

TO LYN

AND OUR PARENTS

GLOBAL PROPERTIES OF
QUANTUM GRAVITY

BY

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PREFACE

The work presented in this thesis was carried out between November 1970 and February 1974 in the Department of Theoretical Physics, Imperial College (until October 1973) and in the Department of Mathematics, King's College, London University under the supervision of Dr. C.J. Isham. I would like to thank him for his friendship and encouragement.

I am particularly grateful for permission to include (in chapters three and four) some results which were obtained in collaboration with Dr. C.J. Isham, and will be submitted for publication in a joint paper. Except where stated in the text, the work described is original and has not been submitted in this or any other University for any other degree.

Finally I am indebted to the British Passenger Lines for the award of a free passage from Australia for my wife and myself.

ABSTRACT

We suggest that the nature of time is such that the Dirac quantization technique is not appropriate for quantum gravity: a canonical approach is to be preferred. Attention is focussed on the mathematical properties that such a (canonical) quantum gravity theory is expected to have. We point out that the Everett-Wheeler interpretation of quantum mechanics is not yet sufficiently general to describe quantum gravity.

We concentrate on models of closed universes and show how many of the previous models proposed have not always respected elementary features of a conventional quantum theory, particularly self-adjointness properties..

We propose a new model: a homogeneous Friedmann model (with the sphere geometry) filled with massless "pions". This is probably the simplest model that is capable of describing (potentially) quantized matter and gravity. Nevertheless intrinsic, extrinsic and "matter-variable" times are discussed.

This model is quantized and attention is given to self-adjointness and orthogonality relations. By dropping the curvature term, a simplified model (that has a very interesting feature: it admits transitions to the non-classical empty Friedmann model) is obtained.

We show that the (minimal) initial value problem (following York) for homogeneous models can be treated very simply and that a massless scalar field can be used to extend all these models. We conjecture that the only quantized matter sources that scale conformally (in the manner of York) are the source-free electro-magnetic field and the above scalar field. We argue that the quantum theory suggests that the configuration space should be extended (à la DeWitt).

We attempt to construct models describing topology change via a conical singularity, or a degenerate metric. The latter is attempted after we define a smoothed addition of metrics.

Finally, there are four appendices discussing standard results for the A.D.M. decomposition, the Friedmann metrics, the scalar field and time dependent Hamiltonians.

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CHAPTER 0. INTRODUCTION.

0.1 Quantum Gravity

Quantum gravity in this thesis is taken to be synonymous with quantization of Einstein's general theory of relativity⁽¹⁾. Einstein's theory of gravity is singled out because of its great attraction for theorists and because recent experimental examination has found a number of competing theories to be invalid⁽²⁾. (The scalar-tensor theory of Brans-Dicke remains acceptable.)

The mathematical structure of general relativity is complicated and can be usefully discussed at four levels⁽³⁾ as follows. The first step is to start with a point set in which the points are associated in a (hazy) one-to-one manner with "physical events" in space-time. The next step is to impose a topology (in the technical sense) on the basic point set. This means that the concepts of continuity, compactness, connectedness etc. are now available.

The third level of increasing mathematical complexity is provided by the introduction of a differentiable manifold structure upon the above space in a way which is compatible with the previously constructed topology. This introduces the notion of local co-ordinate systems and the (fixed) number (the global dimension) that is required to specify uniquely a point in the manifold.

Finally a metric structure is constructed with the physical input that the signature is $(-,+,+,+)$. The entire mathematical system must be such that in any region of the manifold covered by a particular co-ordinate system, the Einstein and stress energy tensors must be such that, when expressed in this co-ordinate system, they satisfy the Einstein field equations:

$$G_{\mu\nu} = K T_{\mu\nu}.$$

To the question "At which level is the theory to be quantized?" many workers have understandably answered "The last!" since this is by far the easiest one with which to deal. (Here too, with the exception of the last chapter, lie the considerations and results of this thesis.)

However this point of view has been criticised on general conceptual grounds by many people, particularly Penrose⁽⁴⁾. The basic trouble is that the initial point set is not operationally measurable since any attempt to localize the position of a "point" will, by virtue of the uncertainty principle, result in a large uncertainty in the energy and momentum of the test particle. This uncertainty in the energy will become so large that copious pair production will occur. Thus the whole situation changes. From this point of view the idea of an underlying continuum is meaningless and quantization should start from this first level (whatever this may mean).

Penrose⁽⁴⁾ also points out that the concepts of open and closed sets, which must also be essentially meaningless in strictly physical terms, are used to great effect by the theoretician (for example, in proving the Hawking-Penrose global "singularity" theorems⁽⁵⁾). But Penrose goes further and criticises the use of the (complex) continuum of probability amplitudes. After all, the universal appearance of the continuum in physics stems from its mathematical utility rather than any physical reality. (In fact, Farrukh⁽⁶⁾ has now developed quantum mechanics and the theory of free quantum fields using a non-standard continuum where, for example, the Dirac delta-functions become effectively "ordinary" functions.)

Penrose provides some answers by constructing his twistor theory for which points are not primitive objects, and sees no objection in principle to being able to reduce the contour integrations that occur to a set of combinatorial rules (He sees quantum physics as essentially discrete and being represented by combinatorial rules such as those for the addition of spin.). Unfortunately, the full implementation of twistor theory remains a distant goal and will not be considered here.

Thus the continuum will be used and quantization of the metric tensor will be considered in this thesis, despite reservations. As Wheeler⁽⁷⁾ (8) has emphasized,

a metric tensor quantization scheme does allow of the possibility of extrapolation back at least to the topology stage. "Pensrose's criticism" is then answered (in principle) by pointing to the highly multiply-connected "foamlike structure" of space where there is a continual creation and annihilation of small "wormholes" which looks like "pair" creation. Unfortunately, this is not creation of pairs of real particles because, as Wheeler⁽⁸⁾ points out, the quantum numbers are probably wrong and so he hopes to interpret particles as resonances, or collective modes, of the foam. However all these ideas rest on the, as yet unproven, existence of "That typically quantum behaviour, topology change"⁽⁹⁾. It is into this highly speculative area that the last chapter of this thesis enters, following "...Wheeler's lively conviction that in certain stage in the development of a theory, speculation may become a useful, or even necessary, tool of progress."⁽¹⁰⁾.

0.2 Model Universes - Quantum Cosmology

General Relativity is a field theory and therefore has an infinite number of degrees of freedom. To solve even the classical equations of general relativity, most of these degrees of freedom must be eliminated. Imposition of space symmetries or algebraic speciality⁽¹¹⁾ is the successful classical procedure because the classical equations respect these restrictions: that is, the solutions so obtained are exact.

The same procedure can be tried in the quantum mechanical case whereby almost all of the degrees of freedom are suppressed completely (i.e. "frozen"), such that quantization of the remaining modes is a tractable problem. Unfortunately, this is incorrect in principle because of the existence of quantum zero point fluctuations in all degrees of freedom: the solutions so obtained can only, at best, be approximate.

But the hope is that as further degrees of freedom are unfrozen and quantized the model becomes progressively less

approximate and provides a convergent sequence. This can be done for the usual quantum field theories⁽¹²⁾. However it has been shown that there are very important differences between finite and infinite dimensional theories.

For example, consider the Schrödinger representation of the canonical commutation relation for a problem with one degree of freedom⁽¹²⁾. (For convenience, $\hbar$ will be set equal to one for this discussion.) The self-adjoint operator $\hat{q}$ is defined on the domain

$$\mathcal{D}(\hat{q}) = \{ \psi \in L^2(\mathbb{R}) \mid q\psi \in L^2(\mathbb{R}) \}$$

by

$$\hat{q}\psi(q) = q\psi(q) ,$$

and is interpreted as the position operator. The action of translations along $\mathbb{R}$ is described by a weakly continuous one-parameter group $\{\hat{U}(a)\}$ of unitary operators defined by

$$(\hat{U}(a)\psi)(q) = \psi(q-a) .$$

The first form of the Schrodinger representation of the canonical commutation relation is given by

$$\hat{U}(a)\hat{q}\hat{U}(-a) = \hat{q} - a\hat{I} \quad \text{on} \quad \mathcal{D}(\hat{q})$$

The generator of $\{\hat{U}(a)\}$ is interpreted as the self-adjoint momentum operator:

$$\lim_{a \rightarrow 0} \frac{1}{a} (\hat{U}(a) - \hat{I}) = -i\hat{p} \quad \text{on} \quad \mathcal{D}(\hat{q})$$

which means that

$$\hat{p} = -i \frac{d}{dq} ,$$

where $\mathcal{D}(\hat{p})$ is the dense linear manifold in $L^2(\mathbb{R})$ consisting of all absolutely continuous functions on $\mathbb{R}$ with derivative in $L^2(\mathbb{R})$. Clearly, the Schrödinger representation of the canonical commutation relations can be rewritten in the Heisenberg form as follows:

$$[\hat{p}, \hat{q}] = -i\hat{I} .$$

In this Heisenberg form, questions about the domains of the operators become rather cumbersome. Also, if the Heisenberg form is used to define a Heisenberg representation, then the Heisenberg representation concentrates essentially on the local aspects of the canonical commutation relation, neglecting the physics contained in the boundary condition of the problem at hand. In fact, if $\hat{q}$ is self-adjoint and bounded, then there does not exist a Heisenberg representation in which $\hat{p}$ is self-adjoint. (This problem occurs in chapter 4 of this thesis.)

The Weyl form of the Schrödinger representation of the canonical commutation relations avoids the domain problems by using only unitary operators as follows. Another weakly continuous, one-parameter group $\{\hat{V}(b)\}$ of unitary operators is defined on $L^2(\mathbb{R})$ with

$$(\hat{V}(b)\psi)(q) = (e^{-i\hat{q}b}\psi)(q) = e^{-iqb}\psi(q).$$

Thus, for all a, b in $\mathbb{R}$, the Weyl form is

$$\hat{U}(a)\hat{V}(b) = e^{iab}\hat{V}(b)\hat{U}(a).$$

This form has the inconvenience of being rather removed from the dynamics as it occurs in the canonical formalism of quantum mechanics which is inherited from the Hamilton relations of classical mechanics.

It is the Weyl form that is used in the Stone-von Neumann theorem. This states that all the irreducible Schrödinger representations are unitarily equivalent to one another. The significance of this is clear since unitary equivalence guarantees that the scalar products (or "overlap" integrals) used to obtain the observable probabilities are invariant.

However the Stone-von Neumann theorem does not generalize to the infinite dimensional field theories. In general, different irreducible representations of the canonical commutation rules are unitarily inequivalent. The embarrassing thing about this for the model field theory builders is that while the model is finite all the quantum mechanical models (with a given choice of time

and Hamiltonian) are unitarily equivalent, but in the limit (of going to an infinite dimensional theory) unitarily inequivalent quantum field theories are produced.

Another serious problem is that in quantum field theory the measure (used for the inner product on the Hilbert space), the canonical commutation relations and the Hamiltonian are all very intimately connected. In a finite quantum mechanical system, a Hamiltonian may be imposed arbitrarily on some representation of the canonical commutation relations. This can not be done in a quantum field theory. This result is known as Haag's Theorem which states that an interaction Hamiltonian may not be imposed on the free field canonical commutation relations; that is, the interaction picture ⁽¹³⁾ does not exist! Thus the algebraic approach ⁽¹²⁾ gives a more appropriate setting for quantum field theory than the usual Fock space techniques.

In quantum gravity these problems are further compounded because of the absence of a natural choice of the time, or for the canonical variables to be quantized. This problem is examined in detail in this thesis.

The Kuchar model of cylindrical waves and the Gowdy inhomogeneous torus, T^3 , model (as analysed by Misner and Berger ⁽¹⁴⁾) are very interesting because they are both infinite dimensional. In view of the recent indications ⁽¹⁵⁾ of the non-renormalizability of quantum gravity using the covariant quantization techniques with dimensional regularization it would seem extremely unlikely that the above models would be renormalizable. This problem deserves further attention.

However, the most popular models (and the ones mainly considered in this thesis) are those with only a finite number of degrees of freedom and these, of course, totally ignore the considerable problem of going from a quantum mechanical problem to a quantum field theory.

Now if a quantum cosmological model is to give some quantitative information, surely the very least required

is that the classical model should be stable. This is because if a classical model is unstable to perturbations in suppressed modes then genuine quantization should excite instability. This is not what happens in the quantum models because these models are obtained by quantizing a classical model with suppressed degrees of freedom. These suppressed modes are not described by the quantum model either. So the question of instability and its relevance enters the list of unsatisfactory aspects of quantum cosmology; especially since the Robertson-Walker models are unstable to certain shearing perturbations⁽¹⁶⁾ and Brill has found some indications of instability of Bianchi type I mixmaster universes⁽¹⁷⁾.

Of course the real universe contains fermions and so models with a source of fermions should be constructed (and this is under active consideration by Isham and Nelson at King's College). In these cases, the models will be inherently quantum theoretical, and the problem of how closely a given model solution approximates the "exact" quantum solution becomes more acute. As emphasized by Isham, it is important to separate the problems that are peculiar to quantum gravity and those that beset any quantum field theory. For example, it would be very interesting if these model techniques were used on a more conventional field theory (such as the usual scalar field with a $\lambda\phi^4$ interaction, which provides nonlinearity) where the "correct answer" is known via Feynman graph perturbation theory, so that a critical comparison is possible.

Despite the inadequacies of these models, their great virtue is that they provide an invaluable testing ground for the validity of concepts such as the nature of time, the configuration space (Is it superspace, extended superspace, conformal superspace,...?), wave-functions of the universe, etc. and for investigating technical problems such as solving the constraint equations, the operator ordering ambiguity, the existence of metrics in superspace, and many more⁽¹⁾.

Since it is well known⁽¹⁾ that many of these problems become particularly acute if the universe is closed, only closed universes are considered in this thesis. In particular, attention is focussed on the fact that the technical requirements of the quantum theory have not always been respected in some of the previous (closed universe) quantum gravity models. In fact, if the mathematical structure of the quantum theory is to be retained, then Dirac quantization is invalid and so super-space is not a useful object in the quantum theory.

0.3 Scheme of the Thesis

In the first chapter the special role that time plays in the quantum theory and the general theory of relativity is discussed generally, within the context of the constraint equations, "operator" time and super-space. It is argued that Dirac quantization (attempting to maintain manifest general covariance) may not be used: in quantum gravity, only the canonical approach is permissible if the mathematical structure of quantum mechanics is to be preserved.

It is also shown that, despite general faith to the contrary, the Everett-Wheeler interpretation is not adequate to describe the quantization of a closed universe.

Chapter two provides a discussion on previous models: how matter has been introduced and the technical shortcomings of many of the "quantum" gravity models. The latter centre around a general lack of elementary features of a conventional quantum theory. For example,

- (i) time should be a parameter which does not enter the definition of the inner product
- (ii) the inner product (for physical states), has to be defined!
- (iii) the observables (which do not include time) should be described by self-adjoint operators.
- (iv) there is a big difference between continuous and discrete spectra

and (v) there is a vast difference between a finite dimensional theory and the true field with its infinite member of degrees of freedom. These points are exposed explicitly in many of the models.

The next chapter introduces a new model that is the simplest possible one that is capable of describing quantized matter and gravity. The source used is a homogeneous massless scalar field. The discussion is classical and it's shown that, despite the overwhelming simplicity of the model, all the different types of time that have been used previously in various models can be defined easily and naturally.

In chapter four, quantization of this model is effected. The easiest time to use is connected with the matter variables and gives a time independent Hamiltonian, which can be proven to be self-adjoint. In the classical model the radius has a maximum which is a dynamical consequence, due to the presence of the curvature term in the equations of motion. Thus a boundary condition (at the radius of maximum expansion) in the quantum model would seem to be inappropriate. However a simplified model is proposed in which the curvature term is dropped and the boundary condition imposed.

A very interesting feature of the simplified model is that it admits transitions to a non-classical model: the empty Friedmann model. This then indicates that Misner's "R-W quantum puff" universe⁽¹⁸⁾ can be given a legitimate quantum mechanical interpretation. However this transition is sensitive to the boundary condition imposed and seems not to be retained in the full theory.

Finally, the full model is also quantized by using intrinsic and extrinsic times, both of which give a time dependent Hamiltonian. It is clear that (in a naive sense) the classical collapse is not averted with any of these quantization schemes. However it must be remarked that a definition and theory of quantum singularities has not yet been developed.

Chapter five introduces York's ⁽¹⁹⁾ results on the minimal set of Cauchy data and the York-Murchadha ⁽²⁰⁾ existence and uniqueness theorems for solutions.

It is shown that homogeneity can be treated simply and that a massless scalar field can be used to extend all the possible homogeneous models.

However it is also argued that conformal superspace ⁽²¹⁾ is only relevant for a very limited class of models since it is conjectured that the only quantized matter sources that scale conformally are the source-free electromagnetic field and the homogeneous and massless scalar field.

