..., (n-1)$. These functions are known as *histories*.

It can be argued that these models can be used as toy models which have some predictive power. The WKB wave function for minisuperspace to the lowest order will be that of the WKB wave function for superspace if we are careful with the minisuperspace ansatz (i.e. the restriction to minisuperspace from the full superspace). By this we mean that the restriction to minisuperspace before varying the action is the same as restricting after varying the action, i.e. that the approach is consistent. For some models this will not be the case; we shall only consider cases for which it is. The minisuperspace solutions are therefore solutions to the full field equations and S will be the action of a solution to the full Einstein equations. For a detailed discussion of the validity of the minisuperspace ansatz, see [65].

The Wheeler-DeWitt equation

We have shown that the sole canonical gravitational variable on Σ is h_{ij}. The quantized momentum constraint will then constrain the wave function to also have h_{ij} and its conjugate momentum as its sole canonical gravitational variables in order for the momentum constraint to be non-trivial. Indeed, as we have shown, the 3-geometry is the carrier of time and the wave function depends on time through this.

The wave function of the universe is indeed taken to be a functional on $Riem(\Sigma)$ or, more precisely, on $\mathcal{S}(\Sigma)$. It depends on the minisuperspace coordinates, q^α, and the Cauchy surface Σ and is written, $\Psi[q^\alpha, \Sigma]$ or $\Psi[h_{ij}, \Phi, \Sigma]$. The central equation of quantum geometrodynamics and that governing the dynamics of the wave function is the *Wheeler-DeWitt equation*, a second order functional differential equation or, more precisely, a set of such equations at each point, $\mathbf{x}$, on Σ,

$$\hat{\mathcal{H}}\Psi = 0 \tag{2.4}$$

where $\hat{\mathcal{H}}$ denotes the full operator Hamiltonian for both the gravitational and non-gravitational fields (usually matter fields). This reduces to a single equation once the minisuperspace ansatz has been imposed. It is obtained from the constraints discussed above in the usual manner; promoting canonical coordinates to operators. There is no prescribed factor ordering for this equation upon quantization. Indeed, there are multiple widely used orderings. We present the two foremost such orderings in *Operator Ordering in the Wheeler-DeWitt Equation, Chapter 3*.

This equation does not contain any classical time variable t due to the reparametrization invariance of the theory which is left over from the diffeomorphism invariance of general relativity (see *The Problem of Time*)

Quantization of the Action

Implementing the procedure described by Dirac [15], one moves to a quantum theory by promoting the canonical variables to operators (note that we will be working in natural units, i.e. $\hbar = 1$, unless otherwise stated),

$$\pi^{ij} \to -i\frac{\delta}{\delta h_{ij}} \quad \pi_\Phi \to -i\frac{\delta}{\delta \Phi} \tag{2.5}$$

$$\pi^{0} \to -i\frac{\delta}{\delta \mathcal{N}} \quad \pi^i \to -i\frac{\delta}{\delta \mathcal{N}_i} \tag{2.6}$$

The primary constraints thus become,

$$\hat{\pi}\Psi = -i\frac{\delta\Psi}{\delta\mathcal{N}} = 0 \tag{2.7}$$

$$\hat{\pi}^i\Psi = -i\frac{\delta\Psi}{\delta\mathcal{N}_i} = 0 \tag{2.8}$$

Promoting the momentum constraint to an operator equation, one finds,

$$\hat{\mathcal{H}}^i\Psi = 0 \tag{2.9}$$

for the momentum constraint. The momentum constraint corresponds to the diffeomorphism invariance of the wave function on the spatial hypersurface Σ. Finally the Hamiltonian constraint yields,

$$\hat{\mathcal{H}}\Psi = 0 \tag{2.10}$$

Thus we have found the Wheeler-DeWitt equation. The Hamiltonian constraint is related to the reparametrization invariance of the theory [29].

Following [29] [98] [79], we shall now consider an arbitrary homogeneous cosmology with a minisuperspace of dimension n and identifying t as the proper time parameter, i.e. $\mathcal{N} = 1$. Using the definition of the DeWitt metric and the expression for the extrinsic curvature (1.9), one finds (*see Appendix*),

$$\mathcal{G}^{ijkl}\dot{h}_{ij}\dot{h}_{kl} = 4\sqrt{h}\mathcal{N}^2(K_{ij}K^{ij} - K^2) \tag{2.11}$$

and inserting this into the Lorentzian action (1.13),

$$S[q^A(t), \mathcal{N}(t)] = \int_0^1 dt \left[\frac{1}{2\mathcal{N}}\mathcal{G}_{AB}\dot{q}^A\dot{q}^B - \mathcal{N}\mathcal{U}(q)\right] \tag{2.12}$$

where we have defined a new 'potential', $\mathcal{U}(q)$,

$$\mathcal{U}(q) = \int d^3x\sqrt{h}\left[\frac{1}{4\kappa^2}(-{}^{(3)}R + 2\Lambda) + \mathcal{V}(\Phi)\right] \tag{2.13}$$

The range of the t integration in the action may always be taken to be from 0 to 1 by shifting t and by scaling the lapse function [29]. In terms of the previous notation, one has,

$$\mathcal{G}_{AB}dq^Adq^B = \int d^3x\left[\frac{1}{8\kappa^2}\mathcal{G}^{ijkl}\delta h_{ij}\delta h_{kl} + \sqrt{h}\delta\Phi\delta\Phi\right] \tag{2.14}$$

This is a 3-surface of homogeneity in minisuperspace. (2.12) is the action of a relativistic point particle with coordinates q^A moving in the potential $\mathcal{U}(q)$. Varying the action with respect to q^A one obtains a geodesic equation in superspace with a driving term (*see Appendix*),

$$\frac{1}{\mathcal{N}}\frac{d}{dt}(\frac{\dot{q}^A}{\mathcal{N}}) + \frac{1}{\mathcal{N}^2}\Gamma^A{}_{BC}[\mathcal{G}]\dot{q}^B\dot{q}^C = -\mathcal{G}^{AB}\frac{\partial\mathcal{U}}{\partial q^B} \tag{2.15}$$

where $\Gamma^A{}_{BC}[\mathcal{G}]$ are the Christoffel connections of the minisuperspace metric, reinforcing our viewpoint that the histories are trajectories in superspace. Variation with respect to $\mathcal{N}$ gives the Hamiltonian constraint,

$$\frac{1}{2\mathcal{N}^2}\mathcal{G}_{AB}(q)\dot{q}^A\dot{q}^B + \mathcal{U}(q) = 0 \tag{2.16}$$

The general solution to this set of equations will have $(2n-1)$ independent parameters. One of these will be t_0, the arbitrary origin of the unobservable time parameter. We thus effectively have $(2n-2)$ independent parameters. We will contrast this with the number of independent parameters in solutions after we restrict ourselves to the semiclassical regime and also after boundary conditions have been imposed later.

The canonical momenta and Hamiltonian are found to be,

$$\pi_A = \frac{\partial L}{\partial \dot{q}^A} = \frac{\mathcal{G}_{AB}\dot{q}^B}{\mathcal{N}} \tag{2.17}$$

$$H = \pi_A q^A - L = \mathcal{N}\left[\frac{1}{2}\mathcal{G}^{AB}\pi_A\pi_B + \mathcal{U}(q)\right] \equiv \mathcal{N}\mathsf{H} \tag{2.18}$$

respectively, where π_A may be related to the momenta (1.16) and (1.17) obtained earlier by integrating over (2.14). The action and Hamiltonian constraint have become,

$$S = \int dt\left[\pi_A \dot{q^A} - \mathcal{N}\mathsf{H}\right] \tag{2.19}$$

$$\frac{1}{2}\mathcal{G}^{AB}\pi_A\pi_B + \mathcal{U}(q) = 0 \tag{2.20}$$

respectively. Under canonical quantization, the Wheeler-DeWitt equation is found to be (where we have the chosen the operator ordering as advocated by [52]),

$$\hat{\mathsf{H}}\Psi = \left[-\frac{1}{2}\nabla^2_{\mathcal{G}} + \mathcal{U}(q)\right]\Psi = 0 \tag{2.21}$$

where,

$$\nabla_{\mathcal{G}} \equiv \frac{1}{\sqrt{-\mathcal{G}}}\partial_A\left[\sqrt{-\mathcal{G}}\mathcal{G}^{AB}\partial_B\right] \tag{2.22}$$

and the curvature term has been absorbed into the potential. $\mathcal{G}$ is the determinant of the minisupermetric and (2.22) is the Laplacian operator of the minisupermetric which we shall write as ∇ in future to simplify notation.

Path Integral Quantization

As in quantum field theory, one may attempt to quantize gravity using path integrals [77] as an alternative to the canonical quantization procedure. As we showed in the previous chapter, the gravitational dependence on Σ is specified by h^{ij} and therefore the wave function which is defined on $\mathcal{S}(\Sigma)$ must also depend on h^{ij}. We may thus naïvely write for a purely gravitational system,

$$\Psi[h_{ij}, \Sigma] = \mathcal{A}\sum_{\mathcal{M}}\int_{\mathcal{C}}\mathcal{D}g_{\mu\nu}exp(iS[g_{\mu\nu}]) \tag{2.23}$$

where $\mathcal{A}$ is some normalization factor, S is the classical Lorentzian action for gravity, the functional integral is over all 4-geometries with spacelike boundary Σ on which the 3-intrinsic metric is h_{ij} and $\mathcal{C}$ are a class of curves that have yet to be specified. The sum over manifolds/topologies $\mathcal{M}$ is usually ignored as it has been proven that 4-manifolds are non-classifiable [19]. It is important to note that the measure is illl-defined and therefore much care must be taken when using these path integrals. The wave function, $\Psi[h_{ij}, \Sigma]$, does not depend on depend on external time in accordance with the lack of time dependence in the Wheeler-DeWitt equation.

Introducing a single scalar field to represent the matter degrees of freedom, the wave function becomes,

$$\Psi[h_{ij}, \Phi, \Sigma] = \int_{\mathcal{C}} \mathcal{D}g_{\mu\nu}\mathcal{D}\phi exp(iS[g_{\mu\nu}, \phi]) \tag{2.24}$$

where $\phi|_{\Sigma} = \Phi$ and we have omitted the sum over topologies and the prefactor. There are now multiple gravitational and matter degrees of freedom.

As we have seen before with path integrals of non-gravitational systems, it is often useful to perform a *Wick rotation*, $t \to -i\tau$ (with τ unrelated to proper time), to Euclidean space with $iS[q^{\alpha}] \equiv -I[q^{\alpha}]$ where $I[q^{\alpha}]$ is the Euclidean action. The path integral thus becomes,

$$\Psi[h_{ij}, \Phi, \Sigma] = \int \mathcal{D}g_{\mu\nu}\mathcal{D}\phi exp(-I[g_{\mu\nu}]) \tag{2.25}$$

where the sum is now taken to be over all metrics with signature $(++++)$, which induce appropriate 3-metrics and matter field configurations on the past and future hypersurfaces. It has also been suggested [68] to Wick rotate in the other direction, i.e. $t \to +i\tau$.

In non-gravitational systems, such a redefinition is necessary to reach a positive definite action that is bounded from below and hence a more convergent path integral. This also converts the extremization equations from a hyperbolic form to a well-posed elliptic form.

There are further complications in the case of gravity however. Recall that $Diff(\mathcal{M})$ is the symmetry group of the manifold, $\mathcal{M}$. The Wick rotation, $t \to -i\tau$ is not a diffeomorphism and, as a result, not every Euclidean metric will have a Lorentzian section, i.e. not every metric will have a Lorentzian signature after a Wick rotation [58].

The gravitational action itself is problematic; even in its Euclidean form the gravitational action is not bounded from below affecting the convergence of the path integral. This inherent unboundedness stems from the existence of a conformal factor in the volume term of the action [21]. Indeed, for the *no-boundary* and *tunneling* proposals for boundary conditions which are the most prominent of the proposals put forth, it becomes necessary to include complex metrics in the sum for convergence.

Note that we may also write the path integral in terms of the lapse function, $\mathcal{N}$ and q^α, with $\alpha = 0, ..., (n-1)$ as,

$$\Psi[\bar{q}^\alpha] = \int \mathcal{D}p_\alpha \mathcal{D}q^\alpha \mathcal{D}\mathcal{N} \delta[G] \Delta_G e^{iS[p,q,\mathcal{N}]} \tag{2.26}$$

where $S[p, q, \mathcal{N}]$ is the Hamiltonian form of the action and Δ_G is a Faddeev-Popov measure of the gauge fixing condition, G. Here, the gauge symmetry of the system is more explicitly seen. For more details on this representation, see [29].

The Semiclassical Approximation and the WKB Wave Function

We discussed earlier the operator ordering issues that arise in the Wheeler-DeWitt equation. Due to the ambiguity arising from this, it is often unreliable to work beyond the semiclassical approximation. In this règime, the wave function is given by the WKB wave function,

$$\Psi \approx \sum_n \Psi_n = \sum_n \mathcal{A}_n e^{-I_n} \tag{2.27}$$

where the sum is over (possibly complex) saddle points of the path integral, the $\mathcal{A}_n$ being the appropriate (possibly complex) prefactors. The Euclidean 4-geometries corresponding to these saddle points are known as *instantons.* Note that the problem of having an ill-defined functional integration measure is no longer present.

We shall assume that, in the case of a superposition of wave functions, *decoherence* (see *Chapter 5: A Consistent Histories Approach to Quantum Cosmology*) occurs within WKB branches. A justification of this is given in [57]. We shall deal with the issue of decoherence for the histories of WKB solutions in the context of the *decoherent histories* to a generalized theory of quantum mechanics.

We shall now follow [29] [98] to examine the properties of WKB solutions for the Wheeler-DeWitt equation derived in *Quantization of the Action*,

$$\left[-\frac{1}{2}\hbar^2\nabla^2 + \mathcal{U}(q)\right]\Psi(q) = 0 \tag{2.28}$$

where $\hbar$ has been included to illustrate the WKB expansion. WKB solutions will be of the form,

$$\Psi_n(q) = \mathcal{A}_n(q)e^{-I_n(q)/\hbar} \tag{2.29}$$

where $I_n(q)$ and $\mathcal{A}_n(q)$ are complex. Inserting (2.29) into (2.28), one finds,

$$0 = \hat{H}\Psi_n = \left[-\frac{1}{2}\hbar^2\nabla^2 + \mathcal{U}(q)\right]\mathcal{A}_n e^{-I_n(q)/\hbar} \tag{2.30}$$

$$= e^{-I_n(q)}\left\{\left[-\frac{1}{2}(\nabla I_n)^2 + \mathcal{U}(q)\right]\mathcal{A}_n + \hbar[\nabla I_n \cdot \nabla\mathcal{A}_n + \frac{1}{2}\mathcal{A}_n\nabla^2 I_n] + \mathcal{O}(\hbar^2)\right\} \tag{2.31}$$

where the dot implies contraction using the minisuperspace metric, $\mathcal{G}_{AB}$. Equating powers of $\hbar$, the pair of equations,

$$-\frac{1}{2}(\nabla I_n)^2 + \mathcal{U}(q) = 0 \tag{2.32}$$

$$\nabla I_n \cdot \nabla\mathcal{A}_n + \frac{1}{2}\mathcal{A}_n\nabla^2 I_n = 0 \tag{2.33}$$

are obtained. These are the $\mathcal{O}(\hbar^0)$ and $\mathcal{O}(\hbar^1)$ consequences respectively of the Wheeler-DeWitt equation.

As we have mentioned I_n are generally complex and can thus be decomposed into real and imaginary parts,

$$I_n(q) \equiv R_n(q) - iS_n(q) \tag{2.34}$$

giving,

$$-\frac{1}{2}(\nabla R_n)^2 + \frac{1}{2}(\nabla S_n)^2 + \mathcal{U}(q) = 0 \tag{2.35}$$

$$\nabla R_n \cdot \nabla S_n = 0 \tag{2.36}$$

Before proceeding further, we must define our notion of classicality as classicality at late times is a necessary condition on any histories. In general the wave function will not be peaked about a region of configuration space but rather some correlation between coordinates and momenta [29]. The Wigner function, $F(p,q)$, may be used to identify such correlations. It is found [28] that, when applied to quantum cosmology, the Wigner function shows no correlation for wave functions of the form e^{-I}, i.e. exponential, and a strong correlation for wave functions of the form e^{iS}, i.e. oscillatory. The latter corresponds to the classically allowed 'Lorentzian' region while the former to the classically forbidden 'Euclidean' region. We shall adopt view of [18] [39]; that Ψ can be considered to "predict" a classical space-time if there exist WKB-type solutions which yield a strong correlation between π_A and q^A according to (2.17). It shall also be assumed that once classical histories have been identified in a region of minisuperspace where the classicality condition holds they may be extended to regions where it does not using the classical equations of motion unless they become classically singular.

So we require a wave function of the form e^{iS} with S satisfying the Lorentzian Hamilton-Jacobi equation,

$$\frac{1}{2}(\nabla S)^2 + \mathcal{U}(q) = 0 \tag{2.37}$$

if we are to have classicality at late times. We see that, provided the imaginary part of the action varies much more rapidly than the real part, i.e.

$$(\nabla R_n)^2 \ll (\nabla S_n)^2 \tag{2.38}$$

that S_n will approximately satisfy (2.37). (2.38) is known as the *classicality condition.* We shall necessarily impose this.

Thus one finds that the Hamilton-Jacobi equation for the Euclidean action is the order $\hbar^0$ consequence of the Wheeler-DeWitt equation when the classicality condition holds. The order $\hbar^1$ is the conservation of a probability measure which will be discussed in *The Probability Measure.*

One finds for (2.35), where we have reverted to natural units ($\hbar = 1$),

$$\frac{1}{2}\mathcal{G}^{AB}\frac{\partial S_n}{\partial q^A}\frac{\partial S_n}{\partial q^B} + \mathcal{U}(q) = 0 \tag{2.39}$$

Comparison with (2.20), suggests a strong correlation between momenta and coordinates,

$$\pi_A = \frac{\partial S_n}{\partial q^A} \tag{2.40}$$

(2.39) can be differentiated with respect to q^C,

$$\frac{1}{2}\mathcal{G}^{AB}{}_{,C}\frac{\partial S_n}{\partial q^A}\frac{\partial S_n}{\partial q^B} + \mathcal{G}^{AB}\frac{\partial S_n}{\partial q^A}\frac{\partial^2 S_n}{\partial q^B \partial q^C} + \frac{\partial \mathcal{U}}{\partial q^C} = 0 \tag{2.41}$$

where $\mathcal{G}^{AB}{}_{,C} \equiv \frac{\partial \mathcal{G}^{AB}}{\partial q^C}$. This equation invites the introduction of a vector,

$$\frac{d}{ds} \equiv \mathcal{G}^{AB}\frac{\partial S_n}{\partial q^A}\frac{\partial}{\partial q^B} \tag{2.42}$$

This identification and (2.40) give,

$$\frac{d\pi_C}{ds} + \frac{1}{2}\mathcal{G}^{AB}{}_{,C}\,\pi_A\pi_B + \frac{\partial \mathcal{U}}{\partial q^C} = 0 \tag{2.43}$$

which is the same as the geodesic equation (2.15). Thus it is clear that the WKB wave function satisfying the classicality condition is peaked about some subset of the set of solutions to the general field equations. This is a key point; for an action, S, approximately satisfying the Hamilton-Jacobi equation, the solutions to (2.43) will involve n independent arbitrary parameters. Recall that the general solution to the full field equations (2.15) and (2.16) involved $(2n-1)$ arbitrary parameters. So the wave function is peaked about a subset of the general solution. In order to get a particular wave function from this set we must impose boundary conditions. We shall introduce the no-boundary and tunneling proposals for boundary conditions in *Chapter 3: Boundary Conditions*.

The Probability Measure

The Wheeler-DeWitt equation is a Klein-Gordon type equation. There is therefore a naturally associated current,

$$\mathcal{J} = \frac{i}{2}(\Psi^\star \nabla \Psi - \Psi \nabla \Psi^\star) \tag{2.44}$$

which is conserved, $\nabla \cdot \mathcal{J} = 0$. There is also a natural inner product associated with this current as with the Klein-Gordon case. Recall, however, the problems associated with that Klein-Gordon inner product; in particular that it is not positive definite, resulting in negative probabilities.

This problem was solved for quantum field theory in flat space-time by introducing the concept of particles and anti-particles, corresponding to waves of positive and negative frequencies respectively. The lack of extrinsic time (or more precisely, the lack of a suitable Killing vector field) prohibits us from making such a prescription in quantum cosmology.

Alternatives have been proposed to this current:

- Use $|\Psi|^2$ directly, i.e.

$$\mathcal{P}(\Omega) \propto \int_\Omega |\Psi|^2 dV \tag{2.45}$$

  where dV is a volume element in superspace and Ω is a region of minisuperspace. This is clearly positive definite; however, it is found [98] that often the wave function is not normalizable. There is also the issue of how to interpret this probability measure; the wave is defined in superspace rather than in space-time and we are integrating over the timelike variable, q^0. Thus the interpretation cannot be the same as that of particle quantum mechanics, i.e. a probability at an instant in time.

- It has also been proposed to promote the wave function Ψ to an operator as in quantum field theory in flat space-time. This introduces the possibilities to create and annihilate universes. It is, however, unclear how measurable probabilities may be extracted from this formalism.

These definitions should coincide for strong peaks in the wave function which will correspond to classical histories, i.e. in the semiclassical limit. We shall also necessarily restrict ourselves to conditional probabilities (see next section for justification).

We shall now find a conserved current in the semiclassical limit on the set of classical trajectories before showing how a probability measure may be constructed from such a current following [29] [98]. Recall the form of the WKB wave function,

$$\Psi(q) = \mathcal{A}(q)e^{-I(q)/\hbar} + \mathcal{O}(\hbar) \tag{2.46}$$

where $I(q) = R(q) - iS(q)$. For classical trajectories we have $|\nabla S| \gg |\nabla R|$ and then have from (2.39),

$$0 = \nabla(-i\nabla S)\cdot\nabla\mathcal{A} + \frac{1}{2}\mathcal{A}(-i\nabla^2 S) \tag{2.47}$$

$$= \nabla S\cdot\nabla\mathcal{A} + \frac{1}{2}\mathcal{A}\nabla^2 S \tag{2.48}$$

$$= \nabla(|\mathcal{A}|^2\nabla S) \tag{2.49}$$

We have thus found the conserved quantity, $j \equiv |\mathcal{A}|^2\nabla S$. The form of the wave function and (2.36) suggest defining another, more natural, current,

$$\mathcal{J} \equiv exp(-2R/\hbar^2)|\mathcal{A}|^2\nabla S \tag{2.50}$$

This may be interpreted as telling us that the coefficients in (2.50) of the vector ∇S provide a conserved measure on the set of classical generated by the tangent vector ∇S. These trajectories are the histories about which the WKB wave function is peaked making it is clear that this conserved current is only valid in the WKB approximation.

We shall now set about constructing a probability measure from such a conserved current. If one has two spatial hypersurfaces, Σ_{t_1} and Σ_{t_2}, let V be the volume spanned by the classical trajectories about which the WKB wave function is peaked. So the histories cross the hypersurfaces at 'times' t_1 and t_2 respectively. As the current is conserved, one has,

$$0 = \int_V dV \nabla \cdot \mathcal{J} = \int_{\partial V} \mathcal{J} \cdot dA \tag{2.51}$$

where dA is the element of area normal to the boundary of V. If we label the union of the trajectories B then the support of $\mathcal{J} \cdot dA$ is on ∂V is $(B \cap \Sigma_{t_1}) \cup (B \cap \Sigma_{t_2})$ and so one has,

$$\int_{B\cap\Sigma_{t_1}} \mathcal{J} \cdot dA = \int_{B\cap\Sigma_{t_2}} \mathcal{J} \cdot dA \tag{2.52}$$

This indicates the independence of this flux on the choice of hypersurface, Σ_t and leads one to identify,

$$d\mathcal{P} \equiv \mathcal{J} \cdot \Sigma \tag{2.53}$$

as the probability measure along the classical trajectories. In the case of the Klein-Gordon equation, one takes the hypersurfaces to be of constant physical time. The analogous case here would be surfaces of $q^0 = constant$, corresponding to surfaces on which $\sqrt{h}$ is zero (see *Time After Quantization*). This choice allows negative values of $\mathcal{J}^0$ as in the Klein-Gordon case.

A natural choice is surfaces of constant S. These are clearly orthogonal to the classical trajectories and therefore the trajectories we are considering will not cross these surfaces more than once. This choice does break down however as the trajectories approach $\mathcal{U}(q) = 0$ as ∇S tends to zero.

The Problem of Time

The concepts of time in general relativity and quantum mechanics are markedly different. Whereas time is an absolute or *external* parameter in quantum theory, it is dynamical in general relativity. This seeming irreconcilability come to bear on quantum cosmology. Indeed, quantum cosmology suffers from the same affliction of any theory based on quantum gravity or any other reparametrization invariant system; the absence of an external time parameter. This can be seen, as we have mentioned, by noting that the Wheeler-DeWitt equation is independent of an external time parameter, t. Thus, there is no preferred evolution parameter. Principally following [56] [58], we shall discuss the three categories of possible solutions to this problem,

1. *Time before quantization*

2. *Time after quantization*

3. *'Timeless' options*

Time Before Quantization

This approach takes the view that the approach in quantum mechanics to the issue of time is the correct one; one puts the classical theory in a form such that, upon quantization, the system takes on the familiar quantum mechanical form of non-relativistic particle quantum mechanics. Such systems are governed by the Schrödinger equation. In this approach, one thus attempts to recover a Schrödinger-type equation by rewriting the classical constraints before quantization. There are two standard approaches in this category,

- obtain a quantum version of Poisson bracket dynamical equations.

- obtain a 'multi-time' Schrödinger equation from the dynamical equations.

The former is found to be restrictive as the 'Schrödinger equation' found is foliation-dependent. Motivated by this, we shall give an outline of the second approach.

The intrinsic 3-geometry, h_{ij}, has six degrees of freedom. Only three of these are physical degrees of freedom; one of which represents the physical time of general relativity. For quantum geometrodynamics, it has been shown [24] that we may locally determine the temporal separation along any timelike world line once we know h_{ij} and $\dot{h}_{ij}$ on the initial Cauchy surface (provided they determine the lapse and shift) for a gravity plus matter action, i.e. one may locally separate this 'temporal' degree of freedom. Towards this goal, perform the canonical transformation,

$$(h_{ij}(\mathbf{x}), \pi^{kl}(\mathbf{x})) \longrightarrow (\mathcal{X}^A(\mathbf{x}), \mathcal{P}_B(\mathbf{x}); \phi^r(\mathbf{x}), p_s(\mathbf{x})) \tag{2.54}$$

where $\mathcal{X}^A$ and $\mathcal{P}_A$ $(A, B = 0, 1, 2, 3)$ are the '*embedding variables*' and their canonical momenta respectively. The embedding variables describe how the hypersurfaces, Σ, are embedded in the pseudo-Riemannian space-time. ϕ_r and p_s $(r, s = 1, 2)$ represent the 'true' degrees of freedom of the gravitational field. One then requires the Hamiltonian constraint to be of the form,

$$\mathcal{P}_A(\mathbf{x}) + h_A(\mathbf{x}; \mathcal{X}^B, p_s) \simeq 0 \tag{2.55}$$

where h_A are simply remaining terms. Upon quantization, one finds (*see Appendix*),

$$i\hbar \frac{\delta\psi[\phi^r(\mathbf{x})]}{\delta\mathcal{X}^A} = h_A\left(\mathbf{x}; \mathcal{X}^B, \hat{\phi}^r, \hat{p}_s\right) \psi[\phi^r(\mathbf{x})] \tag{2.56}$$

on the constraint hypersurface, which is indeed a Schrödinger-type equation. It is in fact a local Schrödinger equation, known as the '*Tomonaga-Schwinger equation*'. Using this 'Hamiltonian', h_A, our notion of 'time' thus originates in the classical theory, *before quantization.*

There are a number of problems[1] with this formulation of a concept of time; the principle being that (2.54) is non-unique and cannot be performed globally [27].

[1] For other problems see [58].

Time After Quantization

One may also attempt to identify time after quantization, i.e. quantize without solving the constraints. Recall the hyperbolic form of the equation; this is suggestive of identifying the "$(-)$" part (the conformal part) of the hyperbolic signature, as a new *intrinsic time* parameter. It makes sense to distinguish this degree of freedom from the others, e.g to impose boundary conditions for $\mathcal{F} = const$ where $\mathcal{F}$ is the conformal part of the minisupermetric.

Kuchař showed [62] that there exists a conformal Killing vector field for the DeWitt metric on $Riem(\Sigma)$ given by h_{ij}. One may thus seek to identify $h^{1/2}$, the square root of the 3-volume, as an intrinsic time variable. Adopting this approach, one would work within a framework such that one describes the evolution of the system with respect to this parameter just as one does with external time in particle quantum mechanics.

In such an approach, the concept of boundary conditions on the wave function becomes somewhat different to that which we are used to with an extrinsic time parameter. An illustration of this is given in [60], which we shall now follow.

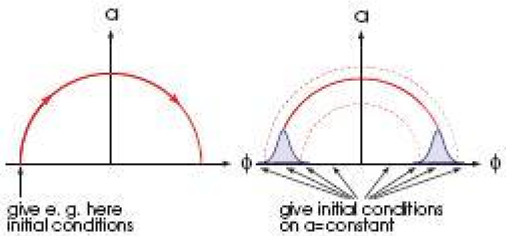

Figure 2: (Taken from [60]) *The classical (left) and quantum (right) evolutions of a recollapsing universe with an initial singularity are shown. The 3-volume of the universe is proportional to the scale factor cubed: $\sqrt{h} \propto a^3$. We identify the scalar field, ϕ as intrinsic time. The arrow shows the direction of the Friedmann time.*

The classical and quantum evolution of a universe with an initial 'Big Bang' singularity and a final 'Big Crunch' singularity are shown in Figure 2. Classically the initial conditions are specified at the left intersection with the $\sqrt{h} = 0$ axis, e.g. at an initial Friedmann time. However, in the quantum picture, initial conditions must be specified at both intersection points on this axis corresponding to the initial and final singularities, i.e. one must impose two initial wave packets. These wave packets must both be evolved forward with respect to $\sqrt{h}$. As they are evolved forward with respect to $\sqrt{h}$ the two singularities become indistinguishable.

There are also many problems associated with this interpretation. The conformal Killing vector field does not induce a positive definite inner product and neither scales in the correct way [56]. In quantum field theory for a scalar field in flat space-time where there was a similar problem, there was a natural motivation for removing the negative energy states. Here, however, these negative energies will simply correspond to a contracting universe as we have seen. Thus, one may not simply exclude them to arrive at a postive definite inner product as they correspond to physically relevant states.

Timeless Options

The final class of approaches is the 'timeless' approach which is that used in the quantum cosmological models that are described in this thesis. In this '*naïve Schrödinger*' picture, time is not interpreted as fundamental, i.e. there is no unique uniformly increasing external parameter with respect to which the evolution of any observables may be defined. Indeed, time in this approach is assumed not to exist at the Planck scale. A Schrödinger equation can thus be seen as, at most, providing an approximate description of the dynamical evolution. One may also identify intrinsic time parameters in this approach. Here, though, they are understood not to provide a fundamental notion of time.

We mentioned earlier that we may not talk about absolute probabilities but rather *conditional* probabilities. This is one of the principle restrictions of the 'timeless' interpretation. In standard non-relativistic quantum mechanics, the wave function Ψ describes a slice of space-time of $t = constant$. Here however, Ψ describes the whole space-time. There is then an inherent divergence in the wave function due to the non-compactness of time [82]. In order to make sense of probabilities, i.e. to ensure finite probabilities, it is necessary to construct some sort of analog of the $t = constant$ restriction; this restriction manifests itself as a conditional probability, i.e. the probability that an event A occurs given that event B occurs. For example one may have,

$$\mathcal{P}(s_0|s_1) = \frac{\int_{S_0} \mathcal{J} \cdot dA}{\int_{S_1} \mathcal{J} \cdot dA} \tag{2.57}$$

where s_0 and s_1 are conditions on the arguments of the wave function and S_0 and S_1 represent the corresponding regions of superspace over which the wave function may be integrated over to satisfy the boundary conditions. Clearly, $S_0 \subset S_1$ is required. Each integral is finite as the domains of integration are finite. The theory makes a prediction when the conditional probabilities are close to zero or one.

The main advantage of the timeless approach is that there is a readily defined positive definite Hilbert space structure such that observables are self-adjoint with respect to the inner product. There is also a natural probability measure. We construct this for the *refined algebraic quantization* procedure for constructing Dirac observables.

Refined Algebraic Quantization

We shall follow closely the six step prescription from [71] for the 'Refined Algebraic Quantization' approach to Dirac quantization. The ultimate goal is to develop a physical Hilbert space, i.e. a space $\mathcal{H}_{phys}$ such that if $|\psi\rangle \in \mathcal{H}_{phys}$ then $\hat{K}|\psi\rangle = 0$ where K is the constraint of the system, with a positive definite inner product.

Consider a constrained classical system with phase space Γ and a non-degenerate symplectic form ω on Γ, defining Poisson brackets on smooth complex valued functions. We label the constraints of the system C_i with $i = 1, ..., n$.

- *Step 1*: Let $\mathbf{T}(\Gamma)$ be the vector space of all smooth complex valued functions, $\{f\}$, on Γ. Identify a subspace, $\mathbf{S} \subset \mathbf{T}$, such that $\mathbf{S}(\Gamma)$ is,
  - large enough such that any $f \in \mathbf{T}(\Gamma)$ may be written as a sum of products of elements in $\mathbf{S}(\Gamma)$.
  - closed under Poisson brackets.
  - closed under complex conjugation.

- *Step 2*: For all $f \in \mathbf{S}(\Gamma)$ identify a corresponding abstract operator, $\hat{F}$. These operators will generate an associative algebra, $\mathcal{B}_{aux}$. Impose,

$$[\hat{F}, \hat{G}] = i\hbar\widehat{\{F, G\}} \tag{2.58}$$

for all $\hat{F}, \hat{G} \in \mathcal{B}_{aux}$ on this algebra.

Before proceeding to Step 3, we must first define an *anti-linear map* and also an *involution operator*,

1. *Anti-linear map*: $f : V \to W$ where V and W are complex vector spaces satisfying,

$$f(a\mathbf{x} + b\mathbf{y}) = a^{cc}f(\mathbf{x}) + b^{cc}f(\mathbf{y}) \tag{2.59}$$

where $a, b \in \mathbb{C}$, $\mathbf{x}, \mathbf{y} \in V$ and 'cc' denotes the complex conjugation operation.

2. *Involution map*: an anti-linear map, $\star : V \to V$, where V is a complex vector space satisfying,

   (a) $(\mathbf{x}\mathbf{y})^\star = \mathbf{y}^\star\mathbf{x}^\star, \quad \forall \mathbf{x}, \mathbf{y} \in V$

   (b) $(\mathbf{x}^\star)^\star, \quad \forall \mathbf{x} \in V$

We may now proceed with our quantization,

- *Step 3*: Induce an involution map, $\star : \mathcal{B}_{aux} \to \mathcal{B}_{aux}$, by identifying the equivalence relation $f^{cc}(\mathbf{x}) = g(\mathbf{x}), \quad \forall \mathbf{x} \in \Gamma$ on $\mathbf{S}(\Gamma)$ with $\hat{F}^\star = \hat{G}$ on $\mathcal{B}_{aux}$. We denote the associated $\star$-algebra $\mathcal{B}_{aux}^{(\star)}$.

- *Step 4*: Next construct a representation, R, of the algebra, $\mathcal{B}_{aux}$, and hence of $\mathcal{B}_{aux}^\star$. This is done using linear operators on some auxiliary Hilbert space, $\mathcal{H}_{aux}$. One then has,

$$R(\hat{A}^\star) = R(\hat{A})^{dagger} \tag{2.60}$$

for all $\hat{A} \in \mathcal{B}_{aux}$. '†' denotes Hermitian conjugation with respect to the inner product on the auxiliary Hilbert space, $\mathcal{H}_{aux}$.

- *Step 5a*: Recall the constraints, $\{C_i\}$. These may be represented by self-adjoint operators on $\mathcal{H}_{aux}$. Doing this, label the corresponding operators, $\hat{C}_i$.

- *Step 5b*: A subspace, $\Phi \subset \mathcal{H}_{aux}$, must now be picked out. Require Φ to be *dense*. [5] defines dense as:

  "A subset A of a topological space X is said to be dense in X if $\bar{A} = X$."

  where the bar denotes the closure of a set. This is well-defined here as all Hilbert spaces are Banach spaces and hence topological vector spaces. Another requirement is that Φ is invariant under the action of the constraints, $\hat{C}_i$. This is equivalent to saying that, for $\hat{A} \in \Phi$, $[\hat{C}_i, \hat{A}] = 0$ for all $\hat{C}_i \in \mathcal{H}_{aux}$. We denote the $\star$-algebra on $\mathcal{H}_{aux}$ corresponding to such $\{\hat{A}\}$ by $\mathcal{B}^{(\star)}_{phys}$ under the additional requirement that both $\hat{A}$ and $\hat{A}^\dagger$ are defined on Φ and map it to itself.

- *Step 5c*: Find an anti-linear map, $\eta : \Phi \to \Phi'$, where Φ' is the topological dual of Φ. This is defined in our case by,

$$\Phi' = \{f : \Phi \to \mathbb{C} | f \textit{ is continuous and linear}\} \tag{2.61}$$

  i.e. the space of all continuous linear functionals from Φ to its base space, $\mathbb{C}$. We require η to satisfy,

  1. $\eta(\phi_1)$ is a solution of the constraints for all $\phi_1 \in \Phi$, i.e.

$$0 = \left(\hat{C}_i(\eta\phi_1)\right)[\phi_2] \equiv (\eta\phi_1)[\hat{C}_i\phi_2] \tag{2.62}$$

     for all $\phi_2 \in \Phi$.

2. η is real and positive, i.e.

$$(\eta\phi_1)[\phi_2] = ((\eta\phi_2)[\phi_1])^\star \tag{2.63}$$

and,

$$(\eta\phi_1)[\phi_1] \geq 0 \tag{2.64}$$

3. η commutes with any $\hat{A} \in \mathcal{B}^{(\star)}_{phys}$, i.e.

$$(\eta\phi_1)[\hat{A}\phi_2] = ((\eta\hat{A}^\dagger\phi_1))[\phi_2] \tag{2.65}$$

η is known as the *rigging map*.

- *Step 5d*: $\{\eta\phi_a\}$ clearly span a vector space, $\mathcal{V}_{phys}$, of solutions of the constraints. An inner product on $\mathcal{V}_{phys}$ may be introduced,

$$\langle\eta\phi_1|\eta\phi_2\rangle_{phys} = (\eta\phi_2)[\phi_1] \tag{2.66}$$

This inner product is well-defined, Hermitian and positive definite.

- *Step 6*: From the third property of the rigging map above, it can be seen that operators $\hat{A} \in \mathcal{B}^{(\star)}_{phys}$ have a well-defined action on Φ'. As these operators commute with the generators of $\mathcal{V}_{phys}$, they leave this space invariant. This may be exploited to induce operators, $\hat{A}_{phys}$ on $\mathcal{H}_{phys}$,

$$\hat{A}_{phys}(\eta\phi) = \eta(\hat{A}\phi) \tag{2.67}$$

It may seem that, although the procedure is well-defined, it is implausible to implement. However, it has been shown [54] [53] that suitable rigging maps may be constructed in certain cases. It has also been argued [71] that, with an additional physical argument, the quantization procedure is unique for typical cases with a single constraint.

Evolving Constants of Motion

A particular 'timeless' approach is the *evolving constants of motion* approach as developed by Rovelli and others. Fundamental to this approach is the interpretation of mechanics as a "theory of relations between observables" rather than the evolution of observables with respect to some external time parameter. We shall now illustrate this approach for *presymplectic* mechanics, a general case of Hamiltonian mechanics, following the example given in [89].

Let $(\Gamma, \omega_\Gamma, H)$ be a Hamiltonian system where Γ is the phase space, ω_Γ is the symplectic form and H is the Hamiltonian[2]. If one labels the canonical coordinates on Γ by q_i and p^i (with $i = 1, ..., n$) then the symplectic form is given by $\omega_\Gamma = dp^i \wedge dq_i$.

In classical mechanics one also has the external time parameter, t. Thus the dynamics of the system are completely described on the space $\mathcal{E} = \Gamma \times \mathbb{R}$ with coordinates q_i, p^i, t. The presymplectic form defined on $\mathcal{E}$ is given by,

$$\omega = \omega_\Gamma - dH(p.q.t) \wedge dt \tag{2.68}$$

Thus, in this form, the system is defined by the presymplectic manifold $(\mathcal{E}, \omega)$[3]. Note the form of the manifold $\mathcal{E}$ and compare it with the form of the manifold $\mathcal{M}$ from *The Hamiltonian Formulation of General Relativity* which was foliated into spacelike hypersurfaces as $\mathcal{M} = \Sigma \times \mathbb{R}$.

The system is thus characterized by $\mathcal{E}$ and ω, i.e. if ω is preserved along a trajectories in $\mathcal{E}$ then the coordinates will obey the same Euler-Lagrange equations along the trajectories. Such curves may thus be considered as 'motions' of the system. Consider a null vector field, Y, with respect to ω, i.e. the interior product, $i_Y\omega$, of Y with ω is zero. The integral curves generated by this vector field will clearly be such trajectories.

[2]For details of how to formulate classical mechanics in this way see, for example, [1]

[3]See [2] for more details.

As we have stated, $\omega(p, q, t) = constant$ along these curves. One may solve this condition by expressing the variables in terms of each other, i.e. find a correlation between variables of the system that characterize such curves. This will prove to be a key observation in this approach; motions of the system are characterized by correlations between variables or *observables* of the system.

We shall now define some quantities, following [89],

- *State*: an integral curve of the null vector field, Y, with respect to the presymplectic form, ω.
- *Observable*: a scalar function, Q, on $\mathcal{E}$ that is constant along the states, i.e.,

$$Y(Q) \equiv Y^a \partial_a Q = 0 \tag{2.69}$$

We shall denote observables by capital letters.

The form of (2.68) is preserved under a change of coordinate system on $\mathcal{E}$. Noting this, recall that a motion characterizes a correlation between variables or equivalently defines one variable as a function of another. Let us suppose that this function is of the form $q(t)$ where t is the external time parameter. Exploiting the conserved form of the presymplectic form under coordinate transformations on $\mathcal{E}$, we may just as have defined the function $q(t')$ had we chosen t' as the time coordinate. This result provides a striking insight; a state cannot be thought of as referring to an instant of time due to this invariance. Rather, the states are 'timeless' and can be thought of as characterizing entire histories.

We have thus demonstrated the lack of time dependence in the definition of a state. The definition of an observable is also evidently independent of any time parameter. A framework is now forming which is suited to describing reparameterization invariant systems.

Reparametrization Invariant Systems

However, we know that we must have at least some approximate notion of time corresponding to the evolution which we observe. Consider a system described by coordinates q^α $(\alpha = 1, ..., n)$ without any external time parameter and let q_1 be a 'clock' variable (*see Appendix*). Suppose one has a system with a function $h(q^1, q^a)$ with $a = 2, ...n$ such that on the integral curves of ω, $h(q^1, q^\alpha) = 0$, or equivalently there is function $q^a(q^1)$ defined on these curves. One may then write the corresponding observable as $Q^a(q^1; q^b)$ provided,

$$Q^a(q^1; q^b) = constant \quad if \ h(q^1, q^a) = 0 \tag{2.70}$$

$$Q^a(q^1; q^b)\Big|_{q^1=T} = q^a(T) \tag{2.71}$$

where $T \in \mathbb{R}$ are fixed values of the clock variable. The first condition keeps Q^a fixed along the trajectories while the second condition determines its value.

The first condition is equivalent with the condition for the Poisson bracket of the quantity with the Hamiltonian constraint defined on that trajectory to vanish, i.e.

$$\{Q^a(q^1; q^b, p_\alpha), H(q^\alpha, p_\alpha)\} = 0 \tag{2.72}$$

and is the definition of an observable used by others [73]. Rovelli's key observation was that these observables represent the evolution in q_1 yet are also constants of motion for the system. We shall simplify the notation and write,

$$Q^a(q^1) = Q^a(q^1; q^b, p_\alpha) \tag{2.73}$$

(2.70) must be satisfied for all values of T in (2.71). Equally, $Q^a(q^1)$ describes the function $q^a(q^1)$, evolving with respect to q^1. It is these properties which lead Rovelli to dub observables satisfying (2.72) and (2.71) as *evolving constants of motion.* Indeed, this system of equations is a more general Hamilton equation of motion. Thus, for the classical system, a complete description of the dynamics of the system has been found which is independent of any external time parameter, t.

Moving to the quantum regime, it is found, via the usual quantization procedure, that (2.72) and (2.71) become (with $p \to \pi$),

$$[\hat{Q}^a(\hat{q}^1), \hat{H}(\hat{q}^\alpha, \hat{\pi}_\alpha)] = 0 \tag{2.74}$$

$$\hat{Q}^a(\hat{q}^1)\Big|_{q^1=T} = \hat{q}^a(T) \tag{2.75}$$

where the second equation is evaluated in a representation such that $\hat{q}^1$ is diagonal and the abuse of notation, $q^1 = T$, is permissible. The dynamics of a quantum system independent of any external time parameter has now been constructed. We first clarify an important distinction between two classes of observables.