We also show that although the classical theory indicates that "extended superspace" ⁽²²⁾ is more natural than superspace, the quantum theory strongly suggests that the configuration space be extended in the manner of De Witt.

In Chapter 6 it is suggested that if models describing topology change (at the geometrical level) are to be found, a dynamical parameter which, in principle, can be extended to produce the topology change must be employed. The construction of such a model is attempted.

The old problem of causality is resurrected and it is suggested that while microscopic causality should not be taken too seriously, a natural description of the "pair annihilation" involves the metric on the wormhole becoming completely degenerate. In order to describe this, a "smoothed addition" of metrics is defined for use with the topological connected direct sum of the two manifolds.

A serious weakness of this approach is that the smoothing function appears explicitly in the constraint equations. Nevertheless, it is speculated that the degenerate metric approach (related to Komorowski's point addition ⁽²³⁾) and conical singularities may play the role that step "functions" and Dirac delta "functions" do (respectively) in ordinary quantum field theory.

Finally, there are four appendices. The first deals with notations and the A.D.M. decomposition ⁽²⁴⁾. The

second provides the explicit calculation of the field equations and the canonical forms for the Friedmann constant curvature models. The third deals similarly with the canonical decomposition of a scalar field. The last appendix sets out the quantum equation of motion for time dependent Hamiltonians.

Upon completion of this thesis, the paper of Kaup and Vitello⁽²⁵⁾ was brought to out attention. They look at the same model that is examined in detail in chapters 3 and 4 of this thesis. Kaup and Vitello use "Klein-Gordon" quantization and "...conclude that this model can be successfully quantized only by using an extrinsic time." Thus their work can only be regarded as preliminary.

CHAPTER 1. THE NATURE OF TIME AND THE INTERPRETATION OF THE WAVE FUNCTION.

1.1 The Nature of Time and its Abuse

Arnowitt, Deser and Misner⁽²⁴⁾⁽²⁶⁾ showed that the sourceless "Einsteinian theory of gravity can be obtained from an action principle with the Lagrangian density

$$\mathcal{L}_G = \pi^{ij} \dot{g}_{ij} - NC^0 - N_i C^i, \quad (1)$$

where

$$C^0 = -\sqrt{g} \cdot {}^3R + \frac{1}{\sqrt{g}} \left[\pi^{ij} \pi_{ij} - \frac{1}{2} (\pi^k_k)^2 \right] \quad (2)$$

$$C^i = -2 \pi^{ij}{}_{|j} . \quad (3)$$

Because the N_μ are Lagrange multipliers, their variation gives the four constraint equations

$$C^\mu(\pi^{ij}, g_{kl}) = 0, \quad (4)$$

(which are the initial value equations). This means that the super-Hamiltonian density, $\mathbb{H}$, is zero:

$$\mathbb{H} = N_\mu C^\mu = 0. \quad (5)$$

Now it might be expected that quantization is achieved by taking the super-Hamiltonian and writing down the obvious time independent Schrödinger equation :

$$\mathbb{H} \psi = 0. \quad (6)$$

But this would mean that the energy eigenstates evolve according to the factor e^{iEt} , where E is zero for closed universes. (For open universes, there is a non zero E which is obtained from the integration over the three-surface at infinity⁽²⁷⁾⁽²⁸⁾. However only closed universes are considered here.) Thus the "quantum" wavefunctions do not evolve in time. This is the "frozen formalism" problem that was encountered very early in quantum gravity⁽²⁹⁾. This ceases to be a problem as soon as it is realized that this "Schrödinger equation" is too time independent: despite its appearance, the theory is still

essentially generally covariant because no coordinate conditions have been imposed, in particular, the time is an arbitrary parameter. So the straight forward solution is to make a choice of coordinates (and solve the constraints classically), thus fixing the "real" canonical Hamiltonian, H , which is (before quantizing) conjugate to the chosen time. This course has been followed by most workers in the field, with the notable exception of DeWitt⁽²⁸⁾.

However theories which are complicated by formal requirements such as manifest covariance and gauge invariance are familiar from quantum field theory, and so considerable effort has been spent on trying to quantize gravity while maintaining general covariance. These attempts would seem to be misdirected because of a failure to recognize the special role that time (as opposed to space) plays in the general theory of relativity and in conventional quantum theory. This criticism will be elucidated following a brief review of how the situation arose by slavishly pursuing the notion of general covariance.

Consider the quantization of the Maxwell Field⁽³⁰⁾. The photon has spin and is usually described by using a vector potential, $A_\mu(x)$. But the photon is not an ordinary vector particle with three helicity states: it has mass zero which restricts it to two helicity states. So a subsidiary (or gauge, or constraint) condition must be imposed to eliminate the extra non-Maxwellian degrees of freedom.

Now this constraint equation may be solved classically and then quantization proceeds along the usual canonical pathway, where only the genuine dynamical variables appear in the canonical commutation relations. However Gupta and Bleuler⁽³¹⁾ showed that the constraint equation may be imposed at the quantum level to project out the physical states from the vector space obtained by using self-adjoint operators and commutation relations.

for even the nonphysical degrees of freedom .

Now the gravitational field is a massless spin two object, and the generally covariant action principle contains many non-dynamical degrees of freedom, although one expects to be able to impose the constraints quantum theoretically. In Dirac's⁽³²⁾ pioneering approach, general covariance is maintained by writing the wave function as

$$\Psi[g_{\mu\nu}] = \Psi[g_{ij}, N_\mu] \quad (7)$$

and treating all the g_{ij} and N_μ as dynamical variables.

The momenta conjugate to the lapse and shift functions are defined by

$$\pi^\mu = \frac{\delta \mathcal{L}}{\delta \dot{N}_\mu} \quad (8)$$

which vanish because the $\dot{N}_\mu$ never appear in the Lagrangian i.e.

$$\pi^\mu = 0. \quad (9)$$

These equations, called the primary constraints, were not written in this simple form until the action was brought into the 3 + 1 form (see appendix I).

However once the status of the N_μ was established to be that of Lagrange multipliers for the constraints(4), which are the initial value equations, it was clear that part of general covariance should be lost by writing the wavefunctional (7) as $\Psi(g_{ij})$, with the constraints (4) imposed quantum theoretically as

$$\hat{C}^0 \Psi(g_{ij}) = 0 \quad (10)$$

$$\hat{C}^i \Psi(g_{ij}) = 0. \quad (11)$$

This is referred to as Dirac quantization.

Most work (in closed universes) has been done in the Wheeler - DeWitt⁽²⁸⁾⁽³³⁾ metric representation where the canonical commutation relations are

$$[\hat{\pi}^{kl}(x), \hat{g}_{ij}(y)] = -i\frac{\hbar}{2} (\delta_i^k \delta_j^l + \delta_i^l \delta_j^k) \delta^{(3)}(x-y). \quad (12)$$

An explicit representation often used is

$$\hat{\pi}^{ij} \rightarrow -i\hbar \frac{\delta}{\delta g_{ij}}. \quad (13)$$

Now the three constraints of (5) can be shown to imply that Ψ is a coordinate-independent functional of the intrinsic geometry, ${}^3\mathcal{G}$, described by the g_{ij} . Thus there is one remaining constraint, which may be written suggestively as

$$\hat{C}^0({}^3\mathcal{G}, \frac{\delta}{\delta {}^3\mathcal{G}}) \Psi({}^3\mathcal{G}) = 0. \quad (14)$$

So the set of all geometries $\{{}^3\mathcal{G}\}$ is the domain space of the state functionals, and was given the name superspace by Wheeler⁽⁸⁾⁽³³⁾. A major problem is to discover the full mathematical structure of superspace: DeWitt⁽²²⁾⁽²⁸⁾ and Fischer⁽³⁴⁾, in particular, have worked on this. The idea of using a metric on superspace has been exploited (mainly to provide some "natural" choice for the factor ordering in the quantum problem)⁽¹⁸⁾⁽²⁸⁾. There has been little progress on the extremely difficult mathematical problem of defining a measure, written hopefully as $(d {}^3\mathcal{G})$, on superspace. This is required so that the inner products

$$(\Psi, \Phi) = \int (d {}^3\mathcal{G}) \Psi^*({}^3\mathcal{G}) \Phi({}^3\mathcal{G}) \quad (15)$$

may be defined, after which the self adjointness of operators and the interpretation of the Ψ may be discussed.

In the quantum theory it is very important from both a physical and mathematical point of view that the operators dealt with are self-adjoint (and so possess a spectral resolution). Now the positive definiteness of g_{ij} precludes any self-adjoint representations of the canonical commutation relations in the metric representation⁽³⁵⁾ in much the same way as the positive definiteness of energy in ordinary quantum mechanics rules out a self-adjoint time operator. Misner⁽¹⁸⁾⁽³⁶⁾ avoids this problem by taking the "exponential route" which is to deal with the variables β_{ij} obtained from the g_{ij} by

$$\{e^{\beta(x)}\}_{ij} = g_{ij}(x). \quad (16)$$

(Other choices of the canonical variables have been also been made^{(19)(35))37.})

However there is a very serious objection (about the nature of time) that criticises the whole superspace philosophy. In fact (14) reproduces the frozen formalism (for closed spaces) and is called the Hamiltonian constraint because C^0 is equivalent to the Hamiltonian density of the generally covariant canonical theory. As mentioned previously, a time has to be chosen as a coordinate condition and so may not appear explicitly in a generally covariant theory. Baierlein et al⁽³⁸⁾ have shown that it is incorrect to think of $\Psi(\mathcal{G})$ as a functional of the geometry intrinsic to space at some "particular time" because the intrinsic geometry itself contains all the dynamically relevant information about time. Thus dynamics can only be introduced by making a choice of the physical time which is a functional of the intrinsic three-geometry and then solving (14).

So Dirac quantization, as used by DeWitt⁽²⁸⁾, Liang⁽³⁹⁾ and Lund⁽⁴⁰⁾ has an "operator time" (since (14) is written as an operator equation, time to be identified later), the canonical commutation relations of (12) may not be interpreted as some kind of equal time canonical commutation relations because they already contain time as a canonical variable and the superspace measure for use in defining inner products contains a " $d(\text{time})$ ". This is not conventional quantization!

The idea that "... time is a measure of change of the existing things, and that in the absence of changing things there would be no time."⁽⁴¹⁾, or more succinctly "Time should simply be considered a reducible parameter denoting change."⁽⁴²⁾ is very basic to both general relativity and quantum mechanics. Time has a special role. It is not on the same footing as space and should not be put there.

Consider the Schrödinger equation, which is the dynamical equation for a non-relativistic particle in a

potential field. The position and momentum of the particle are observable and represented by self-adjoint operators. For a closed system, the Hamiltonian is the energy and is also observable, however the time is just a classical variable. This distinction is preserved in relativistic quantum field theory⁽⁴³⁾ in the sense that a c-number (that is, a classical) time is required for time ordered products which play a central role in the theory. In fact the "covariant" quantization schemes implemented on open universes⁽¹⁾ are this type of field theory with a c-number time defined from a background classical metric, where, as always, time is not an observable.

Thus, if the quantum theory and general relativity are to go together, then the notion of general covariance probably occurs only at the classical level. The canonical procedure should be followed because of time's special role in general relativity and the quantum theory (which seems to have no room for an operator time).

What is required is a measurement theory so that the observables may be identified, as it is these that are central. A long range hope is that the resulting field theory could instead be dealt with by the algebraic approach⁽¹²⁾ which gives a rigorous setting for the usual quantum field theory calculations. Some preliminary model calculations have been attempted⁽⁴⁴⁾⁽⁴⁵⁾.

1.2 Interpretation of the Wave Function

It is well known that the conceptual problems⁽⁴⁶⁾ of the quantum theory of a closed system are particularly serious. The Everett-Wheeler⁽⁴⁷⁾ "relative state" formulation has been advanced to meet these difficulties and fares well. Most objection has come because of the rather bizarre way that they avoid the acausal collapse of the wave function due to an observation.

They start (non-relativistically) with the following collection of mathematical objects: (1) a Hilbert space, (2) a Hamiltonian operator and (3) a Schrödinger equation

for vectors in the Hilbert space. Only one additional postulate is required to give the mathematics physical meaning: the postulate of complexity. This states that the Hamiltonian must be sufficiently complicated so that it can be regarded as describing at least two (but generally many more) distinct dynamical systems which under certain circumstances, but not always, can act as if they are isolated and independent. (In the standard language, this requirement is just that the Hamiltonian describes at least two "almost always" independent systems: the interaction being interpreted as a measurement of one system by the other.)

Everett and Wheeler then prove the following meta-theorem : The mathematical formalism of the quantum theory is capable of yielding its own interpretation. Part of this interpretation is that measurements do not make the wavefunction collapse, because this does not follow from the Schrödinger equation. So, instead, the wavefunction, which is written as a superposition of the various possible outcomes of a measurement, is interpreted as saying that the system splits into equally "real" simultaneous systems. Thus an observer is constantly splitting into all the possible "branches" of the system, although the laws of quantum mechanics do not allow him to feel it. Although it is beautifully self-consistent philosophy, it can never receive operational support in the laboratory.

When the closed system under study is the whole universe, the science-fictional flavour of the Everett-Wheeler interpretation is very clear: the universe is constantly splitting into an incomprehensibly large number of equally "real" branches. However "Apart from Everett's concept of relative states, no self-consistent stem of ideas is at hand to explain what one shall mean by quantizing a closed system like the universe of general relativity."⁽⁴⁸⁾ (For closed universes, there cannot even be a classical observer at asymptotia.)

So most closed universe quantum gravitists have either quoted the Everett-Wheeler interpretation as possible⁽²⁸⁾ or ignored the problem.

However none of the models constructed so far have been complicated enough to describe a measurement process. What is required is a model that satisfies the principle of complexity, so that it can be said that an observation has taken place. An important point that has been missed (also pointed out independently by Clarke⁽⁴⁹⁾) is that the principle of complexity is too severe if gravitation is considered. The gravitational interaction has an infinite range and cannot be shielded, and so the universe can never, in principle, be decomposed into an independent system and apparatus (or observer). So Everett and Wheeler have still not included the observer into the quantum theory intimately enough for quantum gravity.

This leaves quantum gravity in a sorry state: there does not yet exist either a conceptual framework or a complete measurement theory, despite DeWitt's claims⁽⁵⁰⁾. The policy in this thesis is to pay attention to the technical requirements of a quantum theory with the Schrödinger equation as its dynamical equation, in the spirit of the Everett-Wheeler metatheorem: hoping that the mathematical formalism will (eventually) show the way.

CHAPTER 2. PREVIOUS MODELS.

2.1 Introduction of Matter

Most of the classical models which have been quantized so far have been source-less, for example, most of the Bianchi models⁽⁵¹⁾ and Kantowski-Sachs model⁽⁵²⁾ and Gowdy's (inhomogeneous) T^3 model⁽¹⁴⁾. Of course these models are inadequate because the universe does contain mass. This is a deep problem because of the idea, going back at least to Bishop George Berkeley⁽⁵³⁾, that "Empty space is devoid of sign-posts needed to make statements which are operationally meaningful."⁽⁵⁴⁾ In fact, "As viewed by Berkeley and Mach, geometrical concepts are to be associated with the matter content of the universe."⁽⁵⁴⁾ So a consideration of matter is mandatory.

The classical models of Robertson-Walker satisfy the "cosmological principle" in that they are homogeneous and isotropic⁽⁵⁵⁾. They have a perfect fluid as their source. The Friedmann models are special cases obtained by filling the universe with an inert cloud of cold dust. These models have a one parameter family of spacelike hypersurfaces each of which is a space of constant curvature. The Robertson-Walker models seem able to describe most of the "course grain" structure of the universe (if the modern developments⁽⁵⁶⁾ in the field such as quasi-stellar objects, pulsars and black holes are excluded). From these models each of the "Standard Models" of the universe, used to describe its evolution and galaxy formation⁽⁵⁷⁾, etc., even down to the "hadron era" of Frautschi and Carlitz⁽⁵⁸⁾, is derived. This model of the hadron era is very exciting because it puts some elementary particle physics (via Hagedorn's⁽⁵⁹⁾ statistical bootstrap model) into cosmology. It provides some interesting results relevant to the early state of the universe and the formation of the galaxies without requiring initial inhomogeneities. Unfortunately, there are many fundamental features that may be wrong, and so far criticism has centered on the behaviour of super-dense matter⁽⁶⁰⁾. However the most serious criticism from the point of

view of this thesis is that the results of particle physics are extrapolated back to when the universe's radius is one Fermi (the radius of a hadron) and that the particle concept (via super-massive hadron resonances) is still used!

A more conventional attempt to include quantized matter in a classical background gravitational field has been made by Parker and Fulling⁽⁶¹⁾⁽⁶²⁾. They consider a massive scalar field, ϕ , in a Friedmann universe (with $k=1$) using the fundamental equation

$$G_{\mu\nu} = K \langle T_{\mu\nu} \rangle$$

Their major problem is to interpret what the R.H.S. of this equation means: a naive calculation results in a divergent expression. They avoid the problem by considering only special states for which, they believe, the details of renormalization are irrelevant. This point has been reconsidered very recently⁽⁴⁵⁾ and a finite $\langle T_{\mu\nu} \rangle$ has been obtained by abandoning the Fock space representation.