Rovelli introduced this partitioning of observables [90] into two subclassses of *partial* and *complete* observables. His definitions [90] were as follows,

- Partial observable: *"a physical quantity with which can be associated a (measuring) procedure leading to a number."*
- Complete observable: *"a quantity whose value can be predicted by the theory (in classical theory); or whose probability distribution can be predicted by the theory (in quantum theory)."*

Operators are always associated with complete observables and it was indeed complete observables which we referred to as observables in the previous defintion. Consider the clock variable, q^1; this is a partial observable by the criteria above. In contrast $q^a(a^1)$, or more precisely $Q^a(q^1)$, are complete observables. Thus there is no operator associated with q^1; this corresponds to the fact that, in standard non-relativistic quantum mechanics, there is no operator associated with t. These definitions alleviate the issue of a flow of time, i.e. q^1, being observed directly as there is no corresponding operator and thus no notion of commutation.

There has been much debate about the nature of observables in such a construction and particularly with regards to the measurability of Dirac observables. Marolf has shown [74] by defining suitable measurement interactions that single 'evolving constants of motion' observables may be measured.

We now return to the fundamental issue of defining a physical Hilbert space structure. In the Schrödinger picture of standard quantum mechanics these are naturally defined in terms of the external time parameter. We are clearly precluded from such a definition in this system and must search for an alternative formulation of a physical Hilbert space, i.e. $\mathcal{H}_{phys}$ such that $|\Psi\rangle \in \mathcal{H}_{phys} \Rightarrow \hat{H}|\Psi\rangle = 0$.

Marolf studied the dynamics of recollapsing cosmologies [73], specifically finite-dimensional LRS Bianchi IX and Kantowski-Sachs models [73] and a countably infinite-dimensional LRS Bianchi IX model [72] using this construction. He found that the qualitative behaviour of these models was preserved under quantization, i.e. they still exhibited a recollapse.

Recovering Time

In order to recover the properties of time which we observe classically from this formalism, the *thermal time hypothesis* [91] may be invoked,

> *"In nature, there is no preferred physical time variable t. There are no equilibrium states ρ_0 preferred a priori. Rather, all variables are equivalent; we can find the system in an arbitrary state ρ; if the system is in a state ρ, then a preferred variable is singled out by the state of the system. This variable is what we call time."*

There have been notable successes with this proposal; for an initially radiation-filled covariant cosmological model the natural time variable selected by this proposal was found to be the Friedmann time [88]. The notion of time that is recovered is an approximate Schrödinger equation similar to that obtained in the embedding variables approach discussed earlier.

Concluding Remarks on the 'Timeless' Approach

A similar formalism is used in the consistent histories approach to quantum mechanics. We shall discuss this in Chapter 5.

Although such formulations may lead to a well-defined quantum system for parameterized systems, they would be extremely difficult to work with in practice as Hájíček pointed out [26]. This is because we would be required, in this formalism, to solve the theory completely before quantizing.

Chapter 3

Boundary Conditions

In classical cosmology, any predictive power is dependent on the specification of initial conditions and similarly we must impose boundary conditions on the wave function in quantum cosmology. We saw that the restriction to WKB solutions picked out a subset of solutions to the general equations (2.15) and (2.16). A further restriction to pick out one solution is obtained by the imposition of boundary conditions.

Unlike many other quantum systems, there are no natural boundary conditions on physical grounds arising from symmetries. It was initially hoped that a unique solution for the Wheeler-DeWitt equation would be found based purely on mathematical consistency. It is now known that this is not the case. We must impose boundary conditions on our wave function to select specific solution.

Although, in many ways, this is rather unsatisfactory, the various possible prescriptions which we will consider can be viewed as separate, fundamental physical laws.

The No-Boundary Proposal

The no-boundary proposal was first introduced by Hawking and Hartle [38]. It places topological restrictions on the 4-geometries summed over in the path integral representation of the wave function of the universe.

To calculate the no-boundary wave function, $\Psi_{NB}[h_{ij}, \Phi, \Sigma]$, one is instructed to sum only over *compact* Euclidean 4-geometries of all topologies which have the compact three surface Σ as their *only* boundary, such that the 4-metric $g_{\mu\nu}$ induces h_{ij} on Σ and the matter field configuration ϕ matches the value Φ. There is thus no singular boundary in the past. Note that this applies to the Euclideanized wave function and is not to be confused with the possibility for an initial singularity in the universe which is not precluded by the no-boundary condition.

For the globally hyperbolic manifolds which we are considering ($\mathcal{M} = \mathbb{R} \times \Sigma$), the no-boundary condition prescribes conditions on the histories at the initial point in the path integral. We shall be restricting ourselves to the semiclassical approximation, for which the no-boundary proposal reduces to fixing initial conditions for our histories at the classical level. It is found [98] that these conditions are,

1. the 4-geometry closes
2. the saddle-points of the semiclassical wave function correspond to metrics and matter fields which are regular solutions to the classical Einstein equations (satisfying the final conditions on Σ)

We have not yet mentioned the issue of the choice of contour in the path integral. The no-boundary proposal does not offer a prescription for a specific choice of contour and indeed Halliwell and Louko [34] [35] [36] showed that there is no unique contour (which ensures convergence) to integrate over in superspace. Significantly, they also found that the result may also crucially depend on the contour chosen.

Instantons of the No-Boundary Proposal

One area of research has been to find specific 4-geometries or instantons which correspond to the initial boundary condition of the universe. This may be of particular relevance with regard to the string theory landscape. Here, it is hoped that the boundary proposals may provide criteria for selecting the initial vacuum state of the universe [42].

The Hawking-Moss instanton [47] was the first such attempt for the no-boundary proposal. It describes the creation of a closed eternally inflating universe.

The Coleman-De Luccia instanton [8] is a ‘false vacuum’ state. False vacuum states typically tunnel to the true vacuum state. Coleman and De Luccia found that this false vacuum state produced bubble nucleation of open inflationary universes. Some have argued that the condition for the initial state of the universe to be in a false vacuum state is too restrictive and not generic.

Motivated by this, the Hawking-Turok instanton was proposed [49] such that it produces similar results to the Coleman-De Luccia instanton without the requirement that it initially be in a false vacuum state. The disadvantage of this instanton is that the production of singularities in inevitable.

Top-Down Probabilities

Up to this point we have ignored some conceptual issues relating to probabilities in quantum cosmology. In non-relativistic particle quantum mechanics one generally considers experiments which can be repeated a number of times and for which we may vary the initial conditions. The probabilities may then be calculated in the usual ‘S-matrix’ manner. Hawking *et al.* labeled this the ‘bottom-up approach’ to physics [45].

When considering cosmology, it is apparent that such an approach is incompatible. When treating the universe quantum mechanically, it is clear that the situation is not that described above. We are in the middle of the ‘experiment’; one in which there is no control over the initial parameters.

Hawking *et al.* argue that it is necessary to calculate probabilities in quantum cosmology with boundary conditions at late times only, i.e. using the no-boundary wave function. They labeled this approach the ‘top-down approach’ [45]. Essentially, all possible histories which originate in the no-boundary state and give a late universe corresponding to that which we observe are summed over.

In this framework, one may still only speak about conditional probabilities. It is hoped that, using this approach, the precise shape of the CMB fluctuation spectrum may be calculated [43]. The spectrum observed will depend on when and where we observe it, and hence the use of conditional probabilities is justified.

The Anthropic Principle

Anthropic reasoning has been posited as a principle upon which approaches to cosmology should be based. It essentially states that only physically reasonable universes will contain observers. It could, for example, be used to explain/justify the values of the fundamental constants which we observe in Nature and are vital to our existence. It is seen that the anthropic principle may be applied within the top-down approach to probabilities. For example, one may have,

$$p(\alpha|O, H, \Psi) = \frac{p(\alpha, O|H, \Psi)}{p(O|H, \Psi)} \tag{3.1}$$

with O representing a set of conditions that are required for the appearance of complex life and the wave function satisfies the no-boundary condition.

The Tunneling Proposal

An alternative approach to the boundary conditions, developed by Vilenkin [93], is the tunneling proposal. Its name comes from the strong analogy drawn in this interpretation with tunneling in quantum mechanics. This proposal can be seen as saying that the universe tunneled out of nothing. This is best seen in the context of the path integral formulation,

$$\Psi[h_{ij}, \Phi, \Sigma] = \sum_{\mathcal{M}} \int_{\emptyset}^{(h_{ij}, \Phi)} \mathcal{D}g_{\mu\nu}\mathcal{D}\phi e^{iS[g_{\mu\nu}, \phi]} \tag{3.2}$$

where $\emptyset$ is a vanishing 3-geometry and the functional integral is over the Lorentzian 4-metrics that give, Φ, and , h_{ij}, on Σ and initially a vanishing 3-geometry, $\emptyset$.

One may also formulate the proposal using a notion of "incoming" and "outgoing" waves as in quantum field theory in a flat space-time. As we have mentioned, the only Killing vector field on minisuperspace is not suitable for formulating a notion of incoming and outgoing waves in complete analogy with the Klein-Gordon equation. However, we are primarily interested in solutions in the oscillatory WKB region. We saw earlier that there is an associated current,

$$J_n = -|\mathcal{A}_n|^2 \nabla S_n \tag{3.3}$$

In the semiclassical approximation one may define incoming and outgoing modes with respect to this object. A mode is defined to be outgoing at the boundary if ∇S_n points outward there. If the wave function is not oscillatory, this notion is not well-defined.

The tunneling proposal is that *the wave function, Ψ, should be everywhere bounded, and at singular boundaries of superspace Ψ includes only outgoing modes*, i.e. *those that carry a flux out of superspace.*

Geometries in superspace will generally consist of configurations that are in some sense singular, e.g. $h^{1/2}$ will be zero or infinite or quantities relating to the scalar field may be infinite. However, this does not mean that the corresponding 4-geometry is singular. When we refer to singularities, we are referring to parts of the boundary that do correspond to singularities of the 4-geometry.

Instantons in the Tunneling Proposal

The initial instanton of the tunneling proposal is the 4-sphere, S^4. In the proposal, this tunnels to a 4-geometry, $\mathbb{R} \times S^3$. We discuss the possibility of non-trivial topologies in *Topology Change* in which we discuss a 'generalization' of this tunneling. There, the initial instanton is given by the quotient space, S^4/Γ, where Γ is the group of isometries acting on S^4 tunneling to $\mathbb{R} \times (S^3/\Gamma)$.

Operator Ordering in the Wheeler-DeWitt Equation

As in the Klein-Gordon equation for quantum field theory in flat space-time there are operator ordering issues that arise in the Dirac quantization procedure of the Hamiltonian constraint. There are two foremost orderings, one favoured by each of the aformentioned boundary proposals.

It is striking that these proposals both use different factor ordering in the Wheeler-DeWitt equation. Hawking and Page argued [52] for the factor ordering in (3.4),

$$\hat{\mathsf{H}}\Psi = \left[-\frac{1}{2}\nabla^2_{\mathcal{G}} + \mathcal{U}(q)\right]\Psi = 0 \tag{3.4}$$

whilst Vilenkin used a conformally invariant choice of ordering,

$$\hat{\mathsf{H}}\Psi = \left[-\frac{1}{2}\nabla^2 + \frac{n-2}{8(n-1)}\mathcal{R} + \mathcal{U}(q) \right] = 0 \tag{3.5}$$

where $\mathcal{R}$ is the minisupermetric scalar curvature and $n \geq 2$. Note that this was absorbed into the potential, $\mathcal{U}(q)$, in (3.4).

Kontoleon and Wilthsire considered [61] the generality and consistency of the no-boundary and tunneling wave functions for more choices of factor ordering. They considered a closed Friedmann-Robertson-Walker universe with a matter sector described by a scalar field. It was found that whilst the tunneling wave function was consistently defined only for particular choices of factor ordering, the no-boundary wave function may be generically defined.

Symmetric Bounce Proposal

As we will discuss in *Boltzmann Brains, Chapter 4*, Susskind [83] has challenged the no-boundary proposal on the grounds that it is seen to predict that we, as observers, are extremely atypical for a universe with a cosmological constant. In order to avoid this problem, Page [84] recently proposed an alternative boundary condition, the '*symmetric bounce proposal*'.

The proposal can be loosely defined as follows: the initial state is given by [84] the Giddings-Marolf seed state of *"quantum fluctuations about a superposition of macroscopic components that are each time symmetric about a bounce of extremal 3-volume, with the quantum fluctuations being in their ground state at that moment of time symmetry for the macroscopic 4-geometry."*

A Giddings-Marolf seed state is essentially a state in a space $\mathcal{H}^w_{aux}$ which, when operated on by a suitable rigging map, goes to a state in the physical Hilbert space, $\mathcal{H}^w_{phys}$ of weakly coupled perturbative gravity[1].

This proposal was defined such that it would replicate the properties of the no-boundary proposal without the problem described in *Boltzmann Brains.* The price it pays for this is a less natural

[1] See [22] for further details.

definition.

Chapter 4

The Predictions of Quantum Cosmology

We will now examine some of the predictions of quantum cosmology for both the no boundary proposal and the tunneling proposal.

Inflation

Inflation pertains to solve various problems [97] in classical cosmology, e.g the horizon and flatness problems. However, there is no motivation for inflation other than the solving these problems and if inflation is to be a realistic solution then it should be generically possible. It is hoped that quantum cosmology may objectively predict inflation.

We shall not only be asking the question as to whether inflation is predicted by the no-boundary and tunneling proposals but also whether *sufficient* inflation is predicted. It is accepted that ~ 65 *efolds* of inflation are required to solve the aforementioned problems. This therefore provides a lower bound for sufficient inflation. We shall begin with qualitative analysis of a closed Friedmann-Robertson-Walker minisuperspace model with a single scalar field, following [29] [98] [78]. We shall compare the probabilities for the no-boundary and tunneling proposals. We will be working in the WKB limit so that our Klein-Gordon-type current is a reliable probability measure. The metric is given by,

$$ds^2 = -\mathcal{N}^2(\lambda)d\lambda^2 + a^2(\lambda)d\Omega_3^2 \tag{4.1}$$

with λ parameterizing the histories, $q^A(\lambda)$, in superspace.

Ours is a two dimensional minisuperspace model; $q^{(1)}(\lambda) = a(\lambda)$ being the scale factor and $q^{(2)}(\lambda) = \phi(\lambda)$ being the scalar field. The Euclidean action for the model takes the form (*see Appendix*),

$$I[a(\lambda), \phi(\lambda)] = \frac{1}{2}\int_0^1 d\lambda \mathcal{N}\left\{-a\left(\frac{a'}{\mathcal{N}}\right)^2 + a^3\left(\frac{\phi'}{\mathcal{N}}\right)^2 - a^3 V(\phi) + a\right\} \tag{4.2}$$

where prime denotes differentiation with respect to λ. There are three equations of motion, corresponding to extremizing the action with respect to $\mathcal{N}$, ϕ and a respectively,

$$\left(\frac{a'}{\mathcal{N}}\right)^2 + 1 - a^2\left[\left(\frac{\phi'}{\mathcal{N}}\right)^2 + V(\phi)\right] = 0 \tag{4.3}$$

$$\frac{1}{a^3\mathcal{N}}\left(a^3\frac{\phi'}{\mathcal{N}}\right)' + \frac{1}{2}V'(\phi) = 0 \tag{4.4}$$

$$\frac{1}{\mathcal{N}}\left(\frac{a'}{\mathcal{N}}\right)' + 2a\left(\frac{\phi'}{\mathcal{N}}\right)^2 - aV(\phi) = 0 \tag{4.5}$$

Due to the gauge freedom of $\mathcal{N}$, only the first (Hamiltonian constraint) and an arbitrary choice of one of the other two are independent. Note that the canonical momenta are given by,

$$\pi_0 = 0, \quad \pi_a = \frac{-aa'}{\mathcal{N}}, \quad \pi_\phi = \frac{a^3\phi'}{\mathcal{N}} \tag{4.6}$$

Promoting the canonical variables to operators one finds (adopting the operator ordering favoured by the no-boundary proposal) for the Hamiltonian constraint/Wheeler-DeWitt equation,

$$\frac{1}{2}\left[\frac{1}{a^3}\left(a\frac{\partial}{\partial a}a\frac{\partial}{\partial a} - \frac{\partial^2}{\partial\phi^2}\right) - a + a^3V(\phi)\right]\Psi = 0 \tag{4.7}$$

or defining $a \equiv e^{\alpha}$,

$$\frac{1}{2}e^{-3\alpha}\left[\frac{\partial^2}{\partial\alpha^2}-\frac{\partial^2}{\partial\phi^2}-e^{4\alpha}+e^{6\alpha}V(\phi)\right]\Psi=0 \tag{4.8}$$

If one assumes a slowly varying potential which we shall do for the rest of this analysis, then this is just the one-dimensional WKB problem in α with WKB potential $\mathcal{U}(\alpha,\phi)=e^{6\alpha}V(\phi)-e^{4\alpha}$. Thus one finds,

$$\Psi(\alpha,\phi)\approx\mathcal{C}(\phi)\exp\left(\pm\frac{1}{3V(\phi)}(1-e^{2\alpha}V(\phi))^{3/2}\right),\quad \mathcal{U}\ll 0 \tag{4.9}$$

and

$$\Psi(\alpha,\phi)\approx\mathcal{C}(\phi)\exp\left(\pm\frac{i}{3V(\phi)}(e^{2\alpha}V(\phi)-1)^{3/2}\right),\quad \mathcal{U}\gg 0 \tag{4.10}$$

where $\mathcal{C}(\phi)$ is a possibly complex prefactor.

No-Boundary vs Tunneling Wave Function

We shall now compare the predictions of the two wave functions in a heuristic manner for the closed Friedmann model (for analysis of other Friedmann models, see [81]).

The no-boundary proposal may be imposed directly on the wave function, Ψ. Hawking and Page argued [52] that one may approximate the boundary condition here; imposing $\Psi=1$ when $a\to 0$ with ϕ regular and $\Psi=1$ on the null boundaries. Note that this approach to imposing the boundary conditions results in the same wave function as applying 'initial conditions' on the histories (see [98] [29]).

Also Ψ must be regular as $a\to 0$ so one sees that Ψ must be independent of ϕ, i.e. $\frac{\partial\Psi}{\partial\psi}$, to compensate for the factor of a^{-3} in the second term of (4.8). For $a^2V\ll 1$ one finds the prefactor in the wave function (*see Appendix*),

$$\mathcal{C}(\phi) = \frac{1}{\sqrt{\pi}} exp\left(\frac{+1}{3V(\phi)}\right) \tag{4.11}$$

Thus one has found for the no-boundary wave function (using the WKB matching procedure for $a^2V > 1$),

$$\Psi_{NB}(a,\phi) \approx \begin{cases} exp\left(\frac{1}{3V(\phi)}\right) exp\left[\frac{-1}{3V(\phi)}(1-a^2V(\phi))^{3/2}\right], & a^2V < 1 \\ exp\left(\frac{1}{3V(\phi)}\right) cos\left[\frac{-1}{3V(\phi)}(a^2V(\phi)-1)^{3/2} - \frac{\pi}{4}\right], & a^2V > 1 \end{cases} \tag{4.12}$$

Vilenkin carried out an analysis [95] of this model but with the conformal operator ordering in the Wheeler-DeWitt equation,

$$\left[\frac{\partial^2}{\partial a^2} - \frac{1}{a^2}\frac{\partial^2}{\partial \phi^2} + a^4V(\phi) - a^2\right]\Psi(a,\phi) = 0 \tag{4.13}$$

If we restrict ourselves to regions near the boundary then are solutions will be approximately oscillatory,

$$\Psi = \sum_n \mathcal{A}_n e^{iS_n} \tag{4.14}$$

where S_n are solutions to the Hamilton-Jacobi equation. As we mentioned earlier, the tunneling boundary conditions may be specified in the WKB approximation in terms of 'incoming' and 'outgoing' modes at the boundaries. These notions are developed with respect to the current (2.49); one defines a mode to be outgoing is $-\nabla S_n$ points outwards there.

From (4.13), it is apparent that the only non-singular part of the boundary in superspace is at $a = 0$ and ϕ finite. Consider the region $a^2V > 1$; the wave functions are proportional to e^{iS} or e^{-iS} where $S = (a^2V(\phi)-1)^{3/2}/V(\phi)$. The tunneling proposal prescribes that only the outgoing wave function should contribute, i.e. e^{-iS}. One therefore has,

$$\Psi_T(a,\phi) \approx \mathcal{A}(\phi) exp\left(\frac{-i}{3V(\phi)}\left(a^2V(\phi)-1\right)^{3/2}\right) \tag{4.15}$$

For regularity one needs $\frac{\partial\Psi}{\partial\phi} \to 0$ as $a \to 0$. It is thus found,

$$\mathcal{A}(\phi) = exp\left(\frac{-1}{3V(\phi)}\right) \tag{4.16}$$

Thus, we have, using the WKB matchign procedure,

$$\Psi_T(a,\phi) \approx \exp\left(-\frac{1}{3V(\phi)}\left[1-\left(1-a^2V(\phi)\right)^{3/2}\right]\right), \quad for\ a^2V(\phi) < 1 \tag{4.17}$$

$$\Psi_T(a,\phi) \approx \exp\left(-\frac{1}{3V(\phi)}\right)\exp\left(-\frac{i}{3V(\phi)}\left[1-\left(a^2V(\phi)-1\right)^{3/2}\right]\right), \quad for\ a^2V(\phi) > 1 \tag{4.18}$$

Both the no-boundary and tunneling wave functions are peaked about classical trajectories satisfying, $\pi_\alpha = \frac{\partial S}{\partial q^\alpha}$, where $S = \frac{1}{3V(\phi)}\left[1-(a^2V(\phi)-1]^{3/2}\right]$. Such solutions are found to all exhibit inflationary behaviour for slowly varying potential $V(\phi)$ (see [29] [98] for further details). This is a striking result as the set of inflationary solutions to the field equations is relatively small, yet the WKB wave function with the classicality condition and one of the two boundary conditions is seen to objectively predict inflation.

The next question to ask is: how much inflation do these wave functions predict? A measure of the amount of inflation is given by the number of *e-folds*, given here by $E \equiv \int \hat{h}dt$ where t is the Friedmann time and $\hat{h} = \hat{a}_{,t}/\hat{a}$ is the instantaneous Hubble constant.

It has been shown that there is approximate decoherence between the components of the WKB wave function [33]. Thus, in order to study the probabilities, one need only consider one WKB component. We shall choose to examine the outgoing mode. The probability flux, $\mathcal{J}$, should be integrated over the surface separating the tunneling from the oscillatory region, $a^2V(\phi) = 1$. However, the WKB approximation only applies to trajectories with $\dot{\phi} \approx 0$. The answer can then be approximately given by surfaces on which $a = constant$. On such surfaces, it is easy to see that one finds probability fluxes,

$$dP = J \cdot d\Sigma \propto \begin{cases} exp\left(\frac{+2}{3V(\phi)}\right) & \text{no-boundary wave function, } \Psi_{NB} \\ exp\left(\frac{-2}{3V(\phi)}\right) & \text{tunneling wave function, } \Psi_T \end{cases} \tag{4.19}$$

The integral may diverge but one may only talk about conditional probabilities anyway so these divergences will cancel. This conditional probability for sufficient inflation on a surface of constant a is given by,

$$P(\phi_0 > \phi_{suf} | \phi_1 < \phi_0 < \phi_2) = \frac{\int_{\phi_{suf}}^{\phi_2} d\phi_0 exp\left(\frac{\pm 2}{3V(\phi)}\right)}{\int_{\phi_1}^{\phi_2} d\phi_0 exp\left(\frac{\pm 2}{3V(\phi)}\right)} \tag{4.20}$$

where ϕ_1 and ϕ_2 are cut-offs for ϕ_0. ϕ_1 is determined numerically by the requirement for classicality at late times. In their original investigation, Hawking and Page [52] took $\phi_2 = \infty$ and found $P \approx 1$ for inflation for the no-boundary wave function. However, Vilenkin criticized [94] this choice of ϕ_2, claiming that an upper cut-off should be introduced at the Planck scale as the semiclassical approximation breaks down near this value.

For the value of ϕ_2 suggested by Vilenkin, the denominator dominates the probabilities for the no-boundary wave function and we have $P \ll 1$. The tunneling wave function is seen to have $P \approx 1$ for either case. Thus the tunneling proposal would seem to predict more inflation than the no-boundary proposal. However, Hawking has argued that *volume weighting* is necessary.

Volume Weighting

Hawking has argued [50] that the results obtained above should be multiplied by a volume factor, $\exp(3N)$ where N is the number of Hubble volumes in the universe.

The amplitude for a solution to the Wheeler-DeWitt equation gives the probability for the entire universe. However, these predictions are clearly beyond the scope of our observations as we can only observe the Hubble volume surrounding us. Hawking argued that the probabilities must be multiplied by this volume factor to account for other Hubble volumes on our surface of homogeneity that we cannot observe. This is done by integrating over the variables which are unobservable.

In the case of a closed, homogeneous and isotropic model, Hawking *et al.* give us the following prescription for implementing this volume weighting:

> *"Approximate the probability for our data on the past light cone by the probability of data in a Hubble volume on an appropriate surface of homogeneity. Assume that our data are otherwise detailed enough that they occur only once on this surface [44]. The sum is then over the spatial locations of our Hubble volume in that surface of homogeneity in all classical space-times that last sufficiently long."*

It is found that the volume weighted probability distribution has a wide region in which the probability increases with increasing N. Indeed, it is found that, upon implementation of volume weighting, the dominant contribution to the path integral will come from broad saddle-points with one descent direction. For solutions starting at these points, it is found that a large number of efolds are predicted. Thus, the volume weighted no-boundary wave function is seen to predict a large number of efolds which is consistent with the properties of the universe which we observe today. Figure 3 shows heuristic plots of the number of efolds predicted before and after volume weighting.

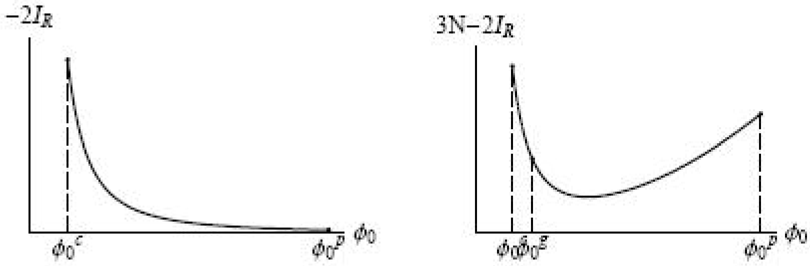

Figure 3: (Taken from [42]) *The left-hand figure shows the approximate argument of the no-boundary wave function before volume weighting and the right-hand side that after volume weighting. The resulting wider distribution is found to predict sufficient inflation.*

Bounces and Initial Singularities

We shall now examining the probabilities for the classical histories of the universe to exhibit a classical bounce or an initial singularity in the no-boundary case. We shall now follow the analysis of [41] for the case of $V(\phi) = m^2\phi$ in the model of the previous section. Following Lyons [70], we introduce,

$$\tau(\lambda) \equiv \int_0^\lambda d\lambda' \mathcal{N}(\lambda') \tag{4.21}$$

$\tau(\lambda)$ defines a contour in the complex τ-plane for each lapse function $\mathcal{N}(\lambda)$. We also introduce the variables,

$$H^2 \equiv \lambda/3, \quad \phi \equiv (4\pi/3)^{1/2}\Phi, \quad \mu \equiv (3/\lambda)^{1/2}m \tag{4.22}$$

H was defined such that it coincides with the usual classical notion of the (Hubble parameter). In terms of these new variables, one has for the action (4.2),

$$I[a(\tau), \phi(\tau)] = \frac{3\pi}{4H^2} \int_{C(0,v)} d\tau \left[-a\dot{a}^2 - a + a^3 + a^3 \left(\dot{\phi}^2 + \mu^2\phi^2\right)\right] \tag{4.23}$$

where $v = X + iY$ is the endpoint of the contour of integration, C. Note that two contours with the same endpoints will give the same value of the action if they can smoothly be distorted into one another [42]. One finds for the equations of motion,

$$\dot{a}^2 - 1 + a^2 + a^2 \left(-\dot{\phi}^2 + \mu^2\phi^2\right) = 0 \tag{4.24}$$

$$\ddot{\phi} + 3(\dot{a}/a)\dot{\phi} - \mu^2\phi = 0 \tag{4.25}$$

$$\ddot{a} + 2a\dot{\phi}^2 + a(1 + \mu^2\phi^2) = 0 \tag{4.26}$$

$\tau = 0$ corresponds to the 'initial' boundary of the universe; it is thus here that we will impose the no-boundary conditions. This point/hypersurface is termed the 'South Pole'. $\tau = v$ corresponds to the present universe. We label the hypersurface at $\tau = v$ as Σ. On this hypersurface, we define,

$$a(\tau)|_{\Sigma} = a(v) \equiv b \qquad \phi(\tau)|_{\Sigma} = \phi(v) \equiv \chi \tag{4.27}$$

Note that b and χ must be (approximately) real to correspond to the universe which we observe.

Now one sets initial conditions on the superspace coordinates, $a(\tau)$ and $\phi(\tau)$ such that the 4-geometry closes and the solution is regular at $\tau = 0$, i.e. imposing the no-boundary condition. Recall the form of the metric, (4.1). We want the 4-geometry to close off regularly as $\tau \to 0$. If one identifies,

$$a(\tau) \sim \pm \mathcal{N}\tau \quad , \quad as \quad \tau \to 0 \tag{4.28}$$

one has the metric of a Euclidean 4-sphere in polar coordinates which clearly closes of regularly as $\tau \to 0$. Closing the metric off in analogy with the 4-sphere suggests,

$$a(0) = 0 \qquad \frac{1}{\mathcal{N}}\frac{da}{d\tau}(0) = 0 \tag{4.29}$$

The first of these conditions suffices as the second is found to follow from (4.3) after the first condition is imposed. For the scalar field, consider (4.5). The second term will diverges unless,

$$\dot{\phi}(0) = 0 \tag{4.30}$$

One thus has the no-boundary condition on the scalar field coordinate. The set of equations with these conditions imposed may be solved analytically only in the limits where $\phi(0)$ is very large and $\phi(0)$ is very small. Elsewhere the equations must be solved numerically.

The problem is well posed as the number of free real parameters is the same as the number of real conditions that must be matched; v and ϕ_0 may be adjusted to fix b and χ. These free parameters must be fine-tuned to result in classicality and real values for the scale factor and scalar field at late time.

Hawking *et al.* found a qualitative difference [42] between $\mu > 3/2$ and $\mu < 3/2$ models. They found that for $\mu > 3/2$ and $\phi_0^c \leq \phi_0 \leq \phi_0^s$ the classically allowed histories of the universe exhibit an initial singularity. Here, ϕ_0^c (found numerically) is the critical value of the scalar field above which the universe will predict classicality at late times and ϕ_0^s is a new critical value.

It is found that for $\phi_0 > \phi_0^s$ the histories bounce at a finite radius $\hat{a}_b$ in the past. Near the bounce, the universe approaches a de Sitter state. Such non-singular classical solutions form only a small subset of all solutions. However, imposing the no-boundary condition and classicality at late times it is found that they have significant probability.

They concluded that for realistic values of parameters, the most likely origin of the universe on a history by history basis is an initial singularity. For the more physical, top-down probabilities however, they found that a bouncing universe is most likely.

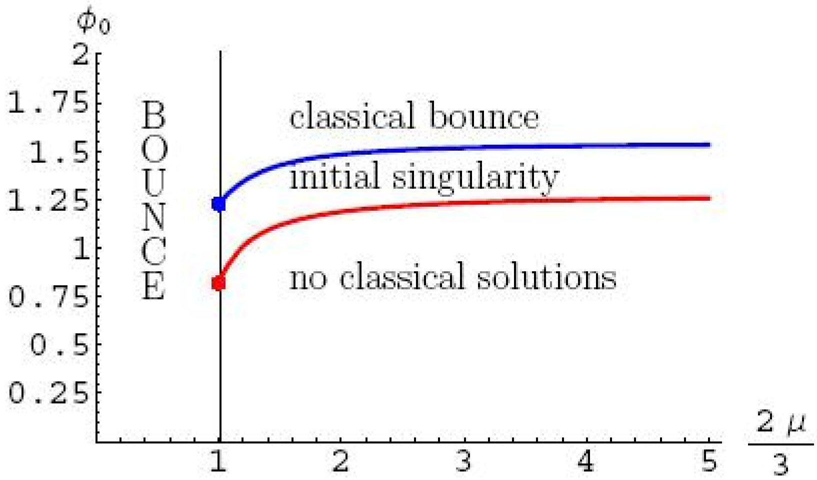

Figure 4: (Taken from [42]) *The 'phase diagram' showing the behaviour at early times for histories of the no-boundary state. For $\mu < 3/2$ all histories are seen to exhibit a bounce whereas for $\mu > 3/2$ this is dependent on the value of ϕ_0.*

Structure Formation

Let us now consider inhomogeneous perturbations about minisuperspace. It is conjectured that such fluctuations are responsible for structure formation. Indeed it is hoped that the data from the MAP and PLANCK satellites may provide verification of the results of such calculations in quantum cosmology and hence indicate a preference for one or more of the various boundary proposals. We shall be considering the closed Friedmann model again. This analysis is essentially a quick overview of that in [29] and for further details we refer the reader there. We shall write the perturbations as,

$$h_{ij}(x,t) = a^2(\Omega_{ij} + \epsilon_{ij}) \tag{4.31}$$

$$\Phi(z,t) = \Phi_0 + \delta\Phi(x,t) \tag{4.32}$$

$$\mathcal{N}(x,t) = \mathcal{N}_0(t) + \delta\mathcal{N}(x,t) \tag{4.33}$$

$$\mathcal{N}_i(x,t) = 0 + \delta\mathcal{N}_i(x,t) \tag{4.34}$$

Halliwell and Hawking [30] showed that these perturbations may be expanded using spherical harmonics on the 3-sphere. For example, one has,

$$\delta\Phi(x,t) = \sum_{nlm} f_{nlm}(t) Q^n{}_{lm}(x) \tag{4.35}$$

where $f_{nlm}(t)$ are coefficients and $Q^n{}_{lm}(x)$ satisfy the 3-dimensional Laplace equation on S^3. Recall the action (1.13); substituting the perturbations (4.31)-(4.34) into (1.13), this may be decomposed,

$$S[g_{\mu\nu}, \Phi] = S_0[q^A, \mathcal{N}_0] + S_2[q^A, \mathcal{N}_0, \epsilon_{ij}, \delta\Phi, \delta\mathcal{N}, \delta\mathcal{N}_i] \tag{4.36}$$

where S_0 is the unperturbed original action and S_2 is the action of the perturbations. Similarly, one may decompose the action,

$$\hat{\mathsf{H}}\Psi = \left[-\frac{1}{2}\nabla^2 + \mathcal{U}(q) + \hat{\mathsf{H}}_2\right]\Psi = 0 \tag{4.37}$$

where H_2 is the Hamiltonian of the perturbations. The part of the Hamiltonian that is linear in the perturbations imposes another momentum constraint,

$$\hat{\mathcal{H}}_i \Psi = 0 \tag{4.38}$$

One may treat still treat q^A semiclassically while treating the perturbations quantum mechanically. One finds solutions of the form,

$$\Psi = \mathcal{C}(q, \Phi) e^{iS_0(q,\Phi)} \psi \tag{4.39}$$

with S_0 satisfying the unperturbed Hamilton-Jacobi equations and ψ satisfying the functional Schrödinger equation (see [29] for details),

$$i \frac{\partial \psi}{\partial t} = \hat{\mathsf{H}} \psi \tag{4.40}$$

The different modes of ψ do not interact. So we have found, from the Wheeler-DeWitt equation, a wave function that is peaked about a set of classical trajectories with corrections governed by ψ. We may apply boundary conditions and pick out a particular wave function from the set of solutions.

We earlier mentioned that it is hoped that quantum cosmology may provide a tool for selecting vacua in string theory landscapes. An example of such vacuum selection is seen here. By solving this Schrödinger equation for both boundary conditions, it is found that both the no-boundary condition [67] and the tunneling condition [94] pick out a particular *Bunch-Davies* vacuum for approximately de Sitter background space. This state is the state often assumed in cosmology as an initial condition when performing calculations. That this is objectively selected by the wave functions lends weight to the validity of quantum cosmology and the boundary proposals.

Boltzmann Brains in the No-Boundary Proposal

Susskind has argued [83] that, in the no-boundary proposal, the presence of a cosmological constant would result in a large Euclidean 4-hemisphere as the dominating extremum in the path integral. This would lead to a dominant probability for a very large, nearly empty de Sitter space, in contradiction to observations. When one talks about observations, one is naturally restricted to parts of the universe for which there are observers. *Boltzmann Brains* (*see Appendix*) are essentially observers born out of quantum fluctuations. As a result, they are obviously extremely unlikely; regardless, they still must be considered as a possibility to provide observers for parts of the universe. Susskind argued that despite this suppressed probability, due to the size of the de Sitter space predicted, Boltzmann Brains are the most likely observer in such a universe. Thus we would be highly atypical in the universe; which must be seen as an incorrect conclusion by the anthropic principle.

Put simple; let $\mathcal{A}$ be the conditions for any kind of observations and $\mathcal{B}$ be the conditions for our kind of observations, i.e. ordered observations. Since $\mathcal{B}$ is what is observed, the conditional probability, $P(\mathcal{B}|\mathcal{A})$, should not be orders of magnitude smaller than unity. Page [83] has performed qualitative calculations and found that $P(\mathcal{B}|\mathcal{A}) \ll 1$.

Page proposed a number of possible resolutions within the no-boundary proposal to remedy this problem in his paper, including that eternal inflation holds resulting in the universe reaching an arbitrarily large sized for which ordered observers will dominate by volume ordering. The proposal that Page sees as most likely is that the integral over inital scalar field values, ϕ_0, will dominate over the probability for de Sitter space. He also, as we have seen, proposed an alternative wave function with very similar properties to the no-boundary wave function that avoids this problem.

The Arrow of Time

It is generally accepted that there is some underlying physical arrow of time. There exist many proposals for defining such an arrow. It is hoped that quantum cosmology may provide a physical basis for this arrow of time. Here, we introduce examples of such proposals.

One of the natural ways to define the direction of time is using entropy. One observes the second law of thermodynamics which states that the entropy of the universe will never decrease with time; thus, it is natural to identify the arrow of time with the direction of increasing entropy. However, it has been argued by many that in order for the second law to hold one must have a low entropy initial state of the universe[1]. Assuming this is the case, then it both the no-boundary and tunneling proposals are seen to predict the second law of thermodynamics.

We shall now describe an alternative approach to how an arrow of time may be defined from the Wheeler-DeWitt equation following [100] [59].

Consider the Wheeler-DeWitt equation (4.8). For this to hold, the potential, V, must be asymmetric with respect to α. Thus, it is seen that, the Wheeler-DeWitt equation is fundamentally asymmetric with respect to the intrinsic time. If one supposes that initially the universe is approximately a product of all possible degrees of freedom,

$$\Psi \stackrel{\alpha \to -\infty}{\longrightarrow} \prod_i \psi_i(x_i) \tag{4.41}$$

i.e. the degrees of freedom are initially not entangled. Then one may define entropy as the entanglement entropy for relevant degrees of freedom, i.e. one integrates out the unobservable degrees of freedom. Entropy would be constrained to increase in the presence of a potential, hence defining the direction of time. This increasing entanglement would cause the universe to assume classical properties due to *decoherence* [57].

Note that as the initial time here is associated with $\alpha \to -\infty$, the scale factor must increase with time. Thus, the expansion of the universe becomes inevitable. For a recollapsing universe, the arrow of time would reverse at the classical turning point. Thus we would see that the Big Bang and Big Crunch become the same with this definition of time. This is just again what we saw in *Time After Quantization*, where we identified the 3-volume as the intrinsic time variable. It has been shown, however, that such a turning point would be constrained to be a purely quantum transition through which no observers could pass [58]. Thus, it is essentially, just two separate expanding universes.

Similar proposals have been made. Penrose suggested [85] using the Weyl tensor as a measure of gravitational entropy and defining the arrow of time accordingly. For example. the big bang has

[1]This has been disputed by some [87].

small Weyl tensor while a big crunch has a large Weyl tensor[2].

Hawking put forth [46] a proposal for the arrow of time conditioned on the no-boundary proposal. He proposed that the fluctuations away from homogeneity and isotropy would be minimized at the South Pole and restricted to increase as they move towards $\lambda = 1$. We earlier, discussed the possibility of a bounce rather than an initial singularity for a closed Friedmann model and found that the volume weighted top-down probability suggested a bounce.

This begs the question as to whether we could observe data from before the bounce if such a bounce had occurred. Furthermore, could an observer pass through such an event? With the definition of the arrow of time given by Hawking, the answer to both questions is no. For a bounce at a finite radius, the arrow of time would point away from the bounce on either 'side' of it. There is hence no causal contact between the two regions and the case is similar to the recollapsing universe described above with the entanglement entropy arrow of time.

Topology Change

In classical general relativity, the topology of space-time is fixed in the absence of closed timelike curves or singularities. These are prohibited for globally hyperbolic space-times. One of the possibilities opened up by a quantum theory of gravity is that of allowed topology changes for globally hyperbolic space-times. Although, one requires a fundamental quantum theory of gravity to determine such changes, we hope that our minisuperspace models may provide some sort of qualitative prediction for such results.

In inflationary scenarios, the strong energy condition is often violated. For the case of Friedmann-Robertson-Walker cosmologies this violation would imply that the curvature, k, is the predominant force at small scale factors. Any topology change would therefore result in a vastly different universe than that if no topology change was assumed. Indeed, Linde has shown [69] that, under certain conditions, the probability for the creation by tunneling from nothing of a topological non-trivial, i.e.

[2] See [100] for further details.

$k = k(t)$, compact universe is not exponentially suppressed whilst for the cases of trivial topologies, i.e. $k = constant$, the corresponding probabilities are suppressed. Thus, it appears more likely than one might have initially thought that topology change may have had a significant bearing on the universe.

De Lorenci *et al.* performed [12] a heuristic analysis of topology changes in such a Friedmann-Robertson-Walker minisuperspace. In order to allow for such topology changes, however, it is necessary to have this minisuperspace embedded in a *midisuperspace* as the the metric will no longer be that of a spatially homogeneous space-time. Midisuperspace is essentially a weaker restriction of superspace than that which results in minisuperspace, i.e. there is less symmetry in the degrees of freedom that one considers. A key property is that midisuperspace is still infinite-dimensional[3].

As the manifold considered is of the form $\Sigma \times \mathbb{R}$ only spacelike topology changes (on Σ) are allowed. For simplicity, we restrict ourselves to boundaryless and compact spatial hypersurfaces. In this case the topology is uniquely determined by the orientability and genus. We have the metric tensor and though this characterizes the corresponding manifold locally, it does not uniquely determine the global structure, i.e. the topology.

The FRW metric we wish to consider is of the form,

$$ds^2 = -\mathcal{N}^2(t)dt^2 + a^2(t)\left\{d\chi^2 + \left[\frac{sin[\sqrt{k(t)}\chi]}{\sqrt{k(t)}}\right]^2 d\Omega^2(\theta,\phi)\right\} \tag{4.42}$$

in minisuperspace which we label $\mathcal{Q}$ here. Note the t-dependence of the spatial curvature, $k(t)$. Generalizing to midisuperspace, $\mathcal{R}$, one finds (with non-vanishing shift vector, $\mathcal{N}_\chi(\chi,t)$),

$$ds^2 = \left[-\mathcal{N}^2(\chi,t) + \frac{\mathcal{N}_\chi^2(\chi,t)}{a^2(\chi,t)}\right]dt^2 + 2\mathcal{N}_\chi(\chi,t)d\chi dt + a^2(\chi,t)[d\chi^2 + \sigma^2(\chi,t)d\Omega^2(\chi,t)] \tag{4.43}$$

Consider this model with a matter sector given by a dust field, $\xi(\chi,t)$, and a scalar field, $\phi(\chi,t)$. It has been proposed [66] that the dust field provides a suitable intrinsic time parameter for such a

[3]For more details on midisuperspace see [63].

system and that is the convention adopted here.

The Wheeler-DeWitt equation in midisuperspace is a functional differential equation rather that the ordinary differential equation of minisuperspace. This is significantly more difficult to solve and we shall restrict ourselves to a minisuperspace subdomain of midisuperspace defined by,

$$a' = 0, \quad \phi' = 0, \quad \xi' = 0, \quad \sigma = \frac{sin[\sqrt{k(t)}\chi]}{\sqrt{k(t)}} \tag{4.44}$$

where prime denotes differentiation with respect to χ. A key point here is that the results obtained for the subdomains at specific values of the spatial curvature will not be the same as those obtained by constructing the minisuperspaces for each value of k separately.

We will be considering only WKB solutions at $\hbar^0$ order as to work to higher orders is too speculative. In order to calcluate any probabilities, one must have a normalizable measure, i.e.

$$\langle\Psi|\Psi\rangle = \int_{\mathcal{R}} \mathcal{D}a\mathcal{D}\sigma\mathcal{D}\phi\Psi[a,\sigma,\phi,\xi]\Psi^{\star}[a,\sigma,\phi,\xi] \tag{4.45}$$

should be normalizable. We only know the wave function, Ψ on the minisuperspace subdomain and so cannot compute this. We must therefore content ourselves with requiring,

$$\langle\Psi|\Psi\rangle_{\mathcal{Q}} \equiv \int_{\mathcal{Q}\subset\mathcal{R}} \mathcal{D}a\mathcal{D}\sigma\mathcal{D}\phi\Psi[a,\sigma,\phi,\xi]\Psi^{\star}[a,\sigma,\phi,\xi] \tag{4.46}$$

to be normalizable. This will depend on both the boundary conditions and the contour of integration chosen.