But there are other problems. They assume that the homogeneous mode of the scalar field is dominating other inhomogeneous modes. At first, the presence of these inhomogeneous modes in the homogeneous Friedmann geometry appears inconsistent. However the situation is confused because the source of the Einstein equations appears as an expectation value, which is not well defined. Also, it seems certain that this universe is not in thermal equilibrium so the discussion of the behaviour of pressure is inadequate.

Even though their argument is not convincing, the result that quantum coherence effects can result in a Friedmann-like contraction being converted into a Friedmann-like expansion is very interesting.

Further work in this direction is currently under consideration by Hu⁽⁶³⁾ and Hu, Fulling and Parker⁽⁶⁴⁾. Their model is the Mixmaster universe⁽³⁶⁾, at the classical

level, filled by scalar waves⁽⁶³⁾ which are to be quantized⁽⁶⁴⁾ The Mixmaster universe was introduced in the hope that anisotropic vibrations of the early universe produces interactions between particles in different parts of the universe and thereby generates a large scale homogeneity. Since it is expected that anisotropy damping is dominated by particle creation processes⁽⁶⁵⁾, this mixmaster universe equipped with a quantized source will be of considerable interest.

In the pioneering work on quantization of gravity, DeWitt⁽²⁸⁾ discusses the $\mathcal{K}=1$ Friedmann model filled by inert dust. One of a number of unsatisfactory features of this model is the use of the old phase - integral techniques which have now been superseded⁽⁶⁶⁾. Misner⁽¹⁸⁾ has also looked at this model from the point of view of his "Klein Gordon" equation approach, suggesting a different factor ordering. Closely related models are those studied by Liang⁽³⁹⁾ and by Lund⁽⁴⁰⁾. Liang studies a class⁽⁶⁷⁾ of cosmologies in an approximation (namely, the curvature term, 3R , is dropped) which is believed to be good in the early stages of the universe. The model of Lund is a quantized Tolman⁽⁶⁸⁾ universe with an inhomogeneous but spherically symmetric cloud of dust. These models (of Liang and Lund) are field theories in that they have an infinite number of degrees of freedom.

All of the previous quantum gravity models should perhaps be called "quantized" because of the very serious difficulties posed by the "quantization" techniques used. Most of these will be exposed explicitly in the other section of this chapter.

However one of the first objections a particle physicist would have to all of the non-empty "quantum" gravity models proposed so far is that these universes have only been filled with a perfect fluid: in fact, dust! This extremely naive view of matter is improved upon in the new model presented here by using quantized matter in the form of a homogeneous massless scalar field,

$\phi(t)$, in a closed Friedmann($\hbar=1$) geometry. The field description is emphasized and this has the merit of avoiding trying to use the particle concept in a closed space where there is no Poincaré group. After all, in field theory, a particle is defined as a unitary irreducible representation of the Poincaré group which is the isometry group of Minkowski space⁽⁶⁹⁾. However, since Quantum Electro-Dynamics is so successful, it's clear that particle physics should have some sort of local validity in a curved space. Thus, loosely speaking, the scalar field $\phi(t)$ may be described as a homogeneous Bose fluid of massless "pions".

2.2 Inadequacies: Klein-Gordon Approach⁽⁷⁰⁾

In one of the earliest model investigations of quantum gravity, Misner found what seems to be a fundamental feature of these models: the appearance of a square root Hamiltonian. This is obtained after making a choice of time and solving the Hamiltonian constraint equation,

$$C^0 = 0,$$

for the Hamiltonian. Typically, the Hamiltonian appears squared in the constraint equation and so the Hamiltonian is written with a square root. Explicit examples are given below and in chapter 3.

As mentioned previously, Misner takes the exponential route by parametrizing the (homogeneous) anisotropic three-geometry by

$$g_{ij}(t) = e^{-2\Omega(t)} \{e^{2\beta}\}_{ij}, \quad (1)$$

where Ω is a scalar and β_{ij} is a traceless matrix. For example, consider the Bianchi type I (or Kasner) metric that is closed (that is, the intrinsic three-geometry is the three torus, T^3):

$$ds^2 = -N^2(t) dt^2 + g_{ij}(t) dx^i dx^j. \quad (2)$$

In fact g_{ij} is diagonal and may be rewritten by setting

$$\beta_{ij} = \text{diag}(\beta_+ + \sqrt{3}\beta_-, \beta_+ - \sqrt{3}\beta_-, -2\beta_+). \quad (3)$$

The A.D.M. action principle may then be written as

$$\mathcal{I} = \int p_+ d\beta_+ + p_- d\beta_- - H d\Omega \quad (4)$$

where the Hamiltonian constraint gives

$$H = \sqrt{p_+^2 + p_-^2} \quad (5)$$

with the coordinate condition $\Omega = t$.

Of course the Hamiltonian really appeared squared, but the other sign is easily interpreted. The parametrization of (1) is only appropriate for the contraction phase of the universe. For expansion, the sign in front of Ω must be changed, and then

$$H = - \sqrt{p_+^2 + p_-^2} \quad (6)$$

(In fact, the Kasner model is too simple because it does not have both expansion and contraction phases. However if this is ignored, the behaviour described is illustrative.)

Because of their bias towards superspace, cosmologists have advocated⁽⁵¹⁾ the use of a "Klein-Gordon" equation quantization. For example

$$-\frac{\partial^2 \psi}{\partial \Omega^2} + \frac{\partial^2 \psi}{\partial \beta_+^2} + \frac{\partial^2 \psi}{\partial \beta_-^2} = 0, \quad (7)$$

for the Kasner model. In quantum cosmology the transition between positive and negative "energy" states is no embarrassment because they just represent the contraction and expansion phases (respectively) of the universe.

However the usual Klein-Gordon equation has more troubles than the transitions to the negative energy states. It is well known⁽⁷¹⁾ that the simple Klein-Gordon quantization does not use self-adjoint position operators, $\hat{x}$. (Thus this simple "first" quantization is not satisfactory and "second" quantization is required.) For Klein-Gordon particles Newton and Wigner⁽⁷²⁾ constructed the genuine self-adjoint position operators $\hat{x}_m$,

usually called the "mean position" operators. It is interesting to note that the "mean position" operators are equivalent to the self-adjoint position operators that are obtained naturally from considering the square root Hamiltonian

$$H = c \sqrt{\mathbf{p} \cdot \mathbf{p} + m^2 c^2}$$

giving the time dependent Schrodinger equation

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = c \sqrt{-\hbar^2 \nabla^2 + m^2 c^2} \psi(\mathbf{x}, t).$$

By using Fourier transforms, this can be rewritten as

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t} = \int d^3 y K(\mathbf{x} - \mathbf{y}) \psi(\mathbf{y}, t) \quad (8)$$

where the kernel is

$$K(\mathbf{x} - \mathbf{y}) = \int \frac{d^3 p}{(2\pi\hbar)^3} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})/\hbar} c \sqrt{\mathbf{p} \cdot \mathbf{p} + m^2 c^2} \quad (9)$$

(This is considered further in chapter 6, section 3.)

Since the anisotropy parameters, $\beta_{\pm}$, are an exponential parametrization of the metric, they do not suffer from the positivity criticism and so they can reasonably be identified as observables, and be described by self-adjoint operators. Under these circumstances, choosing the square root Hamiltonian quantization is obligatory.

Another fundamental feature ⁽⁵¹⁾ of closed universes is that the square root Hamiltonian is time dependent. A model closely resembling the previous example which illustrates the typical behaviour is the Mixmaster universe of Misner ⁽³⁶⁾. In this case the (homogeneous) three-geometry is an anisotropic three sphere, S^3 , that is parametrized in exactly the same form as before in (1), (3) and (4), but with respect to a form basis (independent of time):

$$ds^2 = -N^2(t) dt^2 + g_{ij}(t) \sigma^i \wedge \sigma^j$$

where

$$d\sigma^i = \frac{1}{2} \epsilon^{ijk} \sigma^j \wedge \sigma^k.$$

(In fact homogeneity means with respect to the group $SU(2)$. S^3 is the group space of $SU(2)$ and the forms σ^i are just the duals of the basis vectors of the Lie algebra of $SU(2)$. The anisotropy is introduced by changing the scale in Killing directions.)

For the Mixmaster universe, the Hamiltonian is given by

$$H^2 = p_+^2 + p_-^2 + e^{-4\Omega}(V-1) \quad (10)$$

where

$$V(\beta) = \frac{1}{3} \text{Tr}(e^{4\beta} - 2e^{-2\beta} + 1) \quad (11)$$

Misner "quantizes" this universe by again using a "Klein-Gordon" method giving

$$\hat{H}^2 \psi = -\frac{\partial^2}{\partial \Omega^2} \psi \quad (12)$$

$$\text{i.e.} \quad \left[-\frac{\partial^2 \psi}{\partial \Omega^2} + \frac{\partial^2 \psi}{\partial \beta_+^2} + \frac{\partial^2 \psi}{\partial \beta_-^2} - e^{-4\Omega}(V-1) \right] = 0$$

However this equation, besides having the inadequacies just described, is not even the correct "Klein-Gordon" equation. This is because the "mass" term, $e^{-4\Omega}(V-1)$, is time dependent and so equation (12) should be replaced by

$$\hat{H}^2 \psi = -\frac{\partial^2}{\partial \Omega^2} \psi - i \hat{H} \psi, \quad (13)$$

which can be seen from appendix IV.

It is unfortunate that these errors are present in Misner's ⁽³⁶⁾ analysis showing that the quantized Mixmaster universe always remains in a high quantum number state (that is, looks like the classical model) even as it collapses. If the extra term in (13) is considered the analysis is very much more difficult and has not been carried through.

2.3 Inadequacies: Superspace and Inner Products.⁽⁷⁰⁾

One of the reasons that the "Klein-Gordon" quantization has found favour with cosmologists is that it looks like a natural thing to do⁽⁷³⁾ from the Dirac quantization approach. Then a superspace metric can be used to decide upon a factor ordering.

In the Mixmaster model, if the mini-superspace metric is written as

$$ds^2 = -d\Omega^2 + d\beta_+^2 + d\beta_-^2, \quad (1)$$

then the Klein-Gordon equation used by Misner can be written in a covariant notation as a superspace wave operator⁽¹⁸⁾

$$\Delta_{ds^2} \psi = R \psi, \quad (2)$$

where

$$\begin{aligned} R &= g.^3 R \\ &= -e^{-4\Omega} (V-1) \end{aligned} \quad (3)$$

and

$$\Delta_{ds^2} = - \left(-\frac{\partial^2}{\partial \Omega^2} + \frac{\partial^2}{\partial \beta_+^2} + \frac{\partial^2}{\partial \beta_-^2} \right). \quad (4)$$

So Misner obtains a wave operator which is covariant with respect to transformations of the supercoordinates.

However all this has very little to do with the quantum theory. This is because firstly, the usual Klein-Gordon equation is inadequate; secondly Misner has formalized the wrong Klein-Gordon equation for a time dependent "mass" term present; and thirdly, the superspace approach is wrong because of the way that time is not given the special status (in that it is not an operator and doesn't appear in the inner product measure) that the quantum theory requires. These kinds of errors and omissions are rife in the quantum cosmology literature.

A good example is Misner's "R-W quantum puff" universe.⁽¹⁸⁾

It is well known that a closed, empty Robertson-Walker universe cannot exist classically. This can be seen from the Mixmaster equations (10) and (11) which, for $\beta_+ = \beta_- = 0$, give

$$H^2(\Omega) = -e^{-4\Omega}.$$

This means that the Hamiltonian is purely imaginary! However, this is "quantized" by setting

$$H^2 = -\frac{\partial^2}{\partial \Omega^2}.$$

This gives a differential equation, the solution of which is a Bessel function

$$\psi = K_0\left(\frac{1}{2}e^{-2\Omega}\right).$$

Since $|\psi|$ is exponentially small for a radius, $R \propto e^{-\Omega}$, which is greater than the Planck length, Misner argues that an empty R-W universe can just barely exist, expanding from an initial singularity to a maximum radius of about a Planck length, before recontracting. This is seen as some vindication of Wheeler's foam-like structure ideas at the Planck length.

Whatever this is, it is certainly not conventional quantization. The Ω variable has to be chosen as time, and there are no configuration variables and so there is no inner product for wave functions and no quantum theory.

The problem of not enough variables remains even when an inert dust is used as a source so that there is a classical solution. It is for this reason that DeWitt⁽²⁸⁾ introduced dust with coherent internal degrees of freedom which are governed by the local proper time. Because of this the dust can be used as a clock. Unfortunately, he uses the old quantization rules, following a Dirac quantization procedure and so has "operator valued times".

Liang⁽³⁹⁾ "quantizes" a large class of models in which the curvature scalar term, 3R , is dropped since these should give a good approximation to the behaviour

of the universe near the singularity. His procedure can be specialized to deal with the Mixmaster universe.

Liang uses Dirac quantization, obtaining the "stationary Schrödinger equation"

$$\left[e^{-3\Omega} \left(-\frac{\partial^2}{\partial \Omega^2} + \frac{\partial^2}{\partial \beta_+^2} + \frac{\partial^2}{\partial \beta_-^2} \right) \right] \Psi(\Omega, \beta_{\pm}) = 0 \quad (1)$$

which is subject to some factor ordering. It is "natural" to define the inner product in the usual Schrödinger manner as

$$(\Phi, \Psi) = \int \Phi^* \Psi d\Omega d\beta_+ d\beta_- . \quad (2)$$

Without proof, it is then claimed that the symmetric form of the super Hamiltonian,

$$\left[-\frac{\partial}{\partial \Omega} \left(e^{-3\Omega} \frac{\partial}{\partial \Omega} \right) + e^{-3\Omega} \frac{\partial^2}{\partial \beta_+^2} + e^{-3\Omega} \frac{\partial^2}{\partial \beta_-^2} \right] , \quad (3)$$

is Hermitian. The equation is separable and the Ω solution is easily obtained as

$$\Psi(\Omega) \sim e^{\frac{3}{2}\Omega [1 \pm \sqrt{1-\lambda^2}]} , \quad (4)$$

where

$$\lambda^2 = \frac{4}{9} (p_+^2 + p_-^2) . \quad (5)$$

From (4), it is clear that for anisotropic universes (that is $\lambda \neq 0$), the wave function vanishes at the singularity ($\Omega = -\infty$). As has been usual in quantum cosmology, it is then stated that quantization has removed the singularity.

Of course this is not true because the spectrum for Ω is continuous. In such a case, there is a non zero probability that the universe is in a neighbourhood of any point in the spectrum at some time.

So despite claims to the contrary, it would seem that, even for Liang's factor ordering (which is different from Misner's⁽³⁶⁾), the Mixmaster universe still collapses.

However there is a further serious fault with Liang's work. No time has been chosen and the frozen formalism is used. Liang solves the problem of deciding which are the configuration variables that appear in the measure

for the inner product by using a superspace metric. But, as discussed previously, time must be chosen from the superspace variables.

A natural choice (first taken by Misner⁽³⁶⁾) for the time is Ω . This means that the inner product, (2), can be rewritten as

$$(\Phi, \Psi) = \int \Phi^*(t, \beta_{\pm}) \Psi(t, \beta_{\pm}) dt d\beta_+ d\beta_-.$$

It is clear that this is not a quantum mechanical "overlap integral" because of the "dt". It should be stressed that, although the anisotropy parameters are treated as if they are the position variables of quantum mechanics, the Ω variable is the time.

2.4 Inadequacies: Field Theories⁽⁷⁰⁾

Some remarks have already been made (in chapter 0, section 2) about the large difference between systems with finite or infinite degrees of freedom. Liang⁽³⁹⁾ and Lund⁽⁴⁰⁾ have found another (closely related) pitfall with their field theories.