Recall that we have a spacelike hypersurface, Σ, coordinatized by a and ϕ. Let these coordinates take on values $\bar{a}$ and $\bar{\phi}$ at a specific value of the 'time' variable $\bar{\xi}$. As we have discussed, it is only meaningful to talk about conditional probabilities; the conditional probability for finding spatial curvature k is at 'time' $\bar{\xi}$ is then,

$$P(k|\bar{a},\bar{\phi}) = \frac{|\Psi(k,\bar{a},\bar{\phi})|^2}{\sum_{k=0,\pm1}|\Psi(k,\bar{a},\bar{\phi})|^2} \tag{4.47}$$

In the analysis of De Lorenci *et al.*, boundary conditions were chosen for convenience rather than by physically motivation; hence the wave functions studied are not physical. They imposed boundary conditions on the arbitrary constant, C, on the which the wave function depends; it was chosen to be $C = i$ which ensured convergence of the inner product. Despite the apparent arbitrariness in the choice of boundary conditions, the analysis may still give a taste of some of the properties that such an approach may yield with physical boundary conditions. Indeed this would be an interesting area to look at in the future.

As we mentioned previously, the metric does not uniquely fix the topology of the manifold. De Lorenci *et al.* studied the topologies S^3, D^3 for $k = 1$, T^3 for $k = 0$ and I^3 for $k = -1$. It was found that a topology change between any two topologies of different k was allowed. Moreover, a characteristic 'arrow of topology change' was exhibited, i.e. the direction corresponding to increasing exponent in the wave function is seen to have a much higher probability for topology change than the other direction. This direction was found to be in the opposite direction when $C = -i$ however. It may be possible that this could be linked in some way with the flow of time as discussed in *Arrow of Time*. The cases considered were non-physical, however, and it is naïve to draw any conclusion from the analysis however.

Green Function

Martin *et al.* have explicitly calculated [75] the Green's function for such topology changes in this model. The Green's function, G, will describe the evolution of the wave function, i.e.

$$\Psi(q_f, t_f) = \int dq_i G(q_f, t_f; q_i, t_i)\Psi(q_i, t_i) \tag{4.48}$$

where q_f are final degrees of freedom and q_i initial degrees of freedom. We restrict ourselves to topology changes on large scales, i.e. scales bigger than the Hubble volume, H. This justifies the use of the *long wavelength approximation*[4]. Using both the semiclassical and long wavelength approximations, it is necessary to integrate over complex metrics in order to allow for topology change.

[4] See [75].

They also found that, for large $\Delta\xi$, there was a preferred direction from positive to negative curvatures, i.e. topology change in the other direction was suppressed. This is in keeping with the analysis of De Lorenci *et al.* for the $C = -i$ choice of boundary conditions.

Generalized Tunneling Proposal

e Costa and Fagundes studied [16] tunneling from an open non-trivial S^4/Γ topology into a closed universe of topology $\mathbb{R} \times (S^3/\Gamma)$ where Γ is the group of isometries acting on S^4. In the tunneling boundary proposal, Vilenkin proposed that universes tunnel from an S^4 instanton into an $\mathbb{R} \times S^3$ universe. Thus, the case studied by e Costa and Fagundes can be seen as a 'generalization' of the tunneling proposal allowing for a space-time with a non-trivial topology.

The probability for this manifold with topology $\mathbb{R} \times (S^3/\Gamma)$ to transition to one of topology $\mathbb{R} \times \mathcal{W}$ $(k = +1)$, where $\mathcal{W}$ is the Weeks manifold- a closed hyperbolic 3-manifold with the smallest volume of any hyperbolic 3-manifold, was studied. It was found that this probability approached unity as $\xi \to \infty$. If a more rigourous analysis can be carried out to confirm this result then this result would open up many otherwise excluded histories. For instance, open Friedmann models are generally excluded on the grounds that they do not provide the desired results for the density ratio, $\Omega(t)$, without fine-tuning unlike closed models; they would now no longer be ruled out by this argument, should this result hold.

Symmetric Bounce Proposal

The symmetric bounce proposal was formulated with the desire to essentially 'be' the no-boundary proposal without the Boltzmann Brain problem. Unsurprisingly, it is seen [84] reproduce the prediction of the no-boundary proposal for inflation. From its definition though it is clear that the symmetric bounce wave function always exhibits a bounce and not initial or final singularities.

It is found that it also picks out the Bunch-Davies vacuum as the vacuum state about an approximately de Sitter background space from the calculation of inhomogeneous perturbations, as in

Structure Formation. The arrow of time proposed by Hawking and introduced in *The Arrow of Time* may also be applied, with the same results, to the symmetric bounce proposal.

Further Reading on Predictions of Quantum Cosmology

There has been much research into the predictions of quantum cosmology other that that documented in this chapter. Here we mention a few examples of such research and provide references to the corresponding literature.

Pair Production of Black Holes for the Tunneling Wave Function

The tunneling wave function has been criticised [6] by Bousso and Hawking on the grounds that it leads to a instability of de Sitter space triggering an 'avalanche' of pairs of black holes.

In defense of this criticism, Garriga and Vilenkin countered [17] that the assumptions on which this argument was based were unfounded. Garriga and Vilenkin's analysis found there to be a stable constant production rate rather than the catastrophic rate predicted by Bousso and Hawking.

The Tunneling Wave Function and Open Universes

Generally, closed Friedmann-Robertson-Walker universes have been considered as $k = 1$ models are found to have finite size. The nucleation of locally open regions is allowed in the tunneling proposal. However, Coule and Martin have proposed [10] that, as open universes may also be compact, that it is not necessary to restrict open universes to the case of those created by tunneling from a closed universe. In fact, their argument is a stronger one. They suggest that not only can the universe originated in an open state, but that it should originate in an open state.

Restricting themselves to the tunneling proposal, they found that not only was inflation predicted but that sufficient inflation was predicted.

Quantum Cosmology and Eternal Inflation

For detailed analysis for both both the no-boundary and tunneling perspectives in the règime of eternal inflation, see [40] [92].

Chapter 5

A Consistent Histories Approach to Quantum Cosmology

An issue which we have not yet discussed is that of the quantum mechanical interpretation which we are adopting in the theory. As we have mentioned, a quantum theory of cosmology is clearly incompatible with the Copenhagen interpretation of quantum mechanics, in which the observer and the act of measurement are treated classically, i.e. any quantum system must be embedded in a classical "environment". To provide a completely quantum mechanical description of the universe, we must treat the observer and their measurement quantum mechanically. Such descriptions are known as *generalized quantum mechanics*. We shall focus on the *consistent histories* approach [25] [37] [21].

There is an immediate obstacle to overcome with any quantum mechanical theory that abandons the concept of external observers and the wave collapse mechanism; how does a classical system emerge from the quantum system? The solution lies with the *decoherence mechanism* [99].

Decoherence in Quantum Mechanics

We shall now give a heuristic account of the motivation and role of the wave collapse mechanism in the Copenhagen interpretation and contrast it with the decoherence mechanism of generalized quantum mechanics following [58]. We shall be considering the measurement of a quantum mechanical system, $\mathcal{S}$, to an apparatus, $\mathcal{A}$.

Copenhagen Interpretation

In the Copenhagen interpretation, the interaction Hamiltonian may be written as,

$$H_{int} = \sum_n |n\rangle\langle n| \otimes \hat{\mathcal{A}}_n \tag{5.1}$$

where $\hat{A}_n$ are operators describing the interaction of the system with the measuring apparatus and the states $|n\rangle$ denote the states of the system which may be distinguished by the apparatus. It is assumed here that the apparatus 'measures' the system without affecting it. Suppose that the system is initially in the state $|n\rangle$ and the apparatus in state $|\Phi_0\rangle$. If one evolves the overall system under Schrödinger evolution then one finds,

$$|n\rangle|\Phi_0\rangle \xrightarrow{t} exp(-iH_{int}t)|n\rangle|\Phi_0\rangle = |n\rangle exp\left(-i\hat{\mathcal{A}}_n t\right)|\Phi_0\rangle \tag{5.2}$$

$$\equiv |n\rangle|\Phi_n(t)\rangle \tag{5.3}$$

Now let us consider a superposition of such initial states of the measurable observable,

$$\left(\sum_n c_n|n\rangle\right)|\Phi_0\rangle \xrightarrow{t} \sum_n c_n|n\rangle|\Phi_n(t)\rangle \tag{5.4}$$

Thus, upon evolution, one has a superposition of macroscopic states. This is in clear contradiction to states that we observe and a modification of the theory is required. von Neumann posited the collapse mechanism as this modification. This proposes that the act of 'measuring' automatically imposes a 'collapse' of such a superposition into one of the macroscopic branches of the superposition.

We now examine the same set up in the framework of generalized quantum mechanics. It has been found [99] that macroscopic quantum states exhibit a strong 'coupling' to their environments. In light of this result, it appears necessary that we consider not just our system, $\mathcal{S}$ and our apparatus, $\mathcal{A}$ but also the environment, $\mathcal{E}$. The measurement device itself is 'measured' by the environment and one can write, similarly to (5.3),

$$\left(\sum_n c_n|n\rangle|\Phi_0\rangle\right)|E_0\rangle \xrightarrow{t} \sum_n c_n|n\rangle|\Phi_n(t)\rangle|E_n(t)\rangle \equiv |\psi(t)\rangle \tag{5.5}$$

We are now left with the same problem as before; this is again a superposition of macrostates. However, a key observation is that many of the degrees of freedom of the environmental system are *unobservable*. Such unobservable degrees of freedom must be integrated out if we are to yield measurable predictions from the theory.

For realistic environments, the states, $|E_n(t)\rangle$, for a given value of t will be approximately orthogonal [58], i.e. $\langle E_n|E_m\rangle \approx \delta_{nm}$. Thus the reduced density matrix of the system and apparatus after integration over the unobservable degrees of freedom is approximately given by,

$$\rho_{\mathcal{SA}} \approx \sum_n |c_n|^2|n\rangle\langle n| \otimes |\Phi_n\rangle\langle\Phi_n| \quad if \quad \langle E_n|E_m\rangle \approx \delta_{nm} \tag{5.6}$$

This density matrix does not describe a superposition of macrostates. It rather describes a mixture of macrostates, assigning a probability, $|c_n|^2$, for the system and apparatus to be in state $|n\rangle$ and $|\Phi_n(t)\rangle$ respectively.

Thus we have resolved the issue of having a superposition of macrostates without having to artificially impose a wave collapse mechanism. The result was obtained through the irreversible interaction with the environment or the decoherence mechanism. As a result of this interaction, both the system and apparatus have taken on classical properties.

We now turn our attention back to quantum cosmology. We wish to treat the universe as a closed quantum mechanical system. However, in doing so, we preclude the possibility of an interaction with an environment as, by definition, the universe does not have an environment. Thus it seems that the decoherence mechanism outlined above cannot be used to explain why the universe assumes the classical properties which we observe

However, while the universe itself does not decohere, it is seen that subsystems of the universe will decohere [100]. This is satisfactory as we will never observe the universe as a whole and only deal with subsystems. We may thus apply the decoherence mechanism in quantum cosmology.

Decoherent Histories in Quantum Cosmology

We shall now focus on a particular approach to generalized quantum mechanics, the *decoherent or consistent histories approach* [37]. In this approach, in analogy with the case described in the last section, the histories of the universe decohere to assume classical properties on the present hypersurface, Σ.

A description of the universe in this framework requires three essential elements:

1. *fine-grained histories*: They are the most detailed four dimensional histories of the space-time metric and matter field configurations of the universe.

2. *coarse-grained histories*: They can be thought of as a *"smoothing out"* of the fine-grained histories. More precisely, they are reparametrization invariant classes of fine-grained histories. In other words, the histories are separated into physically meaningful partitions.

3. *decoherence functional*: provides a measure of the quantum mechanical interference between members of a set of histories. Sets of negligible interference between all possible pairs are said to *decohere* or to be *consistent* (there is a distinction between these two; however for our purposes they will be the same). The decoherence functional is vital if one is to assign probability amplitudes. We know that it is not always possible do this in a self-consistent manner if there is not decoherence. Note that the boundary conditions are incorporated into the decoherence functional []. Note, however, that a separate theory of boundary conditions is still required for

this prescription, as before.

We shall now present a more detailed description of these three elements for the case of a non-relativistic system with external time parameter t.

Fine-Grained Histories

Let us consider a physical system, $\mathcal{S}$, with Hamiltonian H. Suppose one has a Hilbert space $\mathcal{H}$ for this system with a family of observables A^α. Let us choose a set of observables A^{α_i}, each corresponding to a time, t_i.

We define $\{h\} = \{a_{k_1}^{\alpha_1}, a_{k_2}^{\alpha_2}, ..., a_{k_n}^{\alpha_n}\}$ where a_k^α are the eigenvalues corresponding to A^α and each k_i runs over all possible eigenvalues. We may regard $\{h\}$ as providing an exclusive, exhaustive set of fine-grained histories for $\mathcal{S}$. Note that these fine-grained histories have 'ends' on which the quantum mechanical boundary conditions must be imposed.

One must also have projections, $P_{a_k}^\alpha$, projecting onto the corresponding eigensubspaces, $\mathcal{S}_{a_k}$, for each eigenvalue, a_k^α. One can construct the propagator,

$$U(t_i, t_j) = e^{-iH(t_i - t_j)/\hbar} \tag{5.7}$$

$$\equiv U(t_i - t_j) \tag{5.8}$$

Using this propagator, Heisenberg projections may be constructed,

$$P_{a_k}^\alpha(t) = U^\dagger(t) P_{a_k}^\alpha U(t) \tag{5.9}$$

Each fine-grained history h may then be represented by its corresponding "class operator",

$$C_h = P_{a_{k_1}}^{\alpha_1}(t_1) P_{a_{k_2}}^{\alpha_2}(t_2) ... P_{a_{k_n}}^{\alpha_n}(t_n) \tag{5.10}$$

$$= U(t_0 - t_1) P_{a_{k_1}}^{\alpha_1} U(t_1 - t_2) ... U(t_{n-1} - t_n) P_{a_{k_n}}^{\alpha_n} U(t_n - t_0) \tag{5.11}$$

(Note: $\sum_h C_h = 1$). They clearly characterizes the history h; given a wave function, they evolve that wave function, then project it onto the eigensubspace corresponding to the eigenvalue of the observable at that time, before evolving it again and so on throughout the entire history.

Using these class operators we may define the "branch wave function",

$$|\psi_h\rangle \equiv C_h^\dagger|\psi\rangle \tag{5.12}$$

$$= U(t_0 - t_n)P^{\alpha_n}_{a_{k_n}}U(t_n - t_{n-1})...U(t_2 - t_1)P^{\alpha_1}_{a_{k_1}}U(t_1 - t_0)|\psi\rangle \tag{5.13}$$

where $|\psi\rangle$ is an initial state (which when we transfer to the case of quantum cosmology will satisfy the Wheeler-DeWitt equation). This is the quantum state which, under Schrödinger evolution, will evolve into the state that has followed the history $\{h\}$. These 'wave functions' are not functions of t and therefore are not solutions of the Schrödinger equation; an appealing property with a view to moving to reparametrization invariant systems.

Coarse-Grained Histories

As we mentioned, one needs not only fine-grained histories for our purposes but also the coarse-grained histories. We wish to identify histories that are the same in the eyes of the theory. In the case of quantum cosmology, the symmetry group is that of reparametrization invariance. After the $3+1$ decomposition, this is the symmetry remaining from the diffeomorphism invarianve of general relativity.

One therefore partitions our fine-grained histories into reparametrization invariant classes. One may implement this partitioning using a reparametrization functional, $F[q^A, N]$, i.e. one partitions the fine-grained histories according to their corresponding values of this functional. Explicitly, for an exclusive set of ranges $\{\Delta_h\}, h = 1, 2, ...$ of the real line, one defines,

$$C_{\bar{h}} = \{(q^A(t), N(t))|F[q^A, N] \in \Delta_h\} \tag{5.14}$$

In order to obtain probabilities, one must therefore ask whether the universe has a given reparameterization invariant property. This allows us to partition in a relevant way our fine-grained histories into the class which has this property and the class which does not. The following are examples of such partitions,

- by largest volume of the three surface of homogeneity giving probabilities for the value of maximum expansion.
- by classes which have a surface of homogeneity with a volume less than ϵ (and the class of those which have no such surface) giving the probability of the universe becoming singular if one takes the $\epsilon \to 0$ limit. We shall study this in *Singularity in a Wheeler-DeWitt Quantum Universe.*
- by the class which remain close to a solution of the classical Einstein equation and the class which do not giving the probability for the universe to remain classical.

One must now find the class operators for these coarse-grained histories. If one denotes ranges of eigenvalues by Δa_k^α, one may identify these histories by grouping together the eigenvalues within these ranges. One thus finds for the class operators of coarse-grained histories,

$$C_{\bar{h}} = \sum_{a_{k_1} \in \Delta a_{\bar{k}_1}} \sum_{a_{k_2} \in \Delta a_{\bar{k}_2}} ... \sum_{a_{k_n} \in \Delta a_{\bar{k}_n}} P^{\alpha_1}_{a_{k_1}}(t_1) P^{\alpha_2}_{a_{k_2}}(t_2) ... P^{\alpha_n}_{a_{k_n}}(t_n) \tag{5.15}$$

The Decoherence Functional

The decoherence functional is defined as,

$$d(h, h') = tr[h^\dagger \rho h'] \tag{5.16}$$

where ρ is the initial density matrix for the state(s). In the simplified case whereby one does not have mixed initial states, this yields,

$$d(h, h') = \langle \psi_{h'} | \psi_h \rangle \tag{5.17}$$

The inner product here is the *"induced" inner product* (*see Appendix*). Normalizing this, one gets,

$$\sum_{h,h'} d(h,h') = \langle\psi|\psi\rangle \tag{5.18}$$

$$= 1 \tag{5.19}$$

When interference between all the members of an exclusive, exhaustive set of coarse-grained histories $\{h\}$ vanishes,

$$d(h,h') = 0 \qquad \forall h \neq h' \tag{5.20}$$

that set of histories is said to decohere, or to be consistent (there are different degrees of decoherence but for our purposes this will be enough). In these sets,

$$\langle\psi|\psi\rangle = \sum_{h} d(h,h) = 1 \tag{5.21}$$

It is evident that the probabilities for the individual histories in this case are given by,

$$p(h) = d(h,h) \tag{5.22}$$

This definition coincides with the familiar Luders-von Neumann formula from ordinary quantum theory.

So (5.20) tells us when it makes sense to talk about probabilities. Using (5.16), one may show that the probability sum rules are satisfied by this definition when the histories are coarse-grained,

$$p(h_1 + h_2) = d(h_1 + h_2, h_1 + h_2) \tag{5.23}$$

$$= tr\left[(h_1 + h_2)^\dagger \rho (h_1 + h_2)\right] \tag{5.24}$$

$$= tr\left[h_1^\dagger \rho h_1\right] + tr\left[h_1^\dagger \rho h_2\right] + tr\left[h_2^\dagger \rho h_1\right] + tr\left[h_2^\dagger \rho h_2\right] \tag{5.25}$$

Then in the case of decoherent histories the second and third terms vanish and one is left with,

$$p(h_1 + h_2) = p(h_1) + p(h_2) \tag{5.26}$$

Thus consistent sets are characterized by a diagonal decoherence functional,

$$d(h, h') = p(h)\delta_{hh'} \tag{5.27}$$

Time and the Probability Measure in the Decoherent Histories Approach

We wish to construct an approach to time in the decoherent histories approach to quantum mechanics is similar to the 'evolving constants of motion' discussed earlier; observables are constructed from operators commuting with the Hamiltonian operator. This is obviously a 'timeless' approach. To illustrate the approach, we shall follow [31] in constructing a well-defined probability for classical trajectories to cross a $(n-1)$-dimensional hypersurface in a n-dimensional configuration space. We shall begin in the classical theory, with the aim being to construct a reparametrization invariant quantity, i.e. one suitable for quantizing gravitational systems. We shall consider the case of a classical Hamiltonian of the form,

$$H = \frac{\mathbf{p}^2}{2M} + V(\mathbf{x}) \tag{5.28}$$

with configuration space, $\mathcal{C}$, coordinatized by $(\mathbf{x}, \mathbf{p}) = (x_i, p_i)$.

This is a suitable candidate to study as the Wheeler-DeWitt equation may usually be put into this form. We shall begin by considering a region, Δ of configuration space and constructing the corresponding probability for classical paths to pass through it. As it is our intention to pass to a quantum regime, we shall label the coordinates of what shall be the classical paths $(\mathbf{x}^{cl}(t), \mathbf{p}^{cl}(t))$ where t is some unobservable parameter that parameterizes curves in the configuration space, as before. We shall assume a classical phase space distribution function, $w(\mathbf{p}, \mathbf{x})$, such that,

$$\int d^n p d^n x w(\mathbf{p}, \mathbf{x}) = 1 \tag{5.29}$$

$$\{H, w\} = 0 \tag{5.30}$$

So w is an observable implying that $w(\mathbf{x}^{cl}(t), \mathbf{p}^{cl}(t)) = w(\mathbf{x}(0), \mathbf{p}(0))$ where $\mathbf{x}(0)$ and $\mathbf{p}(0)$ are the initial coordinates and conjugate momenta of the system respectively.

To construct the desired probability we shall need both quantities characterizing paths which are classical and those characterizing paths which pass through Δ. Consider,

$$\int dt f_\Delta(\mathbf{x}^{cl}(t)) = \int d^n x f_\Delta(\mathbf{x}) \int_{-\infty}^{\infty} dt \delta^{(n)}(\mathbf{x} - \mathbf{x}^{cl}(t)) \tag{5.31}$$

where,

$$f_\Delta(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \Delta \\ 0 & otherwise \end{cases} \tag{5.32}$$

This appears to have both of these desired characteristics; the delta function will ensure that only classical trajectories are included in any integral taken over this and another quantity dependent on the configuration space coordinates whilst the '*window function*', $f_\Delta(\mathbf{x})$, ensures that only paths that pass through Δ will be included. (5.31) may be considered, in a loose sense, the 'time' that the trajectory spends in Δ. From this, it is straightforward to write down the probability,

$$p_\Delta = \int d^n p_0 d^n x_0 w(\mathbf{p}_0, \mathbf{x}_0) \theta \left(\int_{-\infty}^{\infty} dt f_\Delta(\mathbf{x}^{cl}(t)) - \epsilon \right) \tag{5.33}$$

where the integral is over initial points in configuration space. The ϵ is an infinitesimal parameter which will be sent to zero but is needed to ensure the heaviside function is well-defined. We may also write this as,

$$p_\Delta = \frac{M}{\tau}\int d^n x_f d^n x_0 w(\mathbf{p}_0,\mathbf{x}_0)\theta\left(\int_{-\infty}^{\infty} dt f_\Delta(\mathbf{x}_0^f(t)-\epsilon\right) \tag{5.34}$$

where τ is the parameter time such that $x_f = x_0 + \frac{p_0}{M}\tau$ and we have defined $x_0^f = x_0 + \left(\frac{x_f - x_0}{\tau}\right) t$. This has the familiar form from standard quantum mechanics of an integral over 'final' and 'initial' points. Note that the prefactor dependent on τ may be scaled out and we are left with a reparameterization invariant quantity. Key to this invariance is the fact that one is summing over all classical paths passing through both x_0 and x_f rather than just those that pass through these points such that Δ lies between the points.