Liang's⁽³⁹⁾ analysis is more general than was suggested in the last section. It includes inhomogeneous models in which the variables Ω , and $\beta_{\pm}$ are all functions of space and the dust source has a mass distribution function μ . The super-Hamiltonian is then (essentially) written formally in a functional representation, following the Dirac quantization scheme, as

$$\left[-\frac{\delta}{\delta \Omega} \left(e^{-3\Omega} \frac{\delta}{\delta \Omega} \right) + e^{-3\Omega} \frac{\delta^2}{\delta \beta_+^2} + e^{-3\Omega} \frac{\delta^2}{\delta \beta_-^2} - \mu \right] \Psi(\Omega, \beta_{\pm}) = 0. \quad (1)$$

Because of the difficulty in analysing this functional equation, Liang approximates the 3-space continuum by ω^3 infinitesimal cubes, one at each point, $\underline{x}_i$. With the "appropriately averaged" values of Ω and $\beta_{\pm}$ over the volume at $\underline{x}_i$ denoted by $\Omega_i, \beta_{\pm i}$ and μ_i , the functional equation decouples into an infinite system of partial differential equations:

$$\left[-\frac{\partial}{\partial \Omega_i} \left(e^{-3\Omega_i} \frac{\partial}{\partial \Omega_i} \right) + e^{-3\Omega_i} \frac{\partial^2}{\partial \beta_{+i}^2} + e^{-3\Omega_i} \frac{\partial^2}{\partial \beta_{-i}^2} - \mu_i \right] \Psi(\dots \Omega_i, \beta_{\pm i}, \dots) = 0 \quad (2)$$

where

$$i = 1, 2, \dots, \omega^3.$$

In analogy with the homogeneous case, the inner product is "defined" as

$$(\Phi, \Psi) = \int \Phi^* \Psi \prod_{i=1}^{\omega^3} d\Omega_i d\beta_{+i} d\beta_{-i}. \quad (3)$$

Unfortunately, this "infinite Lebesgue measure" does not exist. For any finite dimensional quantum mechanical problem, the Lebesgue measure may be used, and is usually the most natural, since it is in this representation of the canonical commutation relations that the momentum operator is just the partial derivative with respect to the position coordinate. Of course, in quantum mechanics, it doesn't matter which irreducible representation of the canonical commutation relations is used because they are all unitarily equivalent (by the Stone-von Neumann theorem). For example, (in one dimension), if the measure is re-defined with a weight function $\rho(x)$, then the unitarily equivalent theory (in a different Hilbert space) has a transposed position operator:

$$\hat{p} = -i \frac{d}{dx} - i \frac{\rho'}{\rho}. \quad (4)$$

However with a field theory, it matters very much which representation of the canonical commutation relations is used, because the Stone-von Neumann theorem no longer holds. Since an infinite dimensional Lebesgue measure doesn't exist, the usual Schrodinger representation is inappropriate for generalization.

However the representation with a Gaussian weight function, $\rho(x) = e^{-x^2}$, does generalize, since the Kolmogoroff Theorem⁽⁷⁴⁾ ensures the convergence of the sequence of measures

$$e^{-\sum_{i=1}^n x_i^2} dx_1 \dots dx_n \quad (5)$$

as n tends to infinity. It is in this sense that a functional-integral measure (as used in quantum field theory) can be written as

$$e^{-(\varphi, \varphi)} d\varphi(x). \quad (6)$$

It is important to notice also that the representation of the canonical commutation relations is no longer just the simple Heisenberg form

$$[\pi(x), \phi(y)] = -i \delta(x-y)$$

implying that

$$\pi(x) = -i \frac{\delta}{\delta \phi(x)}.$$

This point has been made previously by Isham⁽⁷⁵⁾, but ignored by all workers in the field. In particular, notice that this representation is used to obtain the superspace coordinate-free super-Hamiltonian equation, written formally as

$$C^0({}^3g, \frac{\delta}{\delta {}^3g}) \Psi({}^3g) = 0. \quad (7)$$

Lund⁽⁴⁰⁾ canonically "quantizes" the Tolman universe which is one filled by an inhomogeneous but spherically symmetric dust. By choosing a time which is built from the matter variables, a linear (that is, not a square root) Hamiltonian density appears:

$$H = \dot{x}^2 \pi_x^2 - \left(\frac{q}{32}\right)^{1/3} (1 - \dot{x}^2) x^{2/3}, \quad (8)$$

where x is a field variable that is a function of the radial coordinate r .

The Hamiltonian is obtained by integrating H with respect to r . Lund now makes the same technical error as Liang by taking the "natural" choice of representation of the canonical commutation relations as

$$\pi(r) = -i \frac{\delta}{\delta x(r)},$$

and divides r up into intervals (which must be taken to be infinitesimal). This decouples the problem, with

$$\Psi(x, t) = \prod_j \psi_j(x_j, t),$$

giving a family of Schrödinger equations

$$i \frac{\partial \psi_j}{\partial t} = - \frac{\partial^2 \psi_j}{\partial x_j^2} + a_j x_j^{3/2} \psi_j(x_j) \quad (9)$$

where a_j is a constant, and the measure is, once again, Lebesgue which doesn't exist in the limit as the number of degrees of freedom reach infinity.

Unfortunately Lund's work has a more obvious error. He goes on to treat the homogeneous Friedman model which has the same equation as (9) and is now a genuine quantum mechanical problem, so the Schrödinger equation is adequate.

Noticing that most models, and this one in particular, have a continuous spectrum for the radius of the universe, Lund argues that irrespective of what value the wave function has at the singularity, collapse is avoided. This is because the singularity is just one point of the spectrum and so is of measure zero and may be ignored. This argument is, of course, fallacious.

Finally, it should be mentioned that the "quantum" treatment of Gowdy's inhomogeneous T^3 cosmology by Misner and Berger⁽¹⁴⁾ again tries to use Schrödinger equations with an infinite number of degrees of freedom. But they go further by considering "creation" and "annihilation" operators for modes of the field and also construct "number" operators for these modes, emotively called "graviton" modes.

These are not the spin two objects usually called gravitons because the spin two gravitons are defined as unitary irreducible representations of the Poincaré group⁽⁶⁹⁾. Despite the absence of the vacuum state given by the Poincaré group, it should be possible to use Fock space techniques to construct appropriate number operators. The work of Misner and Berger can be regarded as a step in this direction.

CHAPTER 3. THE MODEL: CLASSICALLY

3.1 Introduction

The importance of considering a theory with matter has already been discussed in chapter 2 section 1. The massless scalar field is used in the present chapter (and the following one) to provide a (potentially quantized) source for the field equations.

A scalar field with mass, m , is easily incorporated into the canonical decomposition, as shown explicitly in appendix III. However the equations of motion are then much more difficult to solve and this problem is still under consideration. (The real problem is that the structure of the initial value equations becomes much more complicated as shown in chapter 5, section 2. It is well known that the effect of a non-zero mass, m , is to change the force from a long range one to a short range "Yukawa" type, although the short range behaviour remains the same in both cases. This argument suggests that the behaviour near the singularity would be the same for both massive and massless "pions" and so only the massless case is considered in this and the following chapter (although the mass term is retained in the first few equations of the next section).

The use of scalar fields is not new in gravity theory. Deser and Higbie⁽⁷⁶⁾ use a massless scalar field in their studies and point out that the Lagrangian density used there and in this thesis

$$\mathcal{L} = {}^4R - \frac{1}{2} \sqrt{{}^4g} g^{\mu\nu} \phi_{,\mu} \phi_{,\nu} , \quad (1)$$

may be rewritten as the Brans-Dicke Lagrangian density,

$$\mathcal{L} = \psi {}^4R - \omega \sqrt{{}^4\bar{g}} \bar{g}^{\mu\nu} \psi_{,\mu} \psi_{,\nu} ,$$

by a conformal transformation on the metric $g_{\mu\nu}$:

$$g_{\mu\nu} = (K\psi) \bar{g}_{\mu\nu}$$

and by a transformation of the scalar field:

$$\sqrt{K} \phi = \sqrt{2\omega+3} \log(K\psi) .$$

Despite the mathematical equivalence of the two classical theories, they almost certainly lead to inequivalent quantum theories. This causes no embarrassment since the physical interpretation is quite different: ψ is part of the gravitational field, while ϕ describes a source of massless "pions".

The model in this thesis uses a homogeneous Friedmann $k = 1$ geometry which has only one degree of freedom (viz the radius of the three-sphere) that is filled with a homogeneous massless scalar field which provides one more degree of freedom. This is (if the closed, isotropic and flat three-torus geometry is excluded) the simplest possible model that has one gravitational degree of freedom and one matter degree of freedom.

Because of its simplicity, field theory difficulties are avoided: the Schrödinger approach is adequate. Nevertheless, a discussion of both intrinsic and extrinsic times as well as time picked out by a matter variable is possible.

3.2 The Classical Model

The geometry (that is, the 3G) of interest here is that of the Friedmann model with constant curvature, $k = 1$. This is the isotropic sphere, S^3 . However the calculations (carried through in appendix II) of the Ricci and Einstein tensors and the canonical form of the Lagrangian keep k arbitrary and so also describe the other Friedmann models (obtained with $k = 0$ or -1). In this work the k will be retained so that the role of the curvature is clear.

The metric is (from AII(1))

$$ds^2 = -N(t)^2 dt^2 + R(t)^2 S_{ij} dx^i dx^j$$

where S_{ij} (not a function of time) is the homogeneous metric for a "unit radius" Friedmann three-geometry which has curvature given by (using AII(20))

$${}^3R = S^{ij} R_{ij} = 6k.$$

This means that the actual curvature for the model is

$${}^3R = \frac{6k}{R^2(t)}.$$

The source of matter used is a massless scalar field, ϕ , which has the Lagrangian density (given in AIII(1))

$$\mathcal{L}_m = -\frac{1}{2} \sqrt{-g} (g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi + m^2 \phi^2).$$

(As a matter of interest, the mass term will be kept for the first few equations of this section.) Appendix III provides the calculations involved with such a field and its canonical decomposition.

It is clear that for the homogeneous Friedmann models, the scalar fields (massive or massless) which fill them must be homogeneous. That is $\phi = \phi(t)$

$$\text{with } \partial_j \phi = 0.$$

(This can be deduced from the form of T_o^i , given in AIII(29) and the fact that $R_{oi} = 0$, derived in AII(11).) In this case, the matter Lagrangian density becomes (from AIII(8))

$$\mathcal{L}_m = \frac{1}{2} \frac{\sqrt{g}}{N} \dot{\phi}^2 - \frac{1}{2} N \sqrt{g} m^2 \phi^2.$$

Since the Hamiltonian in a closed universe has no significance as an energy, and because the field equations are unaffected by multiplying the action by a constant, the factor $\int \sqrt{g} d^3x$ where

$$\sqrt{g} = R^3(t) \sqrt{g_{(i)}} ,$$

in both the gravitational and scalar field actions (AII(25) and AIII(19), respectively) will be dropped.

Thus the Lagrangian can be written in canonical form (using AII(26), AIII(19), AI(17)) as

$$L = \pi_R \dot{R} + \pi_\phi \dot{\phi} + N \left(6\dot{R}^2 R + \frac{\pi_R^2}{24R} - \frac{\pi_\phi^2}{2R^3} - \frac{R^3}{2} m^2 \phi^2 \right) \quad (1)$$

Variation with respect to π_R and π_ϕ reproduce their definitions:

$$\pi_R = -\frac{12 R \dot{R}}{N} \quad (2)$$

$$\text{and } \pi_\phi = \frac{R^3 \dot{\phi}}{N}, \quad (3)$$

while variations of R and N respectively reproduce the G_{λ}^{λ} (AIII(24) and AII(21)) and G_0^0 (AII(22) and AIII(22)) field equations:

$$\frac{\hbar}{R^2} + \frac{\dot{R}^2}{N^2 R^2} + \frac{2\ddot{R}}{N^2 R} - \frac{2\dot{N}\dot{R}}{N^3 R} = -\frac{1}{4} \frac{\dot{\phi}^2}{N^2} + \frac{1}{4} m^2 \phi^2 \quad (4)$$

and

$$3\left(\frac{\hbar}{R^2} + \frac{\dot{R}^2}{N^2 R^2}\right) = \frac{1}{4} \frac{\dot{\phi}^2}{N^2} + \frac{1}{4} m^2 \phi^2. \quad (5)$$

Variation with respect to ϕ reproduces the covariant "Klein-Gordon" equation (AIII(26))

$$\frac{d}{dt} \left(\frac{R^3 \dot{\phi}}{N} \right) + NR^3 m^2 \phi = \pi_{\phi} + NR^3 m^2 \phi = 0 \quad (6)$$

although this is not an independent equation because it can be derived (multiplied by a factor of $\dot{\phi}_N$) from (4) and $\frac{d}{dt}$ (5), by using AII(24). In fact, (6) is part of the Bianchi identities since it is just a consistency condition which ensures the vanishing of the Einstein tensor.)

Equations (4) and (5) can be added and subtracted to give the alternative equations

$$2\left(\frac{\hbar}{R^2} + \frac{\dot{R}^2}{N^2 R^2}\right) + \frac{\ddot{R}}{N^2 R} - \frac{\dot{N}\dot{R}}{N^3 R} = \frac{1}{4} m^2 \phi^2 \quad (7)$$

$$\text{and} \quad \frac{\hbar}{R^2} + \frac{\dot{R}^2}{N^2 R^2} - \frac{\ddot{R}}{N^2 R} + \frac{\dot{N}\dot{R}}{N^3 R} = \frac{1}{4} \frac{\dot{\phi}^2}{N^2}. \quad (8)$$

The "Klein-Gordon" equation, (6), can only be integrated immediately if m is taken to be zero (and this is essentially why the massless case is much easier to solve than the massive theory.). Thus for the rest of this chapter and the next, m will always be set equal to zero. The result of integrating (6) is now

$$\pi_{\phi} = R^3 \dot{\phi} / N = C. \quad (9)$$

To go further, a choice of time must be made. Since the metric is

$$ds^2 = -N(t)^2 dt^2 + R(t)^2 g_{ij} dx^i dx^j,$$

where g_{ij} is not a function of time, it is clear that

setting

$$N = R \quad (10)$$

makes a choice of time. Since this is one of the usual textbook definitions of time for the Friedmann models, it will be called the Friedmann time.

The integrated "Klein-Gordon" equation, (9), now gives

$$R^2 \dot{\phi} = C, \quad (11)$$

while (7) becomes

$$\frac{\ddot{R}}{R^3} + \frac{\dot{R}^2}{R^4} + \frac{2h}{R^2} = 0. \quad (12)$$

setting

$$r = R^2, \quad (13)$$

gives

$$\ddot{r} = \frac{d}{dt}(2R\dot{R}) = 2\dot{R}^2 + 2R\ddot{R} \quad (14)$$

By using (13) and (14), (12) may be rewritten as

$$\ddot{r} + 4hr = 0, \quad (15)$$

which implies that, for h positive,

$$r = a \cos(2\sqrt{h}t) + b \sin(2\sqrt{h}t). \quad (16)$$

However the general solution is not given by just (11) and (16). This is because, as explained previously the "Klein-Gordon" equation, (6), can be derived from the G_{α}^{β} field equations and the time derivative of the G_{α}^{α} field equations. This means that if the "Klein-Gordon" equation is used with another equation to solve the equation of motion, then a consistency check must be made, because some information has been lost.

So to ensure consistency, the integrated "Klein-Gordon" equation, (11), is put into the G_{α}^{α} equation, (5), giving

$$\frac{h}{R^2} + \frac{\dot{R}^2}{R^4} = \frac{1}{12} \frac{C^2}{R^6}$$

i.e.

$$hr^2 + \frac{1}{4} \dot{r}^2 = \frac{1}{12} C^2.$$

(17)

Now (16) is put into (17):

$$k(a \cos[2\sqrt{k}t] + b \sin[2\sqrt{k}t])^2 + \frac{1}{4}(-a \sin[2\sqrt{k}t] + b \cos[2\sqrt{k}t])^2 \cdot 4k = \frac{1}{12}C^2$$

i.e. $12k(a^2 + b^2) = C^2$.

This implies that there exist a δ such that (for positive k)

$$a = \frac{C}{\sqrt{12k}} \sin \delta, \quad b = \frac{C}{\sqrt{12k}} \cos \delta. \quad (18)$$

Thus, from (11), (16) and (18), the solution (for $k > 0$) is

$$R^2 = \frac{C}{\sqrt{12k}} \sin(2\sqrt{k}t + \delta) \quad (19)$$

$$\dot{\phi} = \frac{C}{R^2} = \frac{\sqrt{12k}}{\sin(2\sqrt{k}t + \delta)}. \quad (20)$$

Now it is clear (from (15) and (16)) that the models here do not escape the inevitable classical collapse of the universe⁽⁵⁾. It is also evident that only for $k > 0$ does the radius, R , have a maximum, R_m , which is

$$R_m^2 = \frac{|C|}{\sqrt{12k}}. \quad (21)$$

From (19) and (20), it is obvious that δ merely provides a rescaling of the time. If the time is chosen such that

$$0 \leq t \leq \frac{\pi}{2\sqrt{k}} \quad (22)$$

then two obvious choices for δ are

$$\delta = 0 \text{ implying } C > 0 \text{ implying } \dot{\phi} > 0 \quad (23)$$

or

$$\delta = \pi \text{ implying } C < 0 \text{ implying } \dot{\phi} < 0. \quad (24)$$

Notice that during one of the universes oscillations, only one of either (23) or (24) can apply. Thus one convenient parametrization (for $k > 0$), in which the sign of C does not change, is

$$\left. \begin{aligned}
 0 &\leq t \leq \frac{\pi}{2\sqrt{k}} \\
 R^2 &= R_m^2 \sin(2\sqrt{k}t) \\
 \dot{\phi} &= \sqrt{12k} \operatorname{cosec}(2\sqrt{k}t) \\
 \phi &= \sqrt{3} \log(\tan \sqrt{k}t) + \phi_0
 \end{aligned} \right\} \quad (25)$$

where ϕ was integrated with the help of Gradstein⁽⁷⁷⁾.