We are looking for the probability for classical paths to pass through an $(n-1)$-dimensional hypersurface rather than through a volume. We may adapt our results by considering such a hypersurface, Σ that is 'thickened' by an infinitesimal quantity, Δt, along the direction of classical flow. It is then found that the probability is given by (*see Appendix*),

$$p_\Sigma = \int dt \int d^n p_0 d^n x_0 w(\mathbf{p}_0,\mathbf{x}_0)\int_\Sigma d^{n-1}x\mathbf{n}\cdot\frac{d\mathbf{x}^{cl}(t)}{dt}\delta^n(\mathbf{x}-\mathbf{x}^{cl}(t)) \tag{5.35}$$

With a change of variables at each t, $\mathbf{p}' = \mathbf{p}^{cl}(t)$ and $\mathbf{x}' = \mathbf{x}^{cl}(t)$ one finds,

$$p_\Sigma = \frac{1}{M}\int dt \int_\Sigma d^n p' d^{n-1}x'\mathbf{n}\cdot\mathbf{p}' w(\mathbf{p}',\mathbf{x}') \tag{5.36}$$

The t integral just gives an overall factor and may be dropped.

Let us now consider the quantum règime in the semiclassical approximation. The WKB solutions to the Wheeler-DeWitt equation with momentum given by $\mathbf{p} = \nabla S$. Halliwell found [31] that the probability for crossing a surface, Σ in this règime is given by (5.36) with $w(\mathbf{p},\mathbf{x})$ replaced by the Wigner function, $W(\mathbf{p},\mathbf{x})$. The Wigner function for the WKB solutions is approximately given by,

$$W(\mathbf{p},\mathbf{x}) = |C(\mathbf{x}|^2\delta(\mathbf{p}-\nabla S) \tag{5.37}$$

Thus, one finds,

$$p_\Sigma = \int_\Sigma d^{n-1}x \mathbf{n} \cdot \nabla S |C(\mathbf{x})|^2 \tag{5.38}$$

for the probability measure. Significantly, it is found that this construction agrees heuristically with the probability measure (2.53) defined earlier.

Class Operators for Reparametrization Invariant Systems

As we have mentioned, for reparametrization invariant systems requiring complete observables (which correspond to operators) commute with H,

$$[H, A^{\alpha_i}] = 0 \tag{5.39}$$

ensuring that reparametrization invariance is preserved and also in keeping with the Dirac quantization procedure. These are the operators which we are interested in.

We described earlier how class operators may be constructed for non-relativistic systems described by the Schrödinger equation. The definition must clearly be more subtle due to the lack of an extrinsic time parameter. The use of Heisenberg projections is reliant on such a parameter.

We now ask ourselves how we may construct suitable class operators for this system. The symmetry of the theory is reparametrization invariance. We would like the class operators to also respect this symmetry, i.e. to commute with H. In the absence of an extrinsic time parameter, one may be tempted to replace this parameter in the definition (5.10) of the class operators for a non-relativistic system with an intrinsic time parameter, T.

Let us consider the class operators for histories to enter a region, Δ, in configuration space. We may write,

$$C_\Delta = 1 - \bar{C}_\Delta \tag{5.40}$$

where $\bar{C}_\Delta$ is the class operator corresponding to not entering the region, Δ. If P is the projector onto Δ, then $\bar{P}$ is the projector onto the rest of configuration space. In analogy with the previous definition, we write,

$$\bar{C}_\Delta = \prod_{T=-\infty}^{\infty} \bar{P}_\Delta(T) \tag{5.41}$$

where here T is the intrinsic 'time' parameter. To describe this more rigourously, one writes,

$$\bar{C}_\Delta(T_2, T_1) = \lim_{\epsilon\to 0} \bar{P}(T_2)\bar{P}(T_2-\epsilon)...\bar{P}(T_1+\epsilon)\bar{P}(T_1) \tag{5.42}$$

We wish to find the class operators corresponding to all 'time' and therefore find,

$$\bar{C}_\Delta = \lim_{T_2\to\infty, T_1\to-\infty} \bar{C}_\Delta(T_2, T_1) \tag{5.43}$$

This may be rewritten in terms of the *restricted propagator*, g_r, as,

$$\bar{C}_\Delta = \lim_{T_2\to\infty, T_1\to-\infty} e^{iHT} g_r(T_2, T_1) e^{-iHT_1} \tag{5.44}$$

where,

$$g_r(T_2, T_1) = Pexp(-i(T_2 - T_1)PHP)P \tag{5.45}$$

This definition of the class operator commutes with the Hamiltonian constraint but is found to suffer from the *Zeno effect*. This manifests itself by the wave function never leaving a particular region due to being continually projected onto that region.We thus must come up with a more subtle manner to overcome the lack of external time in order to define a class operator. Motivated by results from the arrival time problem in quantum mechanics [80], in which an analagous problem was observed, Halliwell proposed [32] making the redefinition,

$$g_r(T_2, T_1) \to \exp(-iH(T_2 - T_1) - V(T_2 - T_1)) \tag{5.46}$$

which is essentially the introduction of a complex potential, $-iV$. The potential is given by $V = V_0 P$ where V_0 is a constant. Thus the potential is only defined in the region, Δ. This gives,

$$\bar{C}_\Delta = \lim_{T_2 \to \infty, T_1 \to -\infty} e^{iHT_2} \exp(-iH(T_2 - T_1) - V(T_2 - T_1)) e^{-iHT_1} \tag{5.47}$$

So defined class operators commute with the Hamiltonian constraint,

$$\left[H, \bar{C}_\Delta\right] = 0 \tag{5.48}$$

and do not suffer from the Zeno effect. Note that, due to the unphysical nature of T, we may equally have reversed the order, i.e. $\bar{C}_\Delta \to \bar{C}_\Delta^\dagger$. To account for this, we may write the more general class operator,

$$\bar{C}'_\Delta = \frac{1}{2}(\bar{C}_\Delta + \bar{C}_\Delta^\dagger) \tag{5.49}$$

Thus we have constructed suitable class operators for entering a region, Δ, of configuration space in a reparametrization invariant system using a complex potential.

WKB Solutions to the Wheeler-DeWitt Equation

As you can see, the semiclassical approximation and WKB wave function are vital concepts in quantum cosmology. The decoherence within WKB components and also between WKB components is thus a necessity.

Halliwell has shown [32] that oscillatory WKB solutions to the Wheeler-DeWitt equation approximately decohere in the consistent histories approach. He also examined the more complicated case of superpositions of WKB solutions. We shall outline the simpler case of a single WKB solution and refer the reader to [32] for the case of the superposition of WKB solutions.

Recall that in the oscillatory regime, the single component WKB solutions to the Wheeler-DeWitt equation have the form,

$$\psi = Re^{iS} \tag{5.50}$$

with R and S approximately obeying,

$$(\nabla S)^2 + U = 0 \tag{5.51}$$

$$\nabla \cdot (|R|^2 \nabla S) = 0 \tag{5.52}$$

We saw in the last section that class operators for reparametrization invariant systems may be constructed using a complex potential. Quantum cosmology is an example of such a system and we exploit the results of the previous section here. Consider the case for a single region, Δ, of configuration space. We found the result (5.47) in the last section. This may be rewritten as,

$$C_\Delta = \int_{-\infty}^{\infty} dt V(t) - \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} ds V e^{-i(H-iV)(t-s)} V e^{-iHs} \tag{5.53}$$

Recall that V may be written as $V = V_0 P$ where P is a projector into Δ and V_0 is a constant. In the semiclassical approximation, the V in the argument of the exponential may be approximated by V_0. For the semiclassical approximation to hold, we restrict ourselves to small V_0 and assume that reflection by the potential at the boundary of Δ is negligible for such values of V_0. It is thus found [32],

$$C_\Delta = \int_{-\infty}^{\infty} dt P(t) \int_{-\infty}^{t} ds V_0 e^{-V_0(t-s)} \dot{P}(s) \tag{5.54}$$

where we have noted that we may write the potential, V, as $V = V_0 P$. One may perform the integration to find the action of this operator on an eigenstate of the Hamiltonian H, $|\Psi_\lambda\rangle$, with corresponding eigenvalue λ as,

$$C_\Delta |\Psi_\lambda\rangle = 2\pi V_0 \delta(H - \lambda) P G_V \dot{P} |\Psi_\lambda\rangle \tag{5.55}$$

where P is the projection operator and,

$$G_V = \int_0^\infty dt e^{-i(H-\lambda)t - V_0 t} \tag{5.56}$$

and has the form of a Feynman propagator. This propagator will suppress over time scales above $\frac{1}{V_0}$ and will have a small amount of reflection. One locally considers only incoming modes of the current operator $\dot{P}$ due to the factor PG_V. We denote these incoming modes as $(\dot{P})_{in}$. Upon restriction to these incoming modes, one may neglect the PG_V factors as they have no further purpose to serve. One thus find for the class operator corresponding to the probability for a given trajectory in superspace to enter Δ at least once,

$$C_\Delta |\psi_\lambda\rangle \approx 2\pi\delta(H-\lambda)(\dot{P})_{in}|\psi_\lambda\rangle \tag{5.57}$$

where we have ignored the ingoing modes propagating to a final point outside Δ as these are suppressed over a sufficiently long timescale. H is the Hamiltonian, λ the eigenvalue of $|\psi_\lambda\rangle$, P a projector onto Δ and $(\dot{P})_{in}$ the current operator for incoming momenta. It is found that,

$$(\dot{P})_{in} = -\hat{p}_n\theta(-\hat{p}_n)\delta_\Sigma(\hat{q}) - \delta_\Sigma(\hat{q})\hat{p}_n\theta(-\hat{p}_n) \tag{5.58}$$

with $\delta_\Sigma(\hat{q}) = \int_\Sigma d^{n-1}q|q\rangle\langle q|$. Using this, one finds,

$$\langle q|C_\Delta|\psi_\lambda\rangle = 2\pi i \int_{\Sigma_{in}} d^{n-1}q' \langle q|\delta(H-\lambda)|q'\rangle \overleftrightarrow{\partial_n}\psi_\lambda(q') \tag{5.59}$$

where Σ_{in} denotes sections of the boundary where the flux is ingoing. Semiclassically the evolution of the state $\psi_\lambda(q')$ will be concentrated along the classical trajectories with momenta given by $p = \nabla S(q')$. There will be negligible spreading out of this wave packet provided Δ is sufficiently large. (5.59) may thus be approximately rewritten as,

$$\langle q^a|C_\Delta|\psi_\lambda\rangle \approx \theta(\tau_\Delta - \epsilon)Re^{iS} \tag{5.60}$$

where $\epsilon > 0$ is a small parameter to regularize the θ-function at zero argument and,

$$\tau_\Delta(q) = \int_{-\infty}^{\infty} dt \; f_\Delta(q_{cl}(t)) \tag{5.61}$$

As before this provides a measure of the 'time' spent in Δ. This is still a solution to the Wheeler-DeWitt equation. It is obvious also that,

$$\langle q^a | \overline{C}_\Delta | \psi_\lambda \rangle \approx \theta(\epsilon - \tau_\Delta) R e^{iS} \tag{5.62}$$

This is the WKB state localized on the set of trajectories not entering Δ. Clearly,

$$\langle \psi_{\lambda'} | \overline{C}_\Delta C_\Delta | \psi_\lambda \rangle \approx 0 \tag{5.63}$$

giving approximate decoherence. Halliwell in the same paper examined the decoherence of superposition of WKB components. Approximate decoherence was found over sufficiently large regions. This result was necessary for the validity of our approach to quantum cosmology in this framework.

Singularity in a Wheeler-DeWitt Quantum Universe

We will consider a Wheeler-DeWitt consistent histories quantization of a flat, Friedmann-Robertson-Walker universe with a massless, minimally coupled scalar field and seek to analyze the probability for an initial or final singularity in the Wheeler-DeWitt quantum universe following that of Craig and Singh [11].

We shall identify the scalar field as an intrinsic time parameter and construct the class operators in direct analogy with the non-relativistic case outlined previously. We are thus ignoring the Zeno effect for such constructions. We hope to outline how predictions may be made in the decoherent histories approach.

Before proceeding further, we must first specify precisely what we mean by "singular". In this model, the statement that the universe has zero volume is equivalent to saying that the energy density and space-time curvature invariants diverge. We will thus take this to be our definition of a singularity.

We consider the simplified case of the volume at a given value of the scalar field. By volume we mean the dimensionless volume,

$$\nu \equiv \frac{V}{Cl_p^3} \tag{5.64}$$

where $V = a^3$, C is a dimensionless constant and l_p is the Planck length. We choose the value of the scalar field variable, ϕ, as our (non-monotonic) "time" variable. Initial conditions on the history are chosen such that $\bar{\nu} \gg 1$ and $\bar{\pi}_\phi \gg \hbar$ where π_ϕ is the confugate momentum to the scalar field and the bars denote evaluation at iniitial time, ϕ_0. These conditions are found to ensure that the yet to be specified states remain peaked about the classical solutions. Indeed, the application of the no-boundary or tunneling proposal to the consistent histories approach is an area open for research.

This gives for the class operators corresponding to the volume, ν, of the universe at $\phi = \phi^\star$,

$$C_{\Delta\nu|_{\phi^\star}} = U^\dagger(\phi^\star - \phi_0) P^\nu_{\Delta\nu} U(\phi^\star - \phi_0) \tag{5.65}$$

$$= P^\nu_{\Delta\nu}(\phi^\star) \tag{5.66}$$

where the projectors are given by,

$$P_{\Delta\nu} = \int_{\Delta\nu} \frac{d\nu}{\nu} |\nu\rangle\langle\nu| \tag{5.67}$$

As we mentioned in the previous section, class operators defined in this way are seen to suffer from the Zeno effect. We shall ignore these concerns presently and proceed with the analysis. In order to calculate the probability for an initial singularity or a bounce we need to think carefully about the precise question to ask. Ultimately, that which we choose is essentially: what is the probability that the universe has both a large volume in both the past and the future? Since the class operators are simply projectors, it is straightforward to show that they are orthogonal, i.e.

$$C_{\Delta\nu_i|_{\phi^\star}} \cdot C^\dagger_{\Delta\nu_2|_{\phi^\star}} = C_{\Delta\nu_i|_{\phi^\star}} C_{\Delta\nu_i|_{\phi^\star}} \cdot \delta_{ij} \tag{5.68}$$

From this one gets the relation,

$$\langle \psi_{\Delta\nu_i|_{\phi^\star}} | \psi_{\Delta\nu_j|_{\phi^\star}} \rangle = \langle \psi | C_{\Delta\nu_i|_{\phi^\star}} C^\dagger_{\Delta\nu_j|_{\phi^\star}} | \psi \rangle \tag{5.69}$$

$$= \langle \psi_{\Delta\nu_i|_{\phi^\star}} | \psi_{\Delta\nu_i|_{\phi^\star}} \rangle \cdot \delta_{ij} \tag{5.70}$$

for any $|\psi\rangle$, and we have satisfied the decoherence condition (5.20). Thus this family of histories decoheres and one obtains for the probabilities,

$$p_{\Delta\nu}(\phi^\star) = \langle \psi_{\Delta\nu|_{\phi^\star}} | \psi_{\Delta\nu|_{\phi^\star}} \rangle \tag{5.71}$$

$$= \langle \psi | C_{\Delta\nu|_{\phi^\star}} C^\dagger_{\Delta\nu|_{\phi^\star}} | \psi \rangle \tag{5.72}$$

$$= \langle \psi | U^\dagger(\phi^\star - \phi_0) P^\nu_{\Delta\nu} P^{\nu\dagger}_{\Delta\nu} U(\phi^\star - \phi_0) | \psi \rangle \tag{5.73}$$

$$= \langle \psi | U^\dagger(\phi^\star - \phi_0) P^\nu_{\Delta\nu} U(\phi^\star - \phi_0) | \psi \rangle \tag{5.74}$$

$$= \langle \psi(\phi^\star) | P^\nu_{\Delta\nu} | \psi(\phi^\star) \rangle \tag{5.75}$$

$$= \int_{\Delta\nu} \frac{d\nu}{\nu} |\psi(\nu, \phi^\star)|^2 \tag{5.76}$$

Recall that the gravitational Lagrangian density is given by,

$$\mathcal{L}_g = \sqrt{h}\mathcal{N}\left[K_{ij}K^{ij} - K^2 +^{(3)} R\right] \tag{5.77}$$

for this model with ${}^{(3)}R = \frac{6k}{a^2}$ which will vanish for flat models. This gives as before,

$$S_g = \int dt(-a\dot{a}^2) \tag{5.78}$$

selecting the $\mathcal{N} = 1$ gauge. We find the conjugate momentum corresponding to the scale factor, a, in the ususal manner to be $\pi_a = -\frac{3}{4\pi G} a\dot{a}$. We introduce the matter action,

$$S_{matter} = \int dt a^3 \frac{\dot{\phi}^2}{2} \tag{5.79}$$

giving conjugate momentum $\pi_\phi = a^3\phi$. We thus find for the total Hamiltonian density,

$$H = -\frac{3}{4\pi G} a\dot{a}^2 + a^3\dot{\phi}^2 - \frac{3}{8\pi G} a\dot{a}^2 - \frac{a^3\dot{\phi}^2}{2} \tag{5.80}$$

$$\Rightarrow -a^2\pi_a^2 + \frac{3}{4\pi G}\pi_\phi^2 \cong 0 \tag{5.81}$$

Introducing the volume, V, and its conjugate momentum, $\beta = -\frac{4\pi G}{3}\frac{\pi_a}{a^2}$, this becomes,

$$-\beta^2 V^2 + \frac{4\pi G}{3}\pi_\phi^2 \simeq 0 \tag{5.82}$$

We now introduce the aforementioned dimensionless parameter ν and find upon Dirac quantization,

$$\partial_\phi^2 \Psi(\nu, \phi) = 12\pi G \nu \partial_\nu (\nu \partial_\nu \Psi(\nu, \phi)) \equiv -\Theta(\nu)\Psi(\nu, \phi) \tag{5.83}$$

where the Hilbert space upon which the wave functions are defined is defined by the group averaging procedure of refined algebraic quantization as described in the *Refined Algebraic Quantization, Chapter 2*. Factor ordering has been chosen such that we found $\Theta(\nu)$, the Laplace-Beltrami operator of the DeWitt metric. We may expand solutions of this equation in terms of the eigenfunctions of this operator for this representation, $e_k(\nu)$. These eigenfunctions form an orthonormal basis for the kinematical Hilbert space. The first order expansion of this Wheeler-DeWitt equation may be written as,

$$\mp i\partial_\phi \Psi(\nu, \phi) = \sqrt{\Theta}\Psi(\nu, \psi) \tag{5.84}$$

The minus and plus signs correspond to positive and negative frequencies respectively. These positive and negative frequency sectors are disjoint [11] and hence may be treated separately. We shall concern ourselves with the positive frequency sector. This is of the form of the time-dependent Schrödinger equation, using this analogy, we may write for the positive frequency evolution operator,

$$U(\phi - \phi_0) = e^{i\sqrt{\Theta}(\phi - \phi_0)} \tag{5.85}$$

Thus we may write,

$$\Psi(\nu, \phi) = \Upsilon(\nu)U(\phi - \phi_0) \tag{5.86}$$

where $\psi(\nu) \equiv \Psi(\nu, \phi_0)$. k is the Fourier transform of the variable $\ln(\nu)$ and we have,

$$e_k(\nu) = \frac{1}{\sqrt{w\pi}e^{ik\ln(\nu)}} \tag{5.87}$$

We may also use this fact to rewrite (5.86) as,

$$\Psi(\nu, \phi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\psi(k)e^{ik\ln(\nu)}e^{i\omega(\phi-\phi_0)} \tag{5.88}$$

where ω^2 is the eigenvalue of Θ corresponding to the eigenfunctions $e_k(\nu)$. It can be seen that $\omega = \sqrt{12\pi G}|k|$. This gives,

$$\Psi(\nu, \phi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{0} dk\psi(k)e^{ik(\ln(\nu)-\sqrt{12\pi G}(\phi-\phi_0))} + \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} dk\psi(k)e^{ik(\ln(\nu)+\sqrt{12\pi G}(\phi-\phi_0))} \tag{5.89}$$

$$\equiv \Psi^R(\nu_-) + \Psi^L(\nu_+) \tag{5.90}$$

where $\nu_\pm = \ln(\nu) \pm \sqrt{12\pi G}(\phi - \phi_0)$. In the last step we have partitioned the states into purely expanding, $|\psi^R\rangle$, and purely contracting, $|\psi^L\rangle$, states. We now partition the volume, ν, of the universe into $\Delta\nu^\star = [0, \nu^\star]$ and its complement, $\bar{\Delta\nu}^\star = (0, \infty)$ for some fixed volume $\nu^\star$ at a fixed value of ϕ.

$$p^{L}_{\Delta\nu^{\star}}(\phi) = \int_{0}^{\nu^{\star}} \frac{d\nu}{\nu} |\psi^{L}(\nu_{+})|^{2} \tag{5.91}$$

$$= \kappa \int_{-\infty}^{\phi+\kappa^{-1}ln\nu^{\star}} d\nu_{+} |\psi^{L}(\nu_{+})|^{2} \tag{5.92}$$

and similarly,

$$p^{R}_{\Delta\nu^{\star}}(\phi) = -\kappa \int_{\infty}^{\phi-\kappa^{-1}ln\nu^{\star}} d\nu_{-} |\psi^{R}(\nu_{-})|^{2} \tag{5.93}$$

$$= \kappa \int_{\phi-\kappa^{-1}ln\nu^{\star}}^{\infty} d\nu_{-} |\psi^{R}(\nu_{-})|^{2} \tag{5.94}$$

It is clear from (5.92) and (5.94) that,

$$\underset{\phi\to-\infty}{lim}\, p^{L}_{\Delta\nu^{\star}}(\phi) = 0 \quad \underset{\phi\to+\infty}{lim}\, p^{L}_{\Delta\nu^{\star}}(\phi) = 1 \tag{5.95}$$

$$\underset{\phi\to-\infty}{lim}\, p^{R}_{\Delta\nu^{\star}}(\phi) = 1 \quad \underset{\phi\to+\infty}{lim}\, p^{R}_{\Delta\nu^{\star}}(\phi) = 0 \tag{5.96}$$

for any choice of $\nu^{\star}$. Whilst these results are not very enlightening; they confirm that a contracting universe will shrink to an arbitrarily small volume and an expanding universe will grow from an arbitrarily small volume we have see how probabilities may be determined in this formulation.

The more interesting case is that of a superposition of left-moving and right-moving states. For this case decoherence is no longer apparent yet Craig and Singh found that the system does decohere. They proceeded to find that the probability to a avoid the cosmological singularity approaches zero for this approximately classical flat Friedmann model.

Conclusion

We stated initially that quantum cosmology pertained to provide a guide for candidates providing a fundamental description of the universe. Although many open problems exist in the formulation of the subject as we have mentioned, we hope that we have shown that potential for quantum cosmology to provide such a guide. In particular, that, under certain conditions, a reliable probability measure may be constructed from which observable predictions may be made. We provided a summary in *Chapter 4: The Predictions of Quantum Cosmology* of how predictions may be formulated and some specific example of such results. The principle part of the thesis, however, was concerned with the foundations on which such constructions were laid.

We began in *Chapter 1: Hamiltonian Formulation of General Relativity*, motivated by the incompatibility of space-time with the quantum principle, by decomposing the space-time manifold of general relativity into a set of spacelike hypersurfaces. The system was then found to be characterized by two secondary constraints: the momentum and Hamiltonian constraints. Indeed, it was shown that these constraints may be identified with the generators of surface deformations on three dimensional hypersurfaces, with the classical Poisson bracket algebra defined by them found to construct general relativity under that assumption that the intrinsic 3-metric of the spatial hypersurface and its conjugate momentum are the sole canonical gravitational variables on Σ.

The quantization procedures of the subject were introduced in *Chapter 2: Quantization.* The constraints were promoted by Dirac quantization to operator equations, acting on a wave functional, $\Psi[h_{ij}(\mathbf{x}, \Phi(\mathbf{x}), \Sigma]$, defined using the path integral technique. The path integral formulation here is not well-defined and suffers from the unboundedness of the gravitational action. The quantized

Hamiltonian constraint, $\hat{H}\Psi = 0$, otherwise known as the *Wheeler-DeWitt equation*, is the central equation of quantum cosmology governing the dynamics of the system. This equation is in fact characteristic of any reparametrization invariant system. It is a second order functional differential equation and, just as in the Klein-Gordon equation, there is no prescription for factor ordering when quantizing the classical constraint. There are a number of factor ordering which are prevalent in the literature and this ambiguity is a restriction on the validity of the theory.

The wave function is not defined on space-time, but rather on *superspace*. This is an infinte dimensional configuration space of Euclidean 3-metrics and scalar matter fields. This infinte-dimensionality makes the system difficult to work with and generally it is a finite-dimensional subspace, *minisuperspace*, of this that is considered. This is the space of approximately spatially homogeneous and isotropic 3-metrics and scalar fields. We thus pass from a quantum field theory to quantum mechanics. Indeed, reduction to this space reduces the Wheeler-DeWitt equation from a set of equations, one for each point, $\mathbf{x}$ on Σ, to a single equation. However, despite the physical motivation, the restriction is in violation of the uncertainty principle.

Due to the issues outlined, we often work in the *semiclassical approximation*, on the border between the classical and quantum règimes. In the semiclassical approximation, the wave function is approximated by the *WKB wave function*. Here, the functional integration measure becomes a sum over Euclideanized 4-geometries which are *saddle-points* of the wave function. These 4-geometries are also known as *instantons*. We examined the properties of these WKB solutions for a typical Wheeler-DeWitt equation, imposing classicality at late times. It was found that such solutions selected a subset of solutions to the field equations.

The operator Hamiltonian constraint is a property of all reparametrization invariant systems. It is equivalent to the lack of an external time parameter in the theory. The concept of time in standard quantum mechanics is based on the Schrödinger equation defined with such an external time parameter. So the question arises as to how to formulate a notion of evolution in a quantum theory of a reparametrization invariant system. This is the focus of *The Problem of Time, Chapter 2*. We outlined the three possible approaches to the problem. We focused in particular on the '*timeless*' approach which is that typically used in quantum cosmology. There are fundamental issues with all three approaches, yet this seems to be the most least effected approach. It essentially takes the view that time is not fundamental. Any Schrödinger equations in the theory will be approximate and with respect to a *clock variable*. These are variables providing an approximate measure of time.

The major drawback of this approach was found to be the restriction to *conditional probabilities* due to the non-compact nature of time. Although absolute probabilities are more favourable, the restriction to conditional probabilities may be motivated physically. Firstly, the universe as a whole is never observed, only a section of it. Secondly, the restriction to these probabilities may be seen as the indication of the validity of the *anthropic principle*. Conditional probabilities ask questions such as: what is the probability that A occurs given that B occurs? We may thus view B as an anthropic condition such as the dimensionality of space that must hold for our existence.

A specific case of such an approach is the *evolving constants of motion* approach. The concept of motion as fundamentally a correlation between variables is the underlying philosophy. With this doctrine, it can be shown that *observables* may be constructed describing the evolution of a variable in terms of the clock variable whilst remaining a constant of motion. The single observables constructed in this way have been shown, with additional physical motivation, to be measurable. We have shown how observables may be constructed preserving the reparametrization invariance of the theory. It was also found that the *thermal time hypothesis* may provide a recovery of the local notion of time which we observe. It has been shown for a radiation filled covariant model that this hypothesis is seen to select the Friedmann time as the local time parameter.

The *refined algebraic quantization* approach to constructing a Hilbert space populated by the wave functions was shown. This approach can be used in such a timeless approach as the evolving constants of motion approach. Marolf has shown that under physically motivated restrictions, this construction is typically unique. A stronger statement would lend significant weight to this approach and is perhaps an area of future research.

In order for a specific solution to the field equations to be picked out, one must impose boundary conditions on the wave function. There is no natural choice for the boundary conditions corresponding to the initial hypersurface of the universe. Various proposals have been made prescribing these boundary conditions. The principle two are the no-boundary and tunneling proposals. The no-boundary proposal states that the only boundary of the universe is that corresponding to the present hypersurface. The tunneling proposal describes the birth of the universe as tunneling out of 'nothing'.

It is found that, in the semiclassical approximation, these boundary conditions manifest themselves as initial conditions on the *histories* of the canonical variables.

We examined the predictions of these boundary conditions in *Chapter 4: Predictions of Quantum Cosmology.* We firstly examined the probabilities given by the corresponding wave functions for an epoch of inflation. It was found that both proposal predict a period of inflation in the early universe. Inflation was originally proposed as a solution to various cosmological problems such as the horizon and flatness problems. A minimum 'amount' of inflation is required to produce the universe which we observe. The measure of the amount of inflation is given by the number of *efolds*. It is found that around sixty five efolds of inflation are necessary for *sufficient inflation*. We next asked that question of both wave functions as to whether they predict sufficient inflation. Whilst they are both initially seen to predict sufficient inflation, it has been argued that the upper cut-off for the initial value of the scalar field in these calculations should be finite, whereas it was taken to infinity in there calculations. Vilenkin argued that the upper cut-off should not be above the Planck scale as the semiclassical approximation will break down. It was found that upon imposition of this finite cut-off, the tunneling wave function was found to still predict sufficient inflation whereas the no-boundary wave function was seen to favour a small amount of inflation.

The advocates of the no-boundary proposal countered that, while this result is accurate on a history-by-history basis, it is not the full probability measure. In order to calculate this, they argued, the results must be *volume weighted* by the number of *Hubble volumes* on our surface of homogeneity. We outline this volume weighting in *Volume Weighting, Chapter 4.* The volume weighted probabilities of the no-boundary wave function are seen to predict sufficient inflation.

A no-boundary analysis of the probability for an initial singularity or a bounce was followed. It was found that whilst on a history-by-history basis an initial singularity was predicted. However, for the fully conditioned wave function, a bounce at a finite radius in the past was predicted. This prediction for sufficient inflation by both boundary conditions is a notable success of the proposals.

It was found that the quantum mechanical perturbations about the semiclassical homogeneous and isotropic solutions to the Wheeler-DeWitt equation for a closed Friedmann model may be expressed in terms of spherical harmonics with the perturbations satisfying an approximate Schrödinger equation. Indeed it was found that the no-boundary solutions pick out the *Bunch-Davies* vacuum as the vacuum state of the universe. This is often assumed in classical cosmological models to be the vacuum state of the universe and thus the objective prediction by the no-boundary wave function is encouraging. Indeed, it is hoped that the fluctuation spectrum predicted by quantum cosmology for the CMB may be tested by MAP and PLANCK data.

The analysis of these perturbations also allowed a vacuum state to be selected for an approximately de Sitter background state. The vacuum selected by both the no-boundary and the tunneling wave functions was given by the Bunch-Davies vacuum state, which has been long posited as a vacuum state in cosmology.

We also discussed the possibility for topology change in quantum cosmology. We were considering the case of globally hyperbolic manifolds for which topology change is prohibited classically. The quantum règime opens up the possibility for topology change. Whilst the foliation of the space-time fixes the topology, the wave function itself in the path integral formulation allows for such topology change. We examined the case of Friedmann models with non-trivial topology, i.e. $k = k(t)$. Motivation for such a study was provided by Linde's analysis for the probabilities of non-trivial topologies in such models. He found that, for certain cases, the non-trivial likelihood for non-trivial topologies was enhanced whilst the probabilities for trivial topologies was exponentially suppressed. The analysis carried out was unphysical in the sense that the boundary conditions were not physically motivated. This is an area of potential future research. Here, we rather wished to examine the qualitative behaviour of such models. It was found that using a Green function, the probability in one case for topology change approached unity over large enough intrinsic time. There was also, interestingly, in all cases an *arrow of topology change*, i.e. there was a preferred 'direction' for topology change from positive to negative spatial curvature.

This is a very unexplored area of research in quantum cosmology and for good reason, in many senses despite the motivation given. One would expect topology change to feature prominently only in a purely quantum règime rather than the quasiclassical for which quantum cosmology is reliable. However, there is a seeming qualitative behaviour exhibiting an arrow of topology change for the unphysical models studied. The application of 'physical' boundary conditions such as the no-boundary and tunneling wave function to topology change may also exhibit such

We also introduced a recent boundary proposal by Page, the '*symmetric bounce proposal*'. This proposal was motivated by a criticism of the no-boundary proposal. The criticism is that the no-boundary wave function due to.... will be seen to produce a nearly empty de Sitter universe. In this universe the *normal observer*, such as you or I, is found to be highly atypical. The typical observer is the *Boltzmann brain*, an observer born out of a quantum fluctuation. The observations of such observers would be in contradiction to those which we make, calling into question the no-boundary proposal.

The final chapter, *Chapter 5: A Consistent Histories Approach to Quantum Cosmology*, is concerned with the quantum mechanical foundations and interpretation of quantum cosmology. It was found that if the universe is a closed quantum system, there can be no external observers. This precludes the use of the Copenhagen interpretation. We thus turn to generalized quantum mechanics, in which observers are treated quantum mechanically. We focus, particular, on the consistent histories approach. Here the decoherence mechanism replaces that of the wave collapse.

We outlined the formulation of such a framework; constructing a well-defined notion of *fine-grained histories*, *coarse-grained histories* and the *decoherence functional*. Using these three cornerstones, we built class operators, first for a non-relativistic system then for a reparametrization invariant system. The formulation for the latter was more subtle due to the lack of an external time parameter. The initial attempt, carried out in analogy with the non-relativistic case, was found to suffer from the *Zeno effect*. Suitable class operators were constructed using a complex potential, motivated by recent developments regarding the arrival time problem in quantum mechanics.

We constructed a reparametrization invariant probabiltity measure which was found to coincide with the Klein-Gordon construction of *Probability Measure, Chapter 2*. Motivated by recent developments in the arrival time problem of quantum mechanics, a complex potential was used to define class operators commuting with the Hamiltonian constraint and thus preserving reparametrization invariance. Using these class operators, the proof by Halliwell of approximate decoherence between WKB components was followed. This decoherence is required for the theory to have any validity and therefore is a significant result.

An analysis of the probabilty for an initial singularity or bounce in a flat Friedmann model was carried out in this framework by Craig and Singh. Despite concerns about the class operators regarding the Zeno effect, we follow the analysis. It was found that an inital singularity was predicted. Boundary conditions here were chosen to ensure the states remained peaked about the trajectories of classical solutions. Application of the no-boundary and tunneling proposals to the consistent histories approach remains a relatively untouched area.

Overall, we have shown that whilst the construction of traditional quantum cosmology, i.e. the first four chapters, suffers from some fundamental issues in its definition, combined with the no-boundary or tunneling proposals, it is seen have many successes such as the prediction for sufficient inflation and for the Bunch-Davies vacuum state in its predictions. Perhaps the most relevant test, will be provided by the observations of the spectrum of anisotropies in the universe. There is potential many of the aforementioned problems to be solved, for example, it is only recently that functional integration measure of standard quantum field theory has been properly defined and one may hope that the measure of the gravitational path integral may be found to be well-defined. We may thus see that the predictions of quantum cosmology that have not are not yet testable must be lent at least some weight. They may thus be used as a guide for quantum theories of gravity.

We have seen in particular the evolving constants of motion approach to time. Quantum cosmology provides motivation and a testable framework for implementing approaches to problems such as that of time.

With regards to the two principle boundary proposals, both are seen to have their advantages and disadvantages. In my opinion, while the no-boundary proposal is more geometrically pleasing, the tunneling wave function has the most desirable qualities, allowing for greater freedom by nucleation of universes in a multiverse, or, as we have seen, perhaps through topology change. This is purely a matter of taste however, and hopefully conclusive results will be reached through observations with regards to both of these proposals.

The consistent histories approach of the final chapter is more recent in its application to quantum cosmology. This approach is indeed seems suited to reparametrization invariant systems. The Zeno effect problems appear to be a set back to this approach as the definition of suitable class operators is not as obvious as for non-relativistic systems. We have shown that this may be solved using a complex potential when looking at the probability for crossing a region of configuration space. In this approach boundary conditions are still required to be specified by a separate proposal. The application of the no-boundary and tunneling proposals within the consistent histories approach in future research is thus highly motivated.

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Appendix

Global Hyperbolicity

The definition of global hyperbolicity as in [51],

> *"A set $\mathcal{N}$ is said to be globally hyperbolic if the strong causality assumption holds on $\mathcal{N}$ and if for any two points $p, q \in \mathcal{N}$, $J^+(p) \cap J^-(q)$ does not contain any points on the edge of spacetime, i.e. at infinity or at a singularity"*

where $J^+(p)$ and $J^-(p)$ denote the causal future and past of p respectively. The strong causality condition is given by,

> *"The strong causality condition is said to hold at p if every neighbourhood of p contains a neighbourhood of p which no non-spacelike curve intersects more than once."*

(1.9)

Assuming that the normal vector field $n_\alpha = (-\mathcal{N}, 0, 0, 0)$ is everywhere geodesic, one has,

$$K_{ij} = -\nabla_i n_j \tag{A-1}$$

$$= ^{(4)}\Gamma^\mu{}_{ij} n_\mu \tag{A-2}$$

where ${}^{(4)}\Gamma^{\mu}{}_{\nu\lambda}$ is the Christoffel connection of the 4-metric, $g_{\mu\nu}$ and we have used the fact that we are considering only spatially homogeneous space-times, i.e. $\mathcal{N} = \mathcal{N}(t)$. Writing the Christoffel connections explicitly, one finds,

$$K_{ij} = \frac{1}{2} g^{0\sigma} (g_{\sigma i},_j + g_{j\sigma},_i - g_{ij},_\sigma) n_0 \tag{A-3}$$

In terms of the lapse, shift and intrinsic metric the 4-metric and its inverse are given by,

$$(g_{\mu\nu}) = \begin{pmatrix} -\mathcal{N}^2 + \mathcal{N}^k \mathcal{N}_k & \mathcal{N}_j \\ \mathcal{N}_i & h_{ij} \end{pmatrix} \tag{A-4}$$

$$(g^{\mu\nu}) = \begin{pmatrix} -\frac{1}{\mathcal{N}^2} & \frac{\mathcal{N}^j}{\mathcal{N}^2} \\ \frac{\mathcal{N}^i}{\mathcal{N}^2} & h^{ij} - \frac{\mathcal{N}^i \mathcal{N}^j}{\mathcal{N}^2} \end{pmatrix} \tag{A-5}$$

Inserting the relevant components in (A-3) gives,

$$K_{ij} = \frac{1}{2}\left(\frac{1}{\mathcal{N}^2}\right)(\partial_j \mathcal{N}_i + \partial_i \mathcal{N}_j - \partial_0 h_{ij}(-\mathcal{N}) + \frac{1}{2}\frac{\mathcal{N}^k}{\mathcal{N}^2}(\partial_j h_{ki} + \partial_i h_{jk} - \partial_k h_{ij})\mathcal{N} \tag{A-6}$$

$$= \frac{1}{2\mathcal{N}}(\partial_i \mathcal{N}_j + \partial_i \mathcal{N}_j - \partial_0 h_{ij}) + \frac{1}{\mathcal{N}}\mathcal{N}^k \Gamma_{kij} \tag{A-7}$$

$$= \frac{1}{2\mathcal{N}}(D_i \mathcal{N}_j + D_j \mathcal{N}_i - \dot{h}_{ij}) \tag{A-8}$$

where we have used the symmetry (under interchange of the second and third indices) of the Christoffel connection in the last step.

(1.13)

Consider the Gauss-Codazzi equations,

$$^{(3)}R^{\mu}{}_{\nu\lambda\rho} = h^{\mu}{}_{\bar{\mu}} h_{\nu}{}^{\bar{\nu}} h_{\lambda}{}^{\bar{\lambda}} h_{\rho}{}^{\bar{\rho}} R^{\bar{\mu}}{}_{\bar{\nu}\bar{\lambda}\bar{\rho}} - K^{\mu}{}_{\lambda} K_{\nu\rho} + K_{\nu\lambda} K^{\mu}{}_{\rho} \tag{A-9}$$

$$D_\mu K_{\nu\lambda} - D_\nu K_{\mu\lambda} = h_\mu{}^{\bar{\mu}} h_\nu{}^{\bar{\nu}} h_\lambda{}^{\bar{\lambda}} R_{\bar{\mu}\bar{\nu}\bar{\lambda}\rho} n^\rho \tag{A-10}$$

Contracting the indices in the first equation, we may obtain an expression for the intrinsic 3-curvature scalar, ${}^{(3)}R$,

$$^{(3)}R_{\nu\rho} = h^\mu{}_{\bar{\mu}} h_\nu{}^{\bar{\nu}} h_\mu{}^{\bar{\lambda}} h_\rho{}^{\bar{\rho}} R^{\bar{\mu}}\bar{\nu}\bar{\lambda}\bar{\rho} - K^\mu{}_\mu K_{\nu\rho} + K_{\nu\mu} K^\mu{}_\rho \tag{A-11}$$

$$\Rightarrow^{(3)} R = h^\mu{}_{\bar{\mu}} h^{\nu\bar{\nu}} h_\mu{}^{\bar{\lambda}} h_\nu{}^{\bar{\rho}} R^{\bar{\mu}}{}_{\bar{\nu}\bar{\lambda}\bar{\rho}} - K^\mu{}_\mu K^\nu{}_\nu + K_{\mu\nu} K^{\mu\nu} \tag{A-12}$$

One has $h_{\mu\nu} = g_{\mu\nu} + n_\mu n_\nu$ and using the property that $h_{\mu\nu}$ acts as a projector on Σ_t, i.e. $h_{\mu\nu} n^\nu = 0$, one finds,

$$^{(3)}R + K_\mu{}^\mu K_\nu{}^\nu - K_{\mu\nu} K^{\mu\nu} = R + 2R_{\mu\nu} n^\mu n^\nu \tag{A-13}$$

Consider the Einstein tensor, specifically its 'time-time component', which is projected out using the normal vector field, n^μ,

$$G_{\mu\nu} n^\mu n^\nu = (R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R) n^\mu n^\nu \tag{A-14}$$

$$= R_{\mu\nu} + \frac{1}{2} R \tag{A-15}$$

Substituting this into (A-13), one finds,

$$^{(3)}R + K_\mu{}^\mu K_\nu{}^\nu - K_{\mu\nu} K^{\mu\nu} = 2G_{\mu\nu} n^\mu n^\nu \tag{A-16}$$

In the case of the vacuum Einstein equations this gives,

$$K^2 - K_{ab} K^{ab} +^{(3)} R = 0 \tag{A-17}$$

where $K \equiv K^a{}_a$. These are the 'time-time' components of the Einstein equations. We now have an expression for the scalar curvature,

$$R =^{(3)} R + K^2 - K_{ab}K^{ab} - 2R_{\mu\nu}n^\mu n^\nu \tag{A-18}$$

Recall the definition of the curvature tensor in terms of covariant derivatives (for a commuting algebra),

$$R^\rho{}_{\mu\rho\nu} = \nabla_\rho \nabla_\nu n^\rho - \nabla_\nu \nabla_\rho n^\rho \tag{A-19}$$

Using this definition, one may write the last term in (A-18) as,

$$-2R_{\mu\nu}n^\mu n^\nu = 2(\nabla_\rho n^\nu)(\nabla_\nu n^\rho) - 2\nabla_\rho(n^\nu \nabla_\nu n^\rho) - 2(\nabla_\nu n^\nu)(\nabla_\rho n^\rho) + 2\nabla_\nu(n^\nu \nabla_\rho n^\rho) \tag{A-20}$$

where the second and fourth terms are total divergences. The first term gives $-2(n^\nu \nabla_\nu n^\rho)n_\rho = 0$ (using the symmetry properties) on the boundary while the second gives $2\nabla_\mu n^\mu = -2K$. The latter was found using an alternative form for the extrinsic curvature,

$$K_{\mu\nu} = h_\mu{}^\rho \nabla_\rho n_\nu \tag{A-21}$$

The first and third terms can be written as $2K_{ab}K^{ab}$ and $-2K^2$ respectively. For the volume element one finds [58], $\sqrt{-g} = \mathcal{N}\sqrt{h}$. We will assume that Σ is compact here. Thus, we have for the Einstein-Hilbert action,

$$S_{EH} = \frac{1}{4\kappa^2}\int_{\mathcal{M}} d^4x \mathcal{N}\sqrt{h}\left({}^{(3)}R + K^2 - K_{ab}K^{ab} + 2K_{ab}K^{ab} - 2K^2\right) + \frac{1}{4\kappa^2}\int_{\partial\mathcal{M}} d^3x \sqrt{h}\,(-2\mathcal{N}K + 2K) \tag{A-22}$$

So the surface terms cancel and one has (A-23),

$$S \equiv \int dt L = \frac{1}{4\kappa^2} \int dt d^3x \mathcal{N}\sqrt{h}(K_{ij}K^{ij} - K^2 +^{(3)} R - 2\Lambda) + S_{matter} \tag{A-23}$$

(1.16) and (1.17)

We have the Lagrangian,

$$L = \frac{1}{4\kappa^2}\mathcal{N}\sqrt{h}\left(K_{ij}K^{ij} - K^2 +^{(3)} R - 2\Lambda\right) + L_{matter}(g_{\mu\nu}, \Phi) \tag{A-24}$$