For future reference the range of ϕ , which is from $-\infty$ to $+\infty$, is noted here:

$$\left. \begin{aligned}
 t &= 0 \quad \text{i.e. } \phi - \phi_0 = -\infty \\
 t &= \frac{\pi}{4\sqrt{k}} \quad \text{i.e. } \phi - \phi_0 = 0 \\
 t &= \frac{\pi}{2\sqrt{k}} \quad \text{i.e. } \phi - \phi_0 = +\infty
 \end{aligned} \right\} \quad (26)$$

(In fact there is a time "symmetry" about $t = \frac{\pi}{4\sqrt{k}}$, which is the time of maximum expansion. This can be made explicit by choosing a new time such that

$$-\frac{\pi}{4\sqrt{k}} < t < \frac{\pi}{4\sqrt{k}}$$

with $\zeta = \frac{\pi}{2}$, and C is still always positive.)

It will be useful to have the relation between ϕ and R (since general relativity is really a study of such correlations⁽²⁸⁾.) This can be obtained by eliminating the time from (25), for which the formulae⁽⁷⁸⁾

$$\tan \frac{\theta}{2} = \frac{1 - \cos \theta}{\sin \theta} = \frac{\sin \theta}{1 + \cos \theta} \quad (27)$$

are useful. By using (27),

$$\left. \begin{aligned}
 \theta &= 2\sqrt{k}t, \\
 \tan \frac{\theta}{2} &= \frac{1 \mp \sqrt{1 - \sin^2 \theta}}{\sin \theta},
 \end{aligned} \right\} \quad (28)$$

where $\mp$ correspond to $t \lesseqgtr \frac{\pi}{4\sqrt{k}}$.

Now (25) and (28) imply that

$$\phi - \phi_0 = \sqrt{3} \log \left(\frac{1 \mp \sqrt{1 - \frac{R^4}{R_m^4}}}{\frac{R^2}{R_m^2}} \right) \quad (29)$$

It is clear that there is a change of sign in $\phi - \phi_0$ at $R = R_m$ (i.e. at the maximum of expansion). What is not clear is that there is a time "symmetry", or more precisely, time symmetry for R and antisymmetry for $\phi - \phi_0$. The time symmetry of R is evident and so the antisymmetry of $\phi - \phi_0$ will now be demonstrated from (27), (28) and (25):

$$\tan \frac{\theta}{2} = \sqrt{\frac{1 - \cos \theta}{1 + \cos \theta}},$$

and so

$$\begin{aligned} \phi - \phi_0 &= \sqrt{3} \log \frac{1 - \cos \theta}{1 + \cos \theta} \\ &= \sqrt{3} \log \frac{1 \mp \sqrt{1 - \sin^2 \theta}}{1 \pm \sqrt{1 - \sin^2 \theta}} \\ &= \sqrt{3} \log \left(\frac{1 + \sqrt{1 - \sin^2 \theta}}{1 - \sqrt{1 - \sin^2 \theta}} \right)^{\mp 1} \\ &= \mp \sqrt{3} \log \frac{1 + \sqrt{1 - \sin^2 \theta}}{1 - \sqrt{1 - \sin^2 \theta}} \\ \phi - \phi_0 &= \mp \sqrt{3} \log \frac{R_m^2 + \sqrt{R_m^4 - R^4}}{R_m^2 - \sqrt{R_m^4 - R^4}}. \end{aligned} \quad (30)$$

This change of sign in $\phi - \phi_0$ at the maximum of expansion ($R = R_m$) is an embarrassment if the scalar field is to be considered a function $\phi = \phi(R)$ of the radius since this is one-is-to-two and so not well defined, unless the expansion and contraction phases are considered separately. However the radius as a function $R = R(\phi)$ of the scalar field is well defined (and two-is-to-one) and so (30) will now be inverted:

$$\frac{\phi - \phi_0}{2\sqrt{3}} = \mp \frac{1}{2} \log \frac{1 + \sqrt{1 - \frac{R^4}{R_m^4}}}{1 - \sqrt{1 - \frac{R^4}{R_m^4}}}.$$

But since⁽⁷⁹⁾, for $\zeta < 1$,

$$\frac{1}{2} \log \left(\frac{1+\zeta}{1-\zeta} \right) = \tanh^{-1} \zeta,$$

setting

$$\zeta = \sqrt{1 - \frac{R^4}{R_m^4}}$$

gives

$$R = R_m (1 - \zeta^2)^{1/4}$$

Thus

$$\begin{aligned} \tanh \frac{\phi - \phi_0}{2\sqrt{3}} &= \tanh (\mp \tanh^{-1} \zeta) \\ &= \mp \zeta, \end{aligned}$$

which gives

$$R = R_m \left[1 - \tanh^2 \left(\frac{\phi - \phi_0}{2\sqrt{3}} \right) \right]^{1/4}$$

$$\text{i.e.} \quad R = R_m \cosh^{-1/2} \left(\frac{\phi - \phi_0}{2\sqrt{3}} \right). \quad (31)$$

This expression can easily be inverted to give a simpler form for $\phi = \phi(R)$ than (30):

$$\phi - \phi_0 = \mp 2\sqrt{3} \cosh^{-1} \left(\frac{R_m^2}{R^2} \right), \quad (32)$$

which can also be written as⁽⁷⁹⁾

$$\phi - \phi_0 = \mp 2\sqrt{3} \log \left[\frac{R_m^2}{R^2} + \sqrt{\frac{R_m^4}{R^4} - 1} \right]. \quad (33)$$

3.3 Choices of Time

In general relativity many different choices of time may be made although, because of general covariance, the transformation from one time coordinate to another is very easy. However, in anticipation of quantization, some convenient choices of time will now be discussed, where convenient means that the conjugate Hamiltonian is not too complicated so the (canonical) quantization can be

performed without much difficulty. In this sense, the usual "Friedmann time" is an inconvenient choice.

Now it is well known that for an (empty) closed universe, the intrinsic three-geometry contains information about time. With the superspace philosophy very much in mind, Wheeler⁽⁸⁾⁽³³⁾ and DeWitt⁽²⁸⁾ argue for the identification of one of the parameters of the intrinsic three-geometry with an "intrinsic" time. Following this approach, the natural choice in this model is to set the radius equal to the intrinsic time. (This is clearly an acceptable choice, from the analysis of the previous section.) By examining the Lagrangian (3.2(1))

$$\mathcal{L} = \pi_R \dot{R} + \pi_\phi \dot{\phi} + N \left(6hR + \frac{\pi_R^2}{24R} - \frac{\pi_\phi^2}{2R^3} \right), \quad (1)$$

the Hamiltonian is found to be $-\pi_R$ which can be evaluated from the constraint equation:

$$(\pm \pi_R)^2 = -144hR^2 + 12 \frac{\pi_\phi^2}{R^2}. \quad (2)$$

This parametrization gives a time dependent square root Hamiltonian and it has already been remarked that the appearance of such Hamiltonians seems to be a fundamental feature of quantum gravity Models⁽⁵¹⁾. Unfortunately $R = t$ is specific to the expansion of the universe and a description of the behaviour about the maximum of expansion ($R = R_m$) and the contraction requires a redefinition of the time. The whole procedure requires care, as was foreshadowed by the behaviour (which was discussed in the last section) of $\phi = \phi(R)$. The model with this parametrization is quantized in chapter 4 section 4.

The intrinsic time favoured by Misner⁽¹⁸⁾⁽³⁶⁾ is an exponential one with $x = t$ where

$$R = R_0 e^{\pm x}. \quad (3)$$

(Misner uses the symbol Ω for his "exponential time".) This is really a fairly trivial change because of the equation AII(35):

$$\pi_R \dot{R} + NR^2 \pi_R^2 = \pi_x \dot{x} + N \pi_x^2. \quad (4)$$

Thus the Hamiltonian of the model proposed here transforms, using (1) and (4), to

$$(\mp \pi_x)^2 = -144 R_0^4 e^{\pm 4x} + 12 \pi_\phi^2, \quad (5)$$

while Misner's Mixmaster universe Hamiltonian, 2.2(10), which is more accurately written as

$$(\mp \pi_\Omega)^2 = p_+^2 + p_-^2 + e^{\pm 4\Omega} (V-1),$$

can be transformed back to

$$(\pm \pi_R)^2 = \frac{p_+^2 + p_-^2}{R^2} + R^2 (V-1). \quad (6)$$

Misner's preference for his exponential time is due to his bias towards the superspace

approach : the exponential time looks very much like the "exponential" anisotropy parameters $\beta_\pm$. However it is precisely because R is a time parameter (and therefore not represented by a self-adjoint operator) that positivity of R is irrelevant. Thus there is no advantage, in principle of using an exponential time.

In practice, there is little advantage to using an exponential time. If R_0 (in (3)) is set equal to R_m , then the adjustment (by "hand") that is necessary at the moment of maximum expansion looks fairly "natural". This is because $R = R_m$ at $\Omega = 0$, so that changing the signs in front of π_Ω and Ω at $\Omega = 0$ amounts to just using $|\Omega|$ in the Schrodinger equation.

Neither does the adjustment that is made when the "radius" time is used look too forced: the sign of the Hamiltonian is reversed when it has its zero (This will become clear later.) at $R = R_m$. This corresponds to allowing transitions between positive and negative "energy" levels.

Because of the exponential functions that appear if exponential time is used, the equations are more complicated and so this time variable will not be used.

Since the radius, R , is positive semi-definite (with

$R = 0$ at the singularity), then it would be more natural quantum mechanically to choose R as the Hamiltonian than as the time. Then the conjugate time variable is π_R , because the Lagrangian, (1), may be rewritten as

$$L = \frac{d}{dt} (\pi_R R) - R \dot{\pi}_R + \pi_\phi \dot{\phi} + N \left(6kR + \frac{\pi_R^2}{24R} - \frac{\pi_\phi^2}{2R^3} \right),$$

or, since the total time derivative term doesn't affect the equations of motion it is omitted:

$$L = \pi_\phi \dot{\phi} - R \dot{\pi}_R + N \left(6kR + \frac{\pi_R^2}{24R} - \frac{\pi_\phi^2}{2R^3} \right). \quad (7)$$

That π_R is a suitable time parameter may be seen from examining the model parametrized by the Friedmann time. Using 3.2(2), 3.2(10), 3.2(25),

$$\left. \begin{aligned} \pi_R &= -12 \dot{R} , \\ R^2 &= R_m^2 \sin(2\sqrt{k}t) , \\ \pi_R &= -12\sqrt{k} R_m \frac{\cos(2\sqrt{k}t)}{\sin^{1/2}(2\sqrt{k}t)} . \end{aligned} \right\} \quad (8)$$

These equations show that the "extrinsic" time, π_R , increases steadily from $-\infty$ to $+\infty$ with $\pi_R = 0$ being the moment of maximum expansion.

Unfortunately the Hamiltonian is more complicated than with the other choices of time recommended here. From (7) and 3.2(9)

$$6kR^4 + \frac{\pi_R^2}{24} R^2 - \frac{C^2}{2} = 0, \quad (9)$$

i.e.

$$R^2 = \left(-\frac{t^2}{24} \pm \sqrt{\frac{t^4}{(24)^2} + 12kC^2} \right) \frac{1}{12k} \quad (10)$$

For $k > 0$, $R \geq 0$ and $C^2 \geq 0$, (10) implies that

$$R(t) = \left(\frac{\sqrt{\frac{t^4}{(24)^2} + 12kC^2} - \frac{t^2}{24}}{12k} \right)^{1/2} \quad (11)$$

Setting $\pi_R = \dot{t}$ gives a poor choice of time classically, because of the complications, not only in the Hamiltonian, $R(t)$, that it causes. The lapse function $N(t)$ is given (using 3.2(2)) by

$$N(t) = -12 \frac{dR^2}{dt}$$

and

$$\dot{\phi} = \frac{N \pi_{\phi}}{R^3}.$$

These equations are consistent and may be shown, by some tedious algebra which is omitted here, to give the same $\phi = \phi(R)$ as in the previous section.

This choice of time is called extrinsic because π_R is not a superspace variable. That is, π_R is not one of the variables used to describe the intrinsic geometry, but is conjugate to one such variable, R .

In all previous closed universe models an intrinsic time has been used, because of a bias towards the superspace philosophy. However extrinsic time has been used in Kuchař's model⁽⁴¹⁾ of the Einstein-Rosen cylindrical gravitational waves. (After his discussions about Dirac quantization, operator times and superspace, it is a relief to find that Kuchař really used canonical quantization!)

Since Kuchař's universe is open, the intrinsic or extrinsic curvature of the three-geometry does not carry complete information about time because the boundary conditions make a contribution⁽²⁸⁾. So the time, at some radial position r , is defined as

$$T(r) = T(\infty) + \int_{\infty}^r -\pi_r dr \quad (12)$$

where π_r is conjugate to $r(r)$ which is one of the superspace variables.

The important point in this case, as Kuchař stresses, is that the time T is an extrinsic (or momentum) variable (plus boundary condition) and not a superspace variable. The Hamiltonian appears linearly in the constraint equation and so gives rise to a Schrödinger

equation. Kuchař conjectured that, in general, this is an important feature of an appropriately chosen extrinsic time.

The model presented here provides a counterexample (for closed universes) to Kuchař's conjecture. The Hamiltonian, R , conjugate to the extrinsic time retains the usual features of closed universe Hamiltonians in that it is time dependent and appears in the constraint equation quadratically (not just simply squared, as in previous models using intrinsic time.)

The important advantage that the extrinsic time has over the intrinsic times is that it gives a well defined treatment to the whole dynamical development, with negative time being the expansion and positive time being the contraction phase of the universe.

In fact the extrinsic time is closely related to the "York"⁽¹⁹⁾ time, which occurs as a very natural choice of time if the structure of the initial value (or constraint) equations is considered. York's very important work is general for empty spaces and has not yet been used in model calculations because of the complicated form of the constraint equation. A fuller discussion will be deferred until chapter 5.

However it may be of interest to display the Lagrangian here. If

$$\gamma = R^3 \quad (13)$$

is chosen as the "York" Hamiltonian, then (1) and AII(40) give

$$L = \pi_\phi \dot{\phi} - \gamma \dot{\pi}_\gamma + N \left(6\hbar \gamma^{\frac{1}{2}} + \frac{3}{8} \gamma \pi_\gamma^2 - \frac{\pi_\phi^2}{2\gamma} \right) \quad (14)$$

Evidently the York Hamiltonian is more complicated than the extrinsic Hamiltonian.

The final choice of time to be considered is the most natural for this model, and is obtained by identifying the scalar field, ϕ with time. That ϕ can make a suitable

time can be checked by examining equations 3.2(25), 3.2(26), 3.2(31). With the "scalar" time there are no problems of ambiguity as the universe goes through its maximum of expansion.

The constraint (from (1)) may be rewritten as

$$(-\pi_\phi)^2 = 12\hbar R^4 + \frac{1}{12} R^2 \pi_R^2 . \quad (15)$$

Thus the "scalar" Hamiltonian is a time independent "square root Hamiltonian. Because of the time independence, this choice is to be preferred (despite the absence of a "natural" factor ordering - this is discussed in chapter 4 section1).

The scalar time is a type of extrinsic time. This is because the scalar field appears in the field equations (3.2(4), 3.2(5) with $m = 0$) only as $\frac{\phi}{N}$ and so the "pions" are tuned to the local proper time.

This exhibits the close relationship between the model presented in this thesis and DeWitt's⁽²⁸⁾ "quantum" Friedmann model which is filled with dust. The latter model is too simple: there is just the one parameter, R . To correct this situation, DeWitt allows the dust to have (unspecified) coherent degrees of freedom which are tuned to the local proper time, which is, naturally, extrinsic. However, while the details of DeWitt's model are obscure, the model presented here is simple and clear.

It should be remarked that from a purist's point of view, the observables for some measurement should be chosen first and then these variables assigned self-adjoint operators. In the absence of such a measurement theory, particle physics prejudice indicates that π_ϕ and ϕ should be observables and so ϕ would not be chosen as a time variable. However this simple model shows that it is possible to use a (potentially quantized) matter field variable as the time.

CHAPTER 4. THE MODEL: QUANTIZATION

4.1 Quantization with Scalar Time

The classical Hamiltonian to be quantized is $-\pi_{\phi}$ and its explicit expression is, (from 3.3(15))

$$H^2 = 12 \kappa R^4 + \frac{1}{12} R^2 \pi_R^2. \quad (1)$$

Since ϕ is a good choice of time and H is time independent, the Schrodinger equation

$$\hat{H}(\hat{R}, \hat{\pi}_R) \psi_E(R, t) = E \psi_E(R, t) \quad (2)$$

may be used. The wave function can be separated:

$$\psi_E(R, t) = R_E(R) T_E(t), \quad (3)$$

where

$$T_E(t) = e^{-iEt/\hbar} \quad (4)$$

and

$$\hat{H}(\hat{R}, \hat{\pi}_R) R_E(R) = E R_E(R). \quad (5)$$

Now the Hamiltonian appears in (1) squared. The positive square root of $\hat{H}^2$ may be defined⁽⁸⁰⁾ by using its spectral decomposition, provided that $\hat{H}^2$ is self adjoint so that it possesses a spectral decomposition.

More simply, this means that instead of trying to solve (5) directly, attention may be focussed on

$$\hat{H}^2(\hat{R}, \hat{\pi}_R) R(R) = E^2 R(R), \quad (6)$$

where the positive square of E^2 is used in (4).

The usual (Heisenberg) form of the canonical commutation relation for this one dimensional problem is

$$[\hat{\pi}_R, \hat{R}] = -i\hbar. \quad (7)$$

The "momentum" operator is written as

$$\hat{\pi}_R = -i\hbar \frac{d}{dR} \quad (8)$$

and Lebesgue measure, with respect to R , is used for the inner products of the Hilbert space. Unfortunately because R is bounded, the momentum operator in (8) can not be self-adjoint (see the discussion in chapter 0, section 2). This difficulty is usually avoided (and will be done so in this thesis) by finding the self-adjoint Hamiltonian and defining the self-adjoint momentum operator in terms of (for example, a square root of) the Hamiltonian. Until an expression is found for the Hamiltonian (squared) operator in (15), expressions such as $\hat{\pi}_R \hat{R}^2 \hat{\pi}_R$ will be used with (8) instead of the expression $\hat{\pi}_R \hat{R}^2 \hat{\pi}_R^\dagger$. The difference is essentially one of domains.

The immediate problem is the usual factor ordering problem of quantization. This arises because the combination $R^2 \pi_R^2$ may be written in an infinite number of inequivalent ways in the quantum theory, and the usual quantization rules have nothing to say about the choice to be made. Some of the obvious choices will now be expressed in terms of the choice $\widehat{\pi_R R^2 \pi_R}$ that will be made here. For the following operator algebra the "hat" notation will be suspended to avoid an onslaught of "hats".

The symmetrized factor ordering is $\frac{1}{2}(\pi_R^2 R^2 + R^2 \pi_R^2)$. It is easy to show, using (7), that

$$\frac{1}{2}(\pi_R^2 R^2 + R^2 \pi_R^2) = \pi_R R^2 \pi_R - \hbar^2 \quad (9)$$

The other obvious choices may be parametrized by ν as $R^\nu \pi_R^{2-\nu} \pi_R R^\nu$. Now, using (8),

$$\begin{aligned} [\pi_R, R^\nu] &= -i\hbar \left[\frac{d}{dR}, R^\nu \right] \\ &= -i\hbar \nu R^{\nu-1}. \end{aligned} \quad (10)$$

It can be shown, by commuting factors and using (10), that

$$R^\nu \pi_R R^{2-2\nu} \pi_R R^\nu = \pi_R R^2 \pi_R + \hbar^2 \nu(\nu-1). \quad (11)$$

The quantum equation will be chosen to be, from (1) and (6),

$$(12\hbar R^4 + \frac{1}{12} \pi_R R^2 \pi_R - E^2) \mathcal{R}(R) = 0. \quad (12)$$

It is clear that the other obvious factor orderings merely rescale the "energy". For example, using (11),

$$(12\hbar R^4 + \frac{1}{12} R^\nu \pi_R R^{2-2\nu} \pi_R R^\nu - \nu E^2) \mathcal{R}(R) = 0 \quad (13)$$

which leads to

$$\nu E^2 = E^2 + \hbar^2 \nu(\nu-1). \quad (14)$$

So the differential equation to be solved is from (8) and (12),

$$\left[\frac{d}{dR} \left(R^2 \frac{d}{dR} \right) + \frac{12E^2 - 144\hbar R^4}{\hbar^2} \right] \mathcal{R}_E(R) = 0. \quad (15)$$

i.e.

$$\left[R^2 \frac{d^2}{dR^2} + 2R \frac{d}{dR} + \left(\frac{12E^2}{\hbar^2} - \frac{144\hbar}{\hbar^2} R^4 \right) \right] \mathcal{R}(R) = 0. \quad (16)$$

With the help of Bateman⁽⁸¹⁾, this can be solved. First transform (16) by defining

$$\mathcal{R} = R^2, \quad (17)$$

which gives

$$\left[\frac{d^2}{d\mathcal{R}^2} + \frac{3}{2} \frac{1}{\mathcal{R}} \frac{d}{d\mathcal{R}} + \left(-\frac{36\hbar}{\hbar^2} + \frac{3E^2}{\hbar^2} \cdot \frac{1}{\mathcal{R}^2} \right) \right] \mathcal{R} = 0. \quad (18)$$

The solution of this equation can be written as

$$\mathcal{R} = \mathcal{R}^{-3/4} w(0, \mu, \xi) \quad (19)$$

where

$$\mu = \frac{1}{2} \sqrt{\frac{1}{4} - \frac{12E^2}{\kappa^2}}, \quad (20)$$

$$\xi = \frac{12\sqrt{\kappa}}{\kappa} z, \quad (21)$$

and $w(K, \mu, \xi)$ is an arbitrary solution of the Whittaker equation.

Two linearly independent solutions of the Whittaker equation are given⁽⁸²⁾ by

$$M_{0, \pm\mu}(\xi) = \xi^{\pm\mu - \frac{1}{2}} e^{-\xi/2} \Phi(\pm\mu + \frac{1}{2}, \pm 2\mu + 1, \xi), \quad (22)$$

where $\Phi(a, c; \xi)$ is the confluent hypergeometric function, which is regular and normalized to unity at $\xi = 0$, but undefined if c is an integer. Since 2μ either lies between 0 and $\frac{1}{2}$ or is purely imaginary, these are good solutions, except for $\mu = 0$. These solutions are useful for looking at the behaviour near the singularity. Within multiplicative constants, these two independent solutions (excepting only when $\mu = 0$) are

$$R_{\pm\mu}(R) = R^{\pm 2\mu - \frac{1}{2}} e^{-\frac{6\sqrt{\kappa} R^2}{\kappa}} \Phi(\pm\mu + \frac{1}{2}, \pm 2\mu + 1, \frac{12\sqrt{\kappa} R^2}{\kappa}). \quad (23)$$

Near the singularity, these are

$$R_{\pm\mu}(R) = R^{\pm 2\mu - \frac{1}{2}}, \quad (24)$$

which are irregular at $R = 0$ except for the

$$R_{\mu=\frac{1}{2}}(R) = 1 \quad (25)$$

solution.

It should be noted that regularity of wave functions in quantum mechanics is not required. Consider, for example, a wave function $\frac{1}{\sqrt{z}} R^{-\frac{1}{2}}$ belonging to $L^2(0, 1)$ which is irregular

at $R = 0$. This does not mean that the quantum mechanical probability of being at $R = 0$ is infinite. Instead, the probability of finding the particle in the neighbourhood of $R = 0$ should be asked for :

$$\int_0^\epsilon \frac{1}{3} R^{-2/3} dR = \epsilon^{1/3} \rightarrow 0 \text{ as } \epsilon \rightarrow 0.$$

In fact this is always guaranteed for all physical wave functions: the general theory of Lebesgue integration implies that for all function, $f(R)$, belonging to $L^2(0,1)$

$$\lim_{\epsilon \rightarrow 0} \int_0^\epsilon |f(R)|^2 dR = 0.$$

In this problem $R = 0$ is the singularity. DeWitt has conjectured⁽²⁸⁾ that the boundary condition requiring the wave function to vanish on the singular three-geometries should avoid the classical collapse problem. It has already been pointed out that if the singular three-geometry is part of a continuous spectrum, this is not sufficient and the problem requires further analysis. However it is clear that there are no eigenfunctions for the present problem which satisfy DeWitt's boundary condition.

So if boundary conditions are to be imposed on the eigenfunctions, they must apply at some $R \neq 0$. To study this, the Whittaker solutions are better written in terms of two linearly independent Bessel functions⁽⁸³⁾ :

$$W_{0,\mu}(\pm \xi) = \sqrt{\frac{\xi}{\pi}} K_\mu\left(\pm \frac{\xi}{2}\right). \quad (26)$$

This means that the two linearly independent solutions can be written, within multiplicative constants, using (19), (21) and (26), as

$$R = R^{-1/2} K_\mu\left(\pm \frac{6\sqrt{k}}{\hbar} R^2\right). \quad (27)$$

Since the maximum that the radius R has classically occurs dynamically, then the logical choice (following that for the harmonic oscillator) is not to impose

any boundary condition because it would be artificial. That is, the Hilbert space is taken as $L^2(0, \infty)$.

Now the asymptotic form of the Bessel functions is⁽⁸⁴⁾

$$K_\mu(z) \sim \sqrt{\frac{1}{2} \frac{\pi}{z}} e^{-z}, \quad (28)$$

which means that only

$$R = R^{-1/2} K_\mu \left(+ \frac{6\sqrt{k}}{k} R^2 \right) \quad (29)$$

may belong to $L^2(0, \infty)$.

Naturally, for this to be the wave function, self-adjointness of the $\hat{H}^2$ operator (from (15))

$$\hat{H}^2 = 12k R^4 - \frac{k^2}{12} \frac{d}{dR} \left(R^2 \frac{d}{dR} \right) \quad (30)$$

is required. This is difficult to prove, but the result can be obtained from using Dunford and Schwartz⁽⁸⁵⁾.

Rather than attempt to prove it directly, an attempt can be made to produce the orthogonality relations (since these amount to a resolution of the identity).

One of the orthogonality relations would be obtained, using (29), as

$$\Delta_{\mu, \nu} = \int_0^\infty R^{-1} K_\mu \left(\frac{6\sqrt{k}}{k} R^2 \right) K_\nu \left(\frac{6\sqrt{k}}{k} R^2 \right) dR. \quad (31)$$

$$\text{Setting } \frac{6\sqrt{k}}{k} R^2 = u \quad (32)$$

$$\epsilon \Delta_{\mu, \nu} = 2 \int_0^\infty K_\mu(u) K_\nu(u) u^{-1+\epsilon} du, \quad (33)$$

where ϵ is a parameter which is to be set equal to zero at a later stage. This integral exists and can be evaluated⁽⁸⁶⁾ in terms of a hypergeometric function and gamma functions as

$$\epsilon \Delta_{\mu, \nu} = \frac{2^{-2+\epsilon}}{\Gamma(\epsilon)} \Gamma\left(\frac{\mu+\nu+\epsilon}{2}\right) \Gamma\left(-\frac{\mu+\nu+\epsilon}{2}\right) \Gamma\left(\frac{\mu-\nu+\epsilon}{2}\right) \Gamma\left(-\frac{\mu-\nu+\epsilon}{2}\right) \\ \cdot F\left(\frac{\mu+\nu+\epsilon}{2}, -\frac{\mu+\nu+\epsilon}{2}; \epsilon; 0\right) \quad (34)$$

provided that

$$\epsilon > |\operatorname{Re} \mu| + |\operatorname{Re} \nu|. \quad (35)$$

Thus $\Delta_{\mu, \nu}$ exists in a distribution theoretic sense, as a Dirac delta function. (This is guaranteed by the general Weyl-Kodaira Spectral Theory.)

It is clear that the "solution", (29), on $L^2(0, \infty)$ can not be square integrable and so μ has no point spectrum. Also $\Delta_{\mu, \nu}$ can only exist in a distribution sense if it can be written as

$$\Delta_{\mu, \nu} = \lim_{\epsilon \rightarrow 0} \epsilon \Delta_{\mu, \nu}.$$

From (35), this is not possible if either μ or ν has a real part, so μ may only have a purely imaginary continuous spectrum.

At this stage it may be prudent to see whether some simplification can be made. The obvious thing to do is to impose some kind of reflection condition at $R = R_m$ so that the Hilbert space is constructed on a bounded interval, viz $0 \leq R \leq R_m$. This means that, since $\mathbb{R}^4$ is now bounded, self adjointness of

$$\hat{O} = -\frac{d}{dR} \left(R^2 \frac{d}{dR} \right)$$

implies⁽⁸⁷⁾ self-adjointness of $\hat{H}^2$. This is a much simpler problem to handle, and so the operator $\hat{O}$ will now be considered on the space $L^2(0, 1)$ since the value of R_m merely scales the problem.

4.2. Unitary Transform of the Problem

The operator of interest is

$$\hat{O} \psi = -\frac{d}{dR} \left(R^2 \frac{d\psi}{dR} \right),$$

defined on $L^2(0,1)$. A "change of coordinate" from R to e^{-x} gives a new Hilbert space $L^2(0,\infty)$. This can be obtained by the mapping

$$U: L^2(0,1) \rightarrow L^2(0,\infty),$$

$$\psi \mapsto (U\psi)(x) = e^{-x/2} \psi(e^{-x}).$$

Denote the scalar product in $L^2(0,\infty)$ by $(\cdot, \cdot)_\infty$ and in $L^2(0,1)$ by $(\cdot, \cdot)_1$.

It is easy to prove that the mapping U is unitary:

$$\begin{aligned} (U\psi, U\psi)_\infty &= \int_0^\infty e^{-x} \psi^*(e^{-x}) \psi(e^{-x}) dx \\ &= - \int_1^0 \psi^*(R) \psi(R) dR \\ &= \int_0^1 \psi^*(R) \psi(R) dR \\ &= (\psi, \psi)_1 \end{aligned}$$

Now if $\chi \in L^2(0,\infty)$, then

$$(U^{-1}\chi)(R) = R^{-1/2} \chi(-\log R),$$

so

$$\begin{aligned} (U \hat{O} U^{-1}\chi)(x) &= -U\left(\frac{d}{dR} R^2 \frac{d}{dR} \frac{\chi(-\log R)}{R^{1/2}}\right) \\ &= -U\left(\frac{d}{dR} R^2 \left\{-\frac{1}{2} R^{-3/2} \chi(-\log R) + R^{-1/2} \chi'(-\log R) \cdot \frac{-1}{R}\right\}\right) \\ &= U\left(\frac{d}{dR} R^{1/2} \left\{\frac{\chi(-\log R)}{2} + \chi'(-\log R)\right\}\right) \\ &= U\left(\frac{1}{2} R^{-1/2} \left\{\frac{\chi(-\log R)}{2} + \chi'(-\log R)\right\} + R^{1/2} \left\{-\frac{\chi'(-\log R)}{2R} - \frac{\chi''(-\log R)}{R}\right\}\right) \\ &= \frac{1}{4} R^{-1/2} \chi(-\log R) - R^{-1/2} \chi''(-\log R) \\ &= \left(\frac{1}{4} - \frac{d^2}{dx^2}\right) \chi(x). \end{aligned}$$

That is, the formal unitary transform of the operator is

$$U \hat{O} U^{-1} = -\frac{d^2}{dx^2} + \frac{1}{4}.$$

All the properties of $\hat{O}$ can be deduced from this relation. In particular, $\hat{O}$ has various self-adjoint extensions. It is easier to transcribe the statements about $\hat{O}$ and its domain $\mathcal{D}_{\hat{O}}$ into those about $U \hat{O} U^{-1}$ and $\mathcal{D}_{U \hat{O} U^{-1}}$. The spectrum, $\sigma_{\hat{O}}$ of the operator $\hat{O}$ is given by

$$\sigma_{\hat{O}} = \sigma_{-\frac{d^2}{dy^2}} + \frac{1}{4}$$

where $\mathcal{D}(-\frac{d^2}{dy^2})$ is chosen as above. A complete description of this operator and its spectrum is found in the encyclopedic text by Dunford and Schwartz⁽⁸⁵⁾.

The condition that $\psi'(1) = 0$ in $L^2(0,1)$ transcribes as follows: Let $\varphi \in L^2(0,\infty)$ such that $\varphi = U\psi$, that is

$$\varphi(x) = (U\psi)(x) = e^{-x/2} \psi(e^{-x}),$$

$$\psi(e^{-x}) = e^{x/2} \varphi(x).$$

Differentiating this relation with respect to x gives

$$-e^{-x} \psi'(e^{-x}) = e^{x/2} (\varphi'(x) + \frac{1}{2} \varphi(x)).$$

$$\text{i.e.} \quad -\psi'(1) = \varphi'(0) + \frac{1}{2} \varphi(0),$$

so the transcribed boundary condition is

$$2\varphi'(0) + \varphi(0) = 0.$$

For this case, $-\frac{d^2}{dx^2}$ has a point spectrum, σ_{pp} , of $-\frac{1}{4}$ with eigenfunction $\exp(-\frac{x}{2})$, which transcribes back to $\psi(R) = 1$. The continuous spectrum, σ_{cc} , of $-\frac{d^2}{dy^2}$ is $(0,\infty)$. Thus

$$\sigma_{pp}(\hat{O}) = \{0\} \quad (\psi_0 = 1)$$

$$\sigma_{cc}(\hat{O}) = (\frac{1}{4}, \infty).$$

The other natural boundary condition in $L^2(0,1)$ is $\psi(1)=0$, which transcribes to $\varphi(0)=0$. In this case the operator $-\frac{d^2}{dx^2}$ has no point spectrum and a continuous spectrum of $(0,\infty)$.