For the conjugate momenta of the intrinsic metric one therefore finds,

$$\frac{\partial L}{\partial \dot{h}_{kl}} = \frac{1}{4\kappa^2}\mathcal{N}\sqrt{h}\left(2K^{ij}\frac{\partial K_{ij}}{\partial \dot{h}_{kl}} - 2K\frac{\partial K}{\partial \dot{h}_{kl}}\right) \tag{A-25}$$

Writing the trace of the extrinsic curvature as $K^i{}_i = h^{ij}K_{ij}$ and noting that,

$$\frac{\partial K_{ij}}{\partial \dot{h}_{kl}} = -\frac{\delta_{ik}\delta jl}{2\mathcal{N}} \tag{A-26}$$

one finds,

$$\frac{\partial L}{\partial \dot{h}_{kl}} = \frac{1}{4\kappa^2}\mathcal{N}\sqrt{h}\left(-\frac{2K^{kl}}{2\mathcal{N}} + 2Kh^{kl}\frac{1}{2\mathcal{N}}\right) \tag{A-27}$$

$$= -\frac{1}{4\kappa^2}\sqrt{h}(K^{kl} - h^{kl}K) \tag{A-28}$$

For the conjugate momenta of the canonical matter variable, note that all the $\dot{\Phi}$ dependence is in L_{matter}. L_{matter} is given by,

$$L_{matter} = \sqrt{-g}\left(-\frac{1}{2}g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi - \mathcal{V}(\Phi)\right) \tag{A-29}$$

$$= \mathcal{N}\sqrt{h}\left(-\frac{1}{2}\left[g^{00}\dot{\Phi}^2 + g^{0i}\dot{\Phi}\partial_i\Phi + g^{j0}\partial_j\Phi\dot{\Phi} + ...\right] - \mathcal{V}(\Phi)\right) \tag{A-30}$$

where we have omitted terms without $\dot{\Phi}$-dependence. Using (A-5), one can then write,

$$\frac{\partial L_{matter}}{\partial\dot{\Phi}} = \frac{\partial}{\partial\dot{\Phi}}\left[-\frac{\mathcal{N}\sqrt{h}}{2}\left(\frac{-1}{\mathcal{N}^2}\dot{\Phi}^2 + \frac{2\mathcal{N}^i}{\mathcal{N}^2}\dot{\Phi}\partial_i\Phi + ...\right) - \mathcal{V}(\Phi)\right] \tag{A-31}$$

$$= \frac{\sqrt{h}}{\mathcal{N}}(\dot{\Phi} - \mathcal{N}^i\Phi_{,i}) \tag{A-32}$$

(1.19)

Recall (1.16) (where the indices have been lowered using the intrinsic 3-metric),

$$\pi_{ij} = -\frac{\sqrt{h}}{4\kappa^2}(K_{ij} - h_{ij}K) \tag{A-33}$$

From this one may find the trace of π^{ij},

$$Tr[\pi^{ij}] = -\frac{\sqrt{h}}{4\kappa^2}(K - KTr[h]) \tag{A-34}$$

In Gaussian normal coordinates, this gives,

$$K = \frac{2\kappa^2}{\sqrt{h}}Tr[\pi^{ij}] \tag{A-35}$$

Substituting this into (A-33), one finds,

$$K_{ij} = -\frac{4\kappa^2}{\sqrt{h}}\left(\pi_{ij} - \frac{1}{2}h_{ij}Tr[\pi^{mn}]\right) \tag{A-36}$$

Substituting this into (1.9), gives,

$$\dot{h}_{ij} = -\frac{8\kappa^2\mathcal{N}}{\sqrt{h}}\left(\pi_{ij} - \frac{1}{2}h_{ij}Tr[\pi^{mn}]\right) + D_i\mathcal{N}_j + D_j\mathcal{N}_i \tag{A-37}$$

The gravitational Hamiltonian density is then given by,

$$H = \mathcal{N}\mathbb{H} = \pi^{ij}\dot{h}_{ij} - \mathcal{L} \tag{A-38}$$

where $\mathcal{L}$ is the gravitational Lagrangian density. Substituting in our results,

$$\mathbb{H} = \pi^{ij}\left\{-\frac{8\kappa^2}{\sqrt{h}}\left(\pi_{ij} - \frac{1}{2}h_{ij}Tr[\pi^{mn}]\right)\right\} + D_i\mathcal{N}_j + D_j\mathcal{N}_i - \mathcal{L} \tag{A-39}$$

Recall that the gravitational Lagrangian density is given by,

$$\mathcal{L} = \frac{\sqrt{h}}{4\kappa^2}(K_{ij}K^{ij} - K^2 +^{(3)} R - 2\Lambda) \tag{A-40}$$

In terms of π^{ij} we have,

$$K^{ij}K_{ij} - K^2 = \frac{16\kappa^2\mathcal{N}}{h}\left\{\pi^{ij}\pi_{ij} + (Tr[\pi^{mn}])^2\right\} \tag{A-41}$$

Using the definition of the DeWitt metric, (1.22), one can see,

$$\mathbb{H} = 4\kappa^2\mathcal{G}_{ijkl}\pi^{ij}\pi^{kl} - \frac{\sqrt{h}}{4\kappa^2}(^{(3)}R - 2\Lambda) + \pi^{ij}D_i\mathcal{N}_j + \pi^{ij}D_j\mathcal{N}_i \tag{A-42}$$

π^{ij} is symmetric so the last two terms are the same. Integrating by parts and ignoring the surface term (i.e. assuming Σ is compact), one finds,

$$\mathbb{H} = 4\kappa^2\mathcal{G}_{ijkl}\pi^{ij}\pi^{kl} - \frac{\sqrt{h}}{4\kappa^2}(^{(3)}R - 2\Lambda) - 2\mathcal{N}_iD_j\pi^{ij} \tag{A-43}$$

Writing the Hamiltonian density as,

$$H = \mathcal{N}\mathcal{H} + \mathcal{N}_i\mathcal{H}^i \tag{A-44}$$

one finds,

$$\mathcal{H}^i = -2D_j\pi^{ij} \tag{A-45}$$

$$\mathcal{H} = 4\kappa^2\mathcal{G}_{ijkl}\pi^{ij}\pi^{kl} - \frac{\sqrt{h}}{4\kappa^2}({}^{(3)}R - 2\Lambda) \tag{A-46}$$

as required.

(2.11)

The inverse DeWitt metric is given by,

$$\mathcal{G}^{ijkl} = \frac{\sqrt{h}}{2}(h^{ik}h^{jl} + h^{il}h^{jk} - 2h^{ij}h^{kl}) \tag{A-47}$$

Using the expression (1.9) for the extrinsic curvature in Gaussian normal coordinates, one finds,

$$\begin{aligned}
\mathcal{G}^{ijkl}\dot{h}_{ij}\dot{h}_{kl} &= \frac{\sqrt{h}}{2}(h^{ik}h^{jl} + h^{il}h^{jk} - 2h^{ij}h^{kl})4\mathcal{N}^2K_{ij}K_{kl} && \text{(A-48)}\\
&= 2\sqrt{h}\mathcal{N}^2(K_{ij}K^{ij} + K_{ij}K^{ij} - 2K^2) && \text{(A-49)}\\
&= 4\sqrt{h}\mathcal{N}^2(K_{ij}K^{ij} - K^2) && \text{(A-50)}
\end{aligned}$$

(2.15)

So we have the action,

$$S=\int dt\left[\frac{1}{2\mathcal{N}}\mathcal{G}_{AB}\dot{q}^A\dot{q}^B-\mathcal{N}\mathcal{U}(q)\right] \tag{A-51}$$

We then find for the Euler-Lagrange equations,

$$\frac{\partial L}{\partial q^C}=\frac{1}{2\mathcal{N}}\mathcal{G}_{AB},_C\,\dot{q}^A\dot{q}^B-\mathcal{N}\frac{\partial\mathcal{U}}{\partial q^C} \tag{A-52}$$

$$\frac{\partial L}{\partial\dot{q}^C}=\frac{1}{\mathcal{N}}\mathcal{G}_{AC}\dot{q}^A\Rightarrow\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{q}^C}\right)=\frac{d}{dt}\left(\frac{\dot{q}_C}{\mathcal{N}}\right) \tag{A-53}$$

Raising the indices with the minisuperspace metric and dividing by $\mathcal{N}$, we find (changing some dummy indices),

$$\frac{1}{\mathcal{N}}\frac{d}{dt}\left(\frac{\dot{q}^A}{\mathcal{N}}\right)+\frac{1}{\mathcal{N}^2}\left[-\frac{1}{2}\mathcal{G}^{AB}\mathcal{G}_{EF},_B\right]\dot{q}^E\dot{q}^F=-\mathcal{G}^{AB}\frac{\partial\mathcal{U}}{\partial q^B} \tag{A-54}$$

Noting that the Christoffel connection of the minisuperspace metric is given by,

$$\Gamma^A{}_{BC}=\frac{1}{2}\mathcal{G}^{AD}(\mathcal{G}_{DB},_C-\mathcal{G}_{BC},_D+\mathcal{G}_{CD},_B) \tag{A-55}$$

we may write,

$$\frac{1}{\mathcal{N}}\frac{d}{dt}(\frac{\dot{q}^A}{\mathcal{N}})+\frac{1}{\mathcal{N}^2}\Gamma^A{}_{BC}\dot{q}^B\dot{q}^C=-\mathcal{G}^{AB}\frac{\partial\mathcal{U}}{\partial q^B} \tag{A-56}$$

Time Before Quantization

We have an action of the form,

$$S=\int dt\int_\Sigma d^3x\left(\mathcal{P}_A\dot{\mathcal{X}}^A+p_r\dot{\phi}^r-\mathcal{N}\mathcal{H}-\mathcal{N}^a\mathcal{H}_a\right) \tag{A-57}$$

where all fields are functions of $\mathbf{x}$ and t. Moving to the constraint hypersurface and inserting (2.56), this reduces to,

$$S = \int dt \int_{\Sigma} d^3x \left(p_r \dot{\phi}^r - h_A(\mathbf{x}; \mathcal{X}^B, \phi^r, p_s) \dot{\mathcal{X}}_t^A(\mathbf{x}) \right) \tag{A-58}$$

We can see from the form of this equation that this descibes an ordinary quantum mechanical system with 'true' , unconstrained Hamiltonian,

$$H_{true}(t) = \int_{\Sigma} d^3x h_A(\mathbf{x}; \mathcal{X}^B, \phi^r, p_s) \dot{\mathcal{X}}^A(\mathbf{x}) \tag{A-59}$$

We quantize by making the identification,

$$\mathcal{P}_A(\mathbf{x}) \to -i\hbar \frac{\delta}{\delta \mathcal{X}^A(\mathbf{x})} \tag{A-60}$$

and introducing wave functionals, $\psi[\phi^r(\mathbf{x})]$. $\mathcal{X}^A$ is not turned into an operator in analogy with the external time parameter, t, from quantum mechanics.

Clock Variables

For a long time in physics, the concept of absolute time was taken for granted. In mechanics, one measures the rate of change of position with respect to time by measuring the position at two times t_1 and t_2. Can time actually be measured though? When we measure 'time', we take a reading from a measuring device, a clock. We assume that the time T on the clock to be a function of t, specifically a linear function, $T = \alpha t$. However, how was the clock calibrated? The answer, is of course, by another clock. This continues back to the original clock, the pendulum.

Galileo observed that the period of oscillation is constant for a pendulum by comparing it with his pulse, which of course may only be considered another 'clock'. Thus, we conclude that we may only observe the 'clock time' and never time itself.

We never measure time as an absolute parameter. We always compare two readings, one reading of a clock in terms of another, i.e. $T(T')$ where T' is another clock variable. Assuming that there is an underlying concept of time and that these clock variables give an approximate notion of time, this is not a problem at a classical level.

(4.2)

Recall that the metric is given by,

$$ds^2 = -\mathcal{N}^2(\lambda)d\lambda^2 + a^2(\lambda)d\Omega_3^2 \tag{A-61}$$

We found earlier that the Einstein-Hilbert action takes the form,

$$16\pi S_{EH} = \int_{\mathcal{M}} dtd^3x\mathcal{N}\sqrt{h}\left(K_{ij}K^{ij} - K^2 +^{(3)} R - 2\Lambda\right) \tag{A-62}$$

Setting $\Lambda = 0$, we may calculate this for our Friedmann model. We have for the extrinsic curvature,

$$K_{ij} = \frac{a'}{a\mathcal{N}}h_{ij} \tag{A-63}$$

Which leads us to identify,

$$K = K_{ij}h^{ij} = \frac{a'}{a\mathcal{N}}h_{ij}h^{ij} = \frac{3a'}{a\mathcal{N}} \tag{A-64}$$

If we write,

$$d\Omega_3^2 = d\chi^2 + sin^2\chi(d\theta^2 + sin^2\theta d\phi^2) \tag{A-65}$$

then one has,

$$\sqrt{h}d^3x = a^3 sin^2\chi sin\theta d\chi d\theta d\phi \tag{A-66}$$

The intrinsic scalar curvature is found to be ${}^{(3)}R = \frac{6}{a^2}$ (see [58]). Performing a Wick rotation, one finds that the Euclidean action takes the form (setting $2/3\pi = 1$ for convenience),

$$I_g = \frac{1}{2}\int dt\mathcal{N}\left(-\frac{aa'^2}{\mathcal{N}^2} + a\right) \tag{A-67}$$

Our matter action is similarly given by,

$$I_{matter} = \frac{1}{2}\int dt\mathcal{N}a^3\left(\frac{\phi'^2}{\mathcal{N}^2} - V(\phi)\right) \tag{A-68}$$

so we have for the total action,

$$I[a(\lambda),\phi(\lambda)] = \frac{1}{2}\int_0^1 d\lambda\mathcal{N}\left\{-a\left(\frac{a'}{\mathcal{N}}\right)^2 + a^3\left(\frac{\phi'}{\mathcal{N}}\right)^2 - a^3V(\phi) + a\right\} \tag{A-69}$$

Prefactor for No-Boundary Wave Function

We have the equation,

$$\left[\partial_\alpha^2 - \partial_\phi^2 - e^{4\alpha} + e^{6\alpha}V(\phi)\right]\Psi = 0 \tag{A-70}$$

In the case $a^2V \ll 1$, $V \approx 0$ is a good approximation and the fourth term drops out. We are left with a Bessel equation in $a^2/2$, with approximate solution,

$$I_0(z) = \sum_{n=0}^{\infty}\frac{1}{(n!)^2}\left(\frac{z}{2}\right)^{2n} \tag{A-71}$$

This is the zeroth order modified Bessel function. This has asymptotic behaviour for large a,

$$\Psi \sim \frac{1}{\sqrt{\pi}a}exp(\frac{a^2}{2})[1 + \mathcal{O}(a^{-2})] \tag{A-72}$$

So for large a this will match the previous result ('-' choice) for the wave function,

$$\Psi(a,\phi) \simeq \frac{\mathcal{C}(\phi)}{a(1-a^2V(\phi))^{1/4}} exp\left[\frac{\pm 1}{3V(\phi)}(1-a^2V(\phi))^{3/2}\right] \tag{A-73}$$

$$\approx \frac{\mathcal{C}(\phi)}{a} exp\left[\frac{\pm 1}{3V(\phi)}(1-\frac{3}{2}a^2V(\phi))\right] \tag{A-74}$$

provided,

$$\mathcal{C}(\phi) = \frac{1}{\sqrt{\pi}} \exp\left(\frac{+1}{3V(\phi)}\right) \tag{A-75}$$

We may also consider the $V(\phi) \gg 1$ regime but restricting ourselves to the region in which V is approximately constant. Thus the second term in (A-70) drops out and in the third term is also negligible relative to the fourth term. This is again a Bessel equation with solution,

$$\Psi \simeq c(\phi) J_0(\frac{1}{3}a^3\sqrt{V}) \tag{A-76}$$

where $J_0(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n!)^2} \left(\frac{z}{2}\right)^{2n}$ is the zero order ordinary Bessel function. This has asymptotic behaviour for large a,

$$\Psi \sim \frac{c}{\sqrt{2\pi S}} cos\left(S - \frac{\pi}{4}\right) \tag{A-77}$$

where $S = \frac{1}{3}a^3\sqrt{V}$. For the large V case which we are considering, this is a superposition of two oscillatory WKB modes. Using the WKB matching procedure, we find,

$$c = \sqrt{\frac{2\pi}{3}}\mathcal{C} = \sqrt{\frac{2}{3}} exp\left(\frac{1}{3V(\phi)}\right) \tag{A-78}$$

Boltzmann Brains

Boltzmann brains are 'freak' observers which arise from quantum fluctuations. As Boltzmann brains are random fluctuations, they would most likely observe a predominantly empty universe wherer there is only vacuum energy [13]. This is in contrast with the observations that we make, in which we see a relatively dense universe.

The difference between the observations of regular observers and Boltzmann brains may also described in terms of 'order'. Our observations of the universe are highly ordered. The observations of Boltzmann brains will clearly be highly disordered due to their random quantum nature.

Thus, any theory which is seen to predict the dominance of Boltzmann brains over regular observers is unsatisfactory. There is, in principle, no way to distinguish an observation by a Boltzmann brain and that of a regular observer. As do not see the observations that a typical Boltzmann brain would make, i.e. predominantly empty space, we conclude that the theory must be incorrect or require modification.

Induced Inner Product

Consider the usual Schröodinger inner product for two states $|\psi_1\rangle$ and $|\psi_2\rangle$,

$$\langle\psi_1|\psi_2\rangle = \int d^n q \psi_1^\star(q)\psi_2(q) \tag{A-79}$$

Now consider eigenstates of the Wheeler-DeWitt equation, $|\psi_{\lambda k}\rangle$, with corresponding eigenvalue λ and k labeling degeneracy. We will have,

$$\langle\psi_{\lambda' k'}|\psi_{\lambda k}\rangle = \delta(\lambda - \lambda')\delta(k - k') \tag{A-80}$$

This clearly diverges for $\lambda = \lambda'$.We may loosely define the induced inner product by disregarding $\delta(\lambda - \lambda')$, i.e. the induced inner product is given by,

$$\langle\psi_{\lambda' k'}|\psi_{\lambda k}\rangle_{induced} = \delta(k - k') \tag{A-81}$$

See Ref. [] for a rigourous discussion.

(5.35)

Consider (5.33). The window function, $f_\Delta(\mathbf{x}^{cl}(t))$, describes whether the classical trajectories are in the region Δ. We may also write this as,

$$\int_\Delta d^n x \delta^{(n)}(\mathbf{x} - \mathbf{x}^{cl}(t)) \tag{A-82}$$

This clearly also describes firstly if $\mathbf{x}$ is on a classical trajectory and, secondly, via the integration over the region, Δ, whether it is located in the region Δ. Thus, the argument of the θ-distribution may be written as (neglecting ϵ),

$$\int dt \int_\Delta d^n x \delta^n(\mathbf{x} - \mathbf{x}^{cl}(t)) \tag{A-83}$$

If we let $\Delta = (\Delta t) \times \Sigma$, where Σ is an $(n-1)$-dimensional hypersurface, then this becomes, by Stokes' theorem,

$$\Delta t \int dt \int_\Sigma d^{n-1} x \mathbf{n} \cdot \frac{d\mathbf{x}^{cl}(t)}{dt} \delta^n(\mathbf{x} - \mathbf{x}^{cl}(t)) \equiv \Delta t I[\Sigma, \mathbf{x}^{cl}(t)] \tag{A-84}$$

where we choose $\mathbf{n}$ such that $\mathbf{n} \cdot \frac{d\mathbf{x}^{cl}(t)}{dt} > 0$. It is apparent that $I[\Sigma, \mathbf{x}^{cl}(t)]$ is equal to either 0 or ± 1. It is equal to 0 for no intersections of Σ by the classical trajectories, $\mathbf{x}^{cl}(t)$. For and even number of intersections it is $+1$ while for an odd number it is -1. We consider cases of at most one intersection and are hence restricted to $I = 0, 1$.

We now reconsider the infinitesimal parameter, ϵ. Let us rewrite it in the form, $\epsilon = \Delta t \epsilon'$. Then, for the θ-distribution, one has,

$$\theta(\Delta I - \epsilon) = \theta(I - \epsilon') = I \tag{A-85}$$

and hence we can write p_Σ as,

$$p_\Sigma = \int dt \int d^n p_0 d^n x_0 w(\mathbf{p}_0, \mathbf{x}_0) \int_\Sigma d^{n-1}x\mathbf{n} \cdot \frac{d\mathbf{x}^{cl}(t)}{dt} \delta^{(n)}(\mathbf{x} - \mathbf{x}^{cl}(t)) \tag{A-86}$$

We may rewrite this, as we did (**??**), as,

$$p_\Sigma = \frac{1}{M} \int dt \int_\Sigma d^n p' d^{n-1} x' \mathbf{n} \cdot \mathbf{p}' w(\mathbf{p}', \mathbf{x}') \tag{A-87}$$

where $\mathbf{p}' = \mathbf{p}^{cl}(t)$ and $\mathbf{x}' = \mathbf{x}^{cl}(t)$. We have also exploited the reparametrization invarianve of the system to arrive at this result.

(5.55)

We have,

$$C_\Delta|\Psi_\lambda\rangle = \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} ds P(t) V_0 e^{-V_0(t-s)} \dot{P}(s)|\Psi_\lambda\rangle \tag{A-88}$$

$$= \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} ds e^{-iHt} P e^{iHt} V_0 e^{-V_0(t-s)} e^{-iHs} \dot{P} e^{iHs}|\Psi_\lambda\rangle \tag{A-89}$$

Then acting with the Hamiltonian on $|\Psi_\lambda\rangle$, we have,

$$C_\Delta|\Psi_\lambda\rangle = V_0 \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} e^{-iHt} P e^{iHt - V_0 t} e^{-i(H-\lambda)s + V_0 s} \dot{P}|\Psi_\lambda\rangle \tag{A-90}$$

Performing the s integral, we get,

$$C_\Delta|\Psi_\lambda\rangle = V_0 \int_{-\infty}^{\infty} dt e^{-iHt} P e^{iHt-V_0 t} \left[\frac{1}{-i(H-\lambda)+V_0} e^{-i(H-\lambda)s+V_0 s} \right]_{-\infty}^{t} \dot{P}|\Psi_\lambda\rangle \tag{A-91}$$

$$= V_0 \int_{-\infty}^{\infty} dt e^{-iHt} P e^{iHt-V_0 t} \left\{ \frac{i}{H-\lambda+iV_0} \right\} e^{V_0 t - i(H-\lambda)t} \dot{P}|\Psi_\lambda\rangle \tag{A-92}$$

$$= V_0 \int_{-\infty}^{\infty} dt e^{-i(H-\lambda)t} P G_V \dot{P}|\Psi_\lambda\rangle \tag{A-93}$$

$$= 2\pi V_0 \delta(H-\lambda) P G_V \dot{P}|\Psi_\lambda\rangle \tag{A-94}$$

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