It is apparent that the boundary conditions have to be imposed at $R = 1$ and not $R = 0$ because the natural (unitarily equivalent) "standard" space of the problem uses $0 \leq x < \infty$ where $R = 1$ corresponds to $x = 0$.

4.3 Simplified Model

In the section on quantization of the full problem with scalar time, it was seen that the logical Hilbert space to use is $L^2(0,\infty)$. Unfortunately the wavefunctions for the full problem are complicated and so a simplification is sought.

Self-adjointness has been proven (in the last two sections) for $\hat{H}$ on $L^2(0,R_m)$. However it was noted previously (in chapter 3, section 2) that the occurrence of a maximum of expansion classically is due entirely to the presence of the curvature term. Clearly there is some redundancy in considering the full problem's Hamiltonian with an imposed reflection condition at $R = R_m$.

Thus it is proposed that the curvature term be dropped, since it can be seen classically (from 3.3(2), remembering that π_ϕ is a constant) that the curvature does not play a role in the neighbourhood of the singularity. (In fact this is the approximation made by Liang et al⁽⁶⁷⁾ in their study of a class of models near the singularity, and the starting point of Liang's "quantum" model.) The imposition of a boundary condition at $R = R_m$ now makes more sense since it will mean that the "maximum expansion" still occurs, in an approximate manner, even without the curvature term. The choice of $R = 1$ will be made for simplicity since it merely rescales the problem. (In fact R_m can be taken as part of the Cauchy data for the full classical problem.)

The quantum equation now becomes 4.1(16) with $k = 0$

$$R^2 \frac{d^2}{dR^2} R + 2R \frac{dR}{dR} + \frac{12E^2}{\hbar^2} R = 0. \quad (1)$$

The spectral properties of this differential equation are known rigorously and have been set out in the previous section. However the more usual physicists approach via the orthogonality properties will be taken here. This will be of use in studying the time evolution.

Equation (1) may easily be solved by using the substitution $R = R^\eta$ which gives the indicial equation

$$\eta^2 - \eta + 2\eta + \frac{12E^2}{\hbar^2} = 0,$$

having the solution

$$\begin{aligned} \eta &= -\frac{1}{2} \pm \frac{1}{2} \sqrt{1 - \frac{48E^2}{\hbar^2}} \\ &= -\frac{1}{2} \pm 2\mu, \end{aligned}$$

where

$$2\mu = \sqrt{\frac{1}{4} - \frac{12E^2}{\hbar^2}} \quad (2)$$

which is the same μ as in section 1 of this chapter. Thus the linearly independent solutions of (1) are

$$R = R^{-\frac{1}{2} \pm 2\mu}, \quad (3)$$

except when $\mu = 0$. But it will be seen that $\mu = 0$ is a single point of the continuous spectrum, and so, for the sake of simplicity, this subtlety will be ignored.

It is reassuring to notice that the solutions(3) do accurately reproduce the behaviour near the singularity since they are just the equations 4.1(24) which are the general solutions restricted to small R .

It is interesting to consider which, if any of the solutions(3) are square integrable. The only possibility

is the $\mu = \frac{1}{4}$ solution:

$$R_{\mu=\frac{1}{4}}(R) = 1 \quad (4)$$

(which is the only eigenfunction that is regular at $R = 0$, as was discussed in section 1 of this chapter). This solution is square integrable because the R variable is now bounded.

This means that the only possible discrete point of the μ spectrum is at $\mu = \frac{1}{4}$. (This conclusion can be seen to be rigorous by the results of the previous section.) But this corresponds, from (2), to setting $E = 0$, that is, considering an empty universe. This is Misner's⁽¹⁸⁾ $R - W$ "quantum puff" universe which was discussed in chapter 2, section 3. The importance of its appearance here is that it can now be given a legitimate interpretation, and must be considered just as real as the other possible universes represented in the μ spectrum, despite the fact that it can not exist classically.

It must be stressed that the eigenfunction in this simplified model is quite different from Misner's "eigenfunction", even though the general model solution, equation 4.1(29), obtained earlier is essentially the same. However it has been shown in chapter 4, section 1 that μ may only have a purely imaginary continuous spectrum; that is the empty space solution $\mu = \frac{1}{4}$ does not occur. Thus Misner's argument supporting the foamlike structure of geometrodynamics at the Planck length can not be regarded as validated, except for the present simplified model.

The appearance of the empty universe depends on the boundary conditions. The possible boundary conditions that can be imposed may be written as

$$a R(1) + b R'(1) = 0 \quad (5)$$

It is clear from (4) and (5) that the empty universe solution only appears if the usual reflection condition of quantum mechanics is taken, namely that the first

derivative of the wave function vanishes at the boundary.

In this problem, it turns out that an easier boundary condition to use is the vanishing of the eigenfunction at the boundary. This is because in this case it has already been shown rigorously in the last section that μ has a semi-infinite purely imaginary spectrum. A clear indication of this can be found in the orthogonality relations approach that is more used by physicists and will be demonstrated here. The empty universe solution will not be considered any further here since this simpler boundary condition will be imposed.

Firstly, some more notation will be required:

$$x = -\log R, \quad R = e^{-x}, \quad (6)$$

and

$$\lambda = i2\mu = \sqrt{\frac{12E^2}{R^2} - \frac{1}{4}}. \quad (7)$$

The eigenfunctions satisfying the boundary condition are constant multiples of

$$\begin{aligned} R_\lambda(R) &= R^{-\frac{1}{2}+2\mu} - R^{-\frac{1}{2}-2\mu} \\ &= R^{-\frac{1}{2}-i\lambda} - R^{-\frac{1}{2}+i\lambda} \end{aligned} \quad (8)$$

$$= R_\lambda(x) = e^{x/2} [e^{i\lambda x} - e^{-i\lambda x}] \quad (9)$$

$$= 2i e^{x/2} \sin \lambda x. \quad (10)$$

These wave functions satisfy orthogonality relations:

$$\begin{aligned} \int_0^1 R_\sigma^*(R) R_\lambda(R) dR &= \int_{-\infty}^0 R_\sigma^*(x) R_\lambda(x) \cdot e^{-x} dx \\ &= \int_0^\infty R_\sigma^*(x) R_\lambda(x) e^x dx \end{aligned} \quad (11)$$

$$\begin{aligned}
\int_0^1 R_\sigma^*(R) R_\lambda(R) dR &= \int_0^\infty [e^{-i\sigma^* x} - e^{+i\sigma^* x}] [e^{i\lambda x} - e^{-i\lambda x}] dx \\
&= \int_0^\infty dx [e^{i(\lambda - \sigma^*)x} + e^{i(\sigma^* - \lambda)x} - e^{i(\lambda + \sigma^*)x} - e^{-i(\lambda + \sigma^*)x}] \\
&= \int_{-\infty}^\infty [e^{i(\lambda - \sigma^*)x} - e^{i(\lambda + \sigma^*)x}] dx \\
&= \begin{cases} 2\pi \delta(\sigma - \lambda) - 2\pi \delta(\sigma + \lambda) & \text{if } \lambda, \sigma \in \mathbb{R} \\ \text{if } \lambda, \sigma \notin \mathbb{R} \end{cases} \quad (12)
\end{aligned}$$

This result means that the $R_\lambda(R)$ are not square integrable and implies that the spectrum of λ is real. Since the wave function uses solutions with both signs of λ , to avoid double counting, λ is restricted to

$$\lambda \in \mathbb{R}^+, \quad (13)$$

(which is the correct result given rigorously in the last section).

So this orthogonality relation, (12), can be written as,

$$\int_0^1 R_\sigma^*(R) R_\lambda(R) R dR = 2\pi \delta(\sigma - \lambda) - 2\pi \delta(\sigma + \lambda) \quad (14)$$

This is not quite the correct orthogonality relation because of the two delta functions on the right hand side of (14). However it is clear that because of the range of σ and λ the second delta function can not contribute, except when σ and λ are both zero.

This is the result of ignoring the fact that the solutions, (3), of the quantum equation of motion are only linearly independent for non zero values of the spectrum. This then implies (wrongly) that the solutions $R_\lambda(R)$ constructed from the solutions (3) such that the boundary condition is satisfied, vanish for $\lambda=0$. So it

is clear that the correct orthogonality relation only has $2\pi\delta(\sigma-\lambda)$ as its right hand side and can be written as

$$\int_0^1 R_\sigma^*(R) R_\lambda(R) dR \doteq 2\pi\delta(\sigma-\lambda) \quad (15)$$

By using the notation

$$S = e^{-y}, \quad (16)$$

and (9), the other orthogonality relation may be obtained as follows:

$$\begin{aligned} \int_0^\infty R_\lambda^*(R) R_\lambda(S) d\lambda &= e^{\frac{x+y}{2}} \int_0^\infty (e^{-i\lambda x} - e^{i\lambda x})(e^{-i\lambda y} - e^{i\lambda y}) d\lambda \\ &= e^{\frac{1}{2}(x+y)} \int_{-\infty}^\infty (e^{i\lambda(x-y)} - e^{i\lambda(x+y)}) d\lambda \\ &= e^{\frac{1}{2}(x+y)} 2\pi [\delta(x-y) - \delta(x+y)]. \quad (17) \end{aligned}$$

The relationship between R and x , given in (6), implies that

$$0 \leq R \leq 1 \quad \text{for} \quad \infty \geq x \geq 0, \quad (18)$$

so that the second delta function in (17) merely disallows any contribution at $x = 0$. But this is the boundary, where all wavefunctions must vanish because of the boundary condition. With this complication in mind, (17) will be rewritten as

$$\int_0^\infty R_\lambda^*(R) R_\lambda(S) d\lambda \doteq 2\pi e^y \delta(x-y). \quad (19)$$

It is now simple to use the relation (easily proved by the appropriate integrations of a test function)

$$\delta(\log R - \log S) = S \delta(R-S), \quad (20)$$

to give

$$\int_0^\infty R_\lambda^*(R) R_\lambda(S) d\lambda \doteq 2\pi \delta(R-S). \quad (21)$$

(Note that the term missing from the right hand side of (21) is not $\delta(R+S)$ which would subtract contributions at the singularity, but a term equivalent to $\delta(R+S-2)$ which makes a cancellation at the boundary.)

Since the spectrum of λ is continuous the $R_\lambda(R)$ are not square integrable and so lie outside the simple $L^2(0,1)$ space. Physical wave functions lying in $L^2(0,1)$ are constructed as wave packets, $w(R)$, defined by

$$w(R) = \int_0^\infty f(\lambda) R_\lambda(R) d\lambda. \quad (22)$$

This relation can be inverted because of the orthogonality relations, (15), to give

$$\begin{aligned} \int_0^1 R_\sigma^*(R) w(R) dR &= \int_0^1 R_\sigma^*(R) \int_0^\infty f(\lambda) R_\lambda(R) d\lambda dR \\ &= \int_0^\infty f(\lambda) \int_0^1 R_\sigma^*(R) R_\lambda(R) dR d\lambda \\ &= \int_0^\infty f(\lambda) 2\pi \delta(\sigma-\lambda) d\lambda \\ &= 2\pi f(\sigma). \end{aligned} \quad (23)$$

To build a wave packet, an obvious choice for the weight is the Gaussian form

$$f(\lambda) = e^{-a\lambda^2}, \quad a > 0. \quad (24)$$

Then, using (10) and (22),

$$\begin{aligned} w(R) &= \int_0^\infty e^{-a\lambda^2} 2i e^{x/2} \sin \lambda x d\lambda \\ &= 2i e^{x/2} \int_0^\infty e^{-a\lambda^2} \sin \lambda x d\lambda. \end{aligned}$$

The integral may be evaluated⁽⁸⁸⁾ to give

$$w(R) = i \frac{x}{a} e^{x/2} e^{-\frac{x^2}{4a}} \Phi\left(\frac{1}{2}, \frac{3}{2}; \frac{x^2}{4a}\right) \quad (25)$$

This wave packet can be seen to be irregular at the singularity by using the relation⁽⁸⁹⁾

$$\Phi(a, c; z) = \frac{\Gamma(c)}{\Gamma(a)} e^{-z} z^{a-c} [1 + O(|z|^{-1})] \text{ as } z \rightarrow \infty$$

giving

$$\begin{aligned} \omega(x) &= i \frac{x}{a} e^{x/2} e^{-x^2/4a} \frac{\Gamma(3/2)}{\Gamma(1/2)} e^{x^2/4a} \cdot \frac{4a}{x^2} [1 + O(x^{-2})] \\ &= 4i \frac{\Gamma(3/2)}{\Gamma(1/2)} \frac{e^{x/2}}{x} [1 + O(x^{-2})] \\ &\rightarrow \infty \text{ as } x \rightarrow \infty \end{aligned}$$

However regularity at a point is not important (see the discussion following 4.1(25)). All that is required is that the wave packet $\omega(x)$ is square integrable. This can be seen by considering the form of the confluent hypergeometric function near the origin and near infinity:

$$(\omega(x), \omega(x)) = \int_0^\infty e^{-x} |\omega(x)|^2 dx = \int_0^\infty \frac{x^2}{a^2} e^{-x^2/2a} \Phi^2\left(\frac{1}{2}, \frac{3}{2}; \frac{x^2}{4a}\right) dx$$

The integrand goes as

$$\frac{x^2}{a^2} e^{-x^2/2a} \text{ near } x = 0$$

$$16 \frac{\Gamma^2(3/2)}{\Gamma^2(1/2)} \frac{1}{x^2} \text{ near } x = \infty$$

and so the integral is convergent.

Another wave packet that can be constructed using as its weight function $f(\lambda)$, where

$$f(\lambda) = e^{-a\lambda^2} \sin b\lambda, \quad a, b > 0. \quad (26)$$

This gives

$$\omega(x) = 2i e^{x/2} \int_0^\infty e^{-a\lambda^2} \sin b\lambda \sin x\lambda d\lambda$$

which may be evaluated⁽⁸⁸⁾ as

$$\omega(x) = \frac{i}{2} \sqrt{\frac{\pi}{a}} e^{x/2} \left\{ e^{-\frac{(x-b)^2}{4a}} - e^{-\frac{(x+b)^2}{4a}} \right\}. \quad (27)$$

It is clear the $\omega(x)$ given in (27) is square integrable and

regular everywhere. In particular, it is interesting to note that it vanishes at the singularity.

Now the defining relation, (22), of the wave packet provides a spectral decomposition (with respect to the spectrum of the $\hat{H}$) and so the time development is given by the simple formula

$$\begin{aligned}\psi(R, t) &= e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \psi(R, t_0) \\ &= e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \omega(R) \\ &= \int_0^\infty e^{-\frac{i}{\hbar} E_\lambda(t-t_0)} f(\lambda) R_\lambda(R) d\lambda\end{aligned}\quad (28)$$

where, from (7),

$$E_\lambda^2 = \frac{\hbar^2}{12} \left(\lambda^2 + \frac{1}{4} \right), \quad (29)$$

and the wave packet, $\omega(R)$ was constructed at the initial time t_0 which will now be set equal to zero

Because of the form of (29), it is extremely difficult to perform the integral of (28) in practice. To have a tractable problem, the time dependence of a delta function "wave packet" will be considered instead of the good wave packets constructed in (25) and (27). By using (21),

$$\omega = 2\pi \delta(R-R_0) \quad (30)$$

$$= \int_0^\infty R_\lambda^*(R_0) R_\lambda(R) d\lambda \quad (31)$$

giving

$$f(\lambda) = R_\lambda^*(R_0).$$

Thus

$$\begin{aligned}\psi(R, t) &= \int_0^\infty e^{iEt/\hbar} R_\lambda^*(R_0) R_\lambda(R) d\lambda \\ &= 4e^{\frac{i}{2}(x_0+x)} \int_0^\infty e^{iEt/\hbar} \sin \lambda x_0 \sin \lambda x d\lambda\end{aligned}$$

$$\psi(R,t) = e^{\frac{i}{2}(x_0+x)} \int_0^\infty \exp\left(\frac{i\tau}{2\sqrt{3}} \sqrt{\lambda^2 + \frac{1}{4}}\right) \cdot [\cos \lambda(x-x_0) - \cos \lambda(x+x_0)] d\lambda. \quad (32)$$

The term of the integrand involving the $\cos \lambda(x+x_0)$ is just the boundary correction term discussed before and should only contribute when $x_0 = 0$, providing a cancellation at the boundary for all times! So consider the integral, I , where essentially

$$\psi(R,t) = 2 e^{\frac{i}{2}(x_0+x)} I \quad (33)$$

and

$$I = \int_0^\infty e^{i\tau \sqrt{\lambda^2 + a^2}} \cos \lambda X d\lambda \quad (34)$$

with

$$\left. \begin{aligned} \tau &= \frac{1}{2\sqrt{3}} t, \\ a &= \frac{1}{2}, \\ X &= x - x_0. \end{aligned} \right\} \quad (35)$$

But (34) does not exist, except in a distribution theoretic sense as

$$I = \lim_{\epsilon \rightarrow 0+} \epsilon I, \quad (36)$$

where

$$\epsilon I = \int_0^\infty e^{(\epsilon + i\tau) \sqrt{\lambda^2 + a^2}} \cos \lambda X d\lambda$$

The integral ϵI exists for

$$X \neq 0; \operatorname{Re} a, \operatorname{Re} \epsilon > 0,$$

and is given explicitly as⁽⁹⁰⁾

$$\epsilon I = \frac{a(\epsilon + i\tau)}{\sqrt{X^2 + (\epsilon + i\tau)^2}} K_1 \left[a \sqrt{X^2 + (\epsilon + i\tau)^2} \right] \quad (37)$$

For $\tau = 0$, the distribution is the initial delta function with the "wave function" concentrated at the one point, viz x_0 . Now the K_0 Bessel function is regular everywhere except when its argument becomes zero, so the role of ϵ in (37) is clearly that of preventing the irregularity. So the "wave function" is concentrated at the points where

$$x^2 - \tau^2 = 0 \quad (38)$$

which, by using (35), is

$$x = x_0 \pm \frac{1}{2\sqrt{3}} \tau, \quad (39)$$

or

$$\log \frac{R_0}{R} = \pm \frac{1}{2\sqrt{3}} \tau. \quad (40)$$

From (39), it is clear that the quantization does not stop the universe from evolving to its classically inevitable collapse.

Since the Planck constant does not appear in (40), it is interesting to see whether this reproduces a classical solution. Since the model considered in this section is mathematically just an ordinary quantum mechanical problem, then Ehrenfest's theorem⁽⁶⁶⁾ should apply. Thus, despite the use of a formal argument (with a delta function "wave packet") it is expected that (40) does represent a classical solution.

This classical solution can be derived by solving 3.2(11) and 3.2(15) for $k = 0$, giving precisely (40). The solutions are

$$R^2 = at + b$$

$$\dot{\phi} = \frac{c}{R^2}$$

where

$$a^2 = \frac{1}{3} c^2.$$

Thus

$$\begin{aligned}\phi &= \frac{c}{a} \log R^2 + \phi_0 \\ &= \pm \sqrt{3} \log R^2 + \phi_0.\end{aligned}$$

However the $\pm$ for the classical solution is "either + or -" while in (40), $\pm$ means "both + and -". So the quantum mechanical imposition of a reflection boundary condition, in a model related to the Kasner model, has as its classical limit both the classical expansion and contraction.

Also of interest is the fact that the different factor orderings considered in chapter 4, section 1 merely rescale the "energy" (see equations 4.1(9), 4.1(11), 4.1(14)). Using (29) and (32), this just changes a in (34) and (35) and so (38) remains valid. This means that the factor orderings considered do not affect the classical limit. This result is what would be expected from experience in the ordinary quantum theory.

4.4 Quantization with Radius Time

The classical Hamiltonian to be quantized is $\pm \pi_R$ and its explicit expression is given by (3.3(2)) in which $R=t$:

$$(\pm H)^2 = -144 \hbar t^2 + \frac{12}{t^2} \pi_\phi^2. \quad (1)$$

In this case, there is a natural factor ordering and the quantum equation is

$$\hat{H}^2 = -144 \hbar t^2 + \frac{12}{t^2} \hat{\pi}_\phi^2. \quad (2)$$

It is easy to see that $\hat{H}^2$ is self-adjoint because t is bounded and the usual Schrodinger representation of $\hat{\pi}_\phi$ (which is self-adjoint in this case because ϕ is not bounded)

$$\hat{\pi}_\phi = -i \hbar \frac{\partial}{\partial \phi}, \quad (3)$$

will clearly give a self-adjoint $\hat{\pi}_\phi^2$ on the appropriate domain.

The quantum equation of motion for this time dependent squared Hamiltonian is A IV (6):

$$\hat{H}^2 \psi_E(\phi, t) = E(t)^2 \psi_E(\phi, t). \quad (4)$$

This equation is separable. Let

$$\psi_E(\phi, t) = \Phi_E(\phi) T_E(t). \quad (5)$$

By using (2), (3), (4) this gives

$$\begin{aligned} & \left(-144\hbar t^2 - \frac{12}{t^2} \hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \Phi(\phi) = E^2(t) \Phi(\phi) \\ \text{i.e.} \quad & \Phi''(\phi) + \frac{t^2}{12\hbar^2} (E^2(t) + 144\hbar t^2) \Phi(\phi) = 0 \end{aligned} \quad (6)$$

Now

$$\Phi''(\phi) \Phi'(\phi) = f(\phi) = -\frac{t^2}{12\hbar^2} (E^2(t) + 144\hbar t^2)$$

gives

$$f(\phi) = -\frac{\lambda^2}{\hbar^2},$$

where C is a constant. Thus

$$E^2(t) = \frac{12}{t^2} \lambda^2 - 144\hbar t^2, \quad (7)$$

and the condition that $E^2 > 0$ implies that (for $k > 0$)

$$\frac{\lambda^2}{12\hbar} > t^4. \quad (8)$$

It is clear that the equation (7) with the eigenvalues E^2 and λ is the same as the classical equation with the classical E^2 and λ given in 3.3(2). The maximum of expansion is given by

$$t_m = R_m = \left(\frac{\lambda^2}{12\hbar} \right)^{1/4}, \quad \lambda^2 = 12\hbar R_m^4. \quad (9)$$

The Φ part of the wave function is easily seen to be

$$\Phi_E(\phi) = A e^{i\lambda\phi/\hbar} + B e^{-i\lambda\phi/\hbar}$$

$$\Phi_E(\phi) = A e^{i2\sqrt{3}R_m^2 \phi/\hbar} + B e^{-i2\sqrt{3}R_m^2 \phi/\hbar} \quad (10)$$

From AIV(9), AIV(6), AIV(8) the Schrödinger equation is

$$i\hbar \frac{d}{dt} T_E(t) = E(t) T_E(t) \\ = \pm \sqrt{\frac{12\lambda^2}{t^2} - 144\hbar t^2},$$

giving

$$i\hbar \frac{dT}{T} = \pm \frac{12\sqrt{\hbar}}{t} \sqrt{R_m^4 - t^4} dt \quad (11)$$

Consider the integral

$$I = \int \frac{dt}{t} \sqrt{a+bt^4}, \quad a=R_m^4, b=-1.$$

The substitution

$$u = t^4, \quad \frac{du}{4u} = \frac{dt}{t},$$

gives

$$I = \frac{1}{4} \int \frac{du}{u} \sqrt{a+bu}.$$

This may be evaluated⁽⁹⁰⁾, giving

$$I = \frac{1}{4} \left\{ 2\sqrt{a+bu} + \sqrt{a} \log \frac{\sqrt{a+bu} - \sqrt{a}}{\sqrt{a+bu} + \sqrt{a}} \right\}.$$

Thus (11) is

$$\log T - \log D = \mp \frac{i}{2} 12\sqrt{\hbar} I$$

$$\text{i.e.} \quad \log \frac{T}{D} = \mp \frac{i}{\hbar} 3\sqrt{\hbar} \left\{ 2\sqrt{R_m^4 - t^4} + R_m^2 \log \frac{\sqrt{R_m^4 - t^4} - R_m^2}{\sqrt{R_m^4 - t^4} + R_m^2} \right\} \quad (12)$$

This may also be written as

$$T = D \exp \left\{ \frac{-i}{\hbar} \left[\frac{tE(t)}{2} \pm iR_m^2 \log \frac{\mp tE(t) - 12\sqrt{\hbar}R_m^2}{\mp tE(t) + 12\sqrt{\hbar}R_m^2} \right] \right\} \quad (13)$$

It is clear that the spectra of λ and E are continuous. From the eigenvalue equation (7), which is just the classical equation, it is clear that the singularity at $\lambda(R)=0$ is not avoided. However if the physical wave functions are required, they can (formally) be constructed as wave packets in the usual way, despite the time dependence of the Hamiltonian, as follows:

$$\omega_{t_0}(\phi) = \int \psi_E(\phi, t_0) f(\lambda) d\lambda, \quad (14)$$

with the time development given, using AIV(3), by

$$\begin{aligned} \psi(\phi, t) &= \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t \hat{H}(\phi) ds \right\} \omega_{t_0}(\phi) \\ &= \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t \hat{H}(\phi) ds \right\} \int \psi_E(\phi, t_0) f(\lambda) d\lambda \\ &= \int \exp \left\{ -\frac{i}{\hbar} \int_{t_0}^t \hat{H}(\phi) ds \right\} \psi_E(\phi, t_0) f(\lambda) d\lambda \\ &= \int \psi_E(\phi, t) f(\lambda) d\lambda. \end{aligned} \quad (15)$$

4.5 Quantization with Extrinsic Time

With π_R chosen as the time, the classical Hamiltonian to be quantized is the radius $R(t)$, given in quadratic form in the constraint equation, 3.3(9),

$$12\hbar R^4 + \frac{t^2}{12} R^2 - \pi_\phi^2 = 0 \quad (1)$$

which may be solved to give

$$R(t) = \frac{1}{\sqrt{12\hbar}} \left(\sqrt{\frac{t^4}{(24)^2} + 12\hbar\pi_\phi^2} - \frac{t^2}{24} \right)^{1/2} \quad (2)$$

Note that because $\pi_R = t$, there is no factor ordering problem with the $\pi_R^2 R^2$ term in the constraint equation because π_R can not be represented by an operator. With the usual Schrödinger representation of $\hat{\pi}_\phi$, viz

$$\hat{\pi}_\phi = -i\hbar \frac{\partial}{\partial \phi}, \quad (3)$$

the Hamiltonian is certainly expected to be self-adjoint and positive. Turning (1) into an operator equation gives the same result as interpreting (2) by means of a spectral resolution of $\hat{\pi}_\phi^2$. Using AIV(5) and AIV(6), (1) becomes

$$\left(12\hbar \hat{H}^4 + \frac{t^2}{12} \hat{H}^2 + \hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \psi = 0$$

$$\text{i.e.} \quad \left(12\hbar E^4(t) + \frac{t^2}{12} E^2(t) + \hbar^2 \frac{\partial^2}{\partial \phi^2} \right) \psi_E(\phi, t) = 0$$

Letting

$$\psi_E(\phi, t) = \Phi_E(\phi) T_E(t),$$

gives

$$\left(12\hbar E^4(t) + \frac{t^2}{12} E^2(t) \right) \Phi(\phi) + \hbar^2 \Phi''(\phi) = 0$$

i.e.

$$\Phi''(\phi) = -\frac{\lambda^2}{\hbar^2} \Phi(\phi)$$

where λ is a constant. So

$$\Phi(\phi) = A e^{i\lambda\phi/\hbar} + B e^{-i\lambda\phi/\hbar} \quad (4)$$

and

$$12\hbar E^4(t) + \frac{t^2}{12} E^2(t) - \lambda^2 = 0 \quad (5)$$

which means that once again the equation of the eigenvalues looks like the classical equation, with the solution

$$E = \frac{1}{\sqrt{12\hbar}} \left(\sqrt{\frac{t^4}{(24)^2} + 12\hbar\lambda^2} - \frac{t^2}{24} \right)^{1/2}, \quad (6)$$

which is positive definite for λ real. The singularity now corresponds to vanishing "energy" and occurs when the

time is infinite. The Hamiltonian eigenvalue is symmetric with respect to time, with a maximum

$$E(0) = \sqrt{\frac{|\lambda|}{12\hbar}} = R_m. \quad (7)$$

Because the wave function is separable, the Schrödinger equation is

$$\begin{aligned} i\hbar \frac{dT_E(t)}{dt} &= E(t) T_E(t) \\ \text{i.e.} \quad \frac{dT}{T} &= \frac{-i}{\hbar} \frac{1}{\sqrt{12\hbar}} \left(\sqrt{\frac{t^4}{(24)^2} + 12\hbar\lambda^2} - \frac{t^2}{24} \right)^{1/2} dt \\ &= \frac{-i}{\hbar} \frac{1}{12\sqrt{2\hbar}} \left(\sqrt{t^4 + 4 \cdot 12^3 \hbar \lambda^2} - t^2 \right)^{1/2} dt \quad (8) \end{aligned}$$

This can be evaluated by considering the integral

$$I = \int \left(\sqrt{t^4 + a^2} - t^2 \right)^{1/2} dt \quad (9)$$

where

$$a^2 = 4 \cdot 12^3 \hbar \lambda^2.$$

Since the integrand is an even function, consider positive time and set

$$t^2 = a \sinh u,$$

with

$$dt = \frac{\sqrt{a}}{2} \frac{\cosh u}{\sinh^{1/2} u} du.$$

This gives

$$I = \frac{a}{2} \int \sqrt{\frac{\cosh u - \sinh u}{\sinh u}} \cosh u du$$

Integration by parts gives

$$\begin{aligned} I &= \frac{a}{2} \sqrt{\frac{u}{2}} + \frac{a}{4} \int \frac{du}{\sqrt{\frac{u}{2}}} \\ &= \frac{a}{2} \sqrt{\frac{u}{2}} + I_1 \end{aligned}$$

where

$$\frac{u}{2} = \cosh u \sinh u - \sinh^2 u$$

$$\frac{w}{2} = \frac{t^2}{a^2} (\sqrt{t^4 + a^2} - t^2), \quad (10)$$

$$\begin{aligned} w(u) &= \sinh 2u - \cosh 2u + 1 \\ &= 1 - e^{-2u}. \end{aligned}$$

So $w(u)$ is a monotonically increasing function, with

$$w(0) = 0, \quad w(\infty) = 1$$

and

$$\begin{aligned} dw &= 2(\cosh 2u - \sinh 2u) du \\ &= 2(1 - w) du. \end{aligned}$$

Thus the remaining integral I_1 can be evaluated by a change of variable to w :

$$I_1 = \frac{a}{4\sqrt{2}} \int \frac{dw}{(1-w)\sqrt{w}}$$

giving⁽⁹¹⁾

$$I_1 = \frac{a}{4\sqrt{2}} \log \frac{1+\sqrt{w}}{1-\sqrt{w}}.$$

Thus

$$I = \frac{a}{2\sqrt{2}} \sqrt{w} + \frac{a}{4\sqrt{2}} \log \frac{1+\sqrt{w}}{1-\sqrt{w}}$$

where

$$\sqrt{w} = \frac{\sqrt{2}}{a} t \sqrt{t^4 + a^2} - t^2.$$

Using (8) gives

$$\sqrt{w} = \frac{t E(t)}{\sqrt{12\lambda}}, \quad (11)$$

so that it is clear that the result for all t is given by

$$I = \frac{a}{4} \left(\frac{t E(t)}{\sqrt{3\lambda}} + \log \frac{\sqrt{12\lambda} + t E(t)}{\sqrt{12\lambda} - t E(t)} \right).$$

Thus, the solution of (8) is

$$T_E(t) = D \exp \left[-\frac{i\lambda}{\hbar} \sqrt{\frac{3}{2}} \left\{ \frac{t E(t)}{\sqrt{3\lambda}} + \log \frac{\sqrt{12\lambda} + t E(t)}{\sqrt{12\lambda} - t E(t)} \right\} \right] \quad (12)$$

To get physical wave functions, wave packets must be constructed from (4) and (12). Since the spectrum of the

Hamiltonian (which is the radius) is continuous and includes the singularity, it is clear that any wave packet that is constructed must evolve in time towards an inevitable collapse.

CHAPTER 5. YORK TIME AND CONFIGURATION SPACE

5.1 Introduction

When space-time was decomposed in a $3 + 1$ formalism to obtain a Lagrangian density in canonical form⁽²⁴⁾ it was found⁽³⁸⁾ that the intrinsic three-geometry contains information about time. Indeed, in a closed universe, the intrinsic three-geometry contains all the information about time. In a series of papers, York⁽¹⁹⁾ (and lately with Murchadha⁽²⁰⁾) has shown that there is a choice of time which is, in a sense, canonical.

The "York time", τ , arises naturally in a study of the initial value problem for empty universes (and also in the case of a charge free electromagnetic field^{(19IV)(20)}). Instead of specifying the three-geometry, only the conformal degrees of freedom (giving a conformal three-geometry, ${}^3\tilde{g}$) should be given.

The object that may be initially freely specified is the conformal geometry, ${}^3\tilde{g}$ (defined on some given manifold.) This is obtained from considering a three-metric $\bar{g}_{ab}$ on the manifold and taking equivalence classes under the conformal scaling given in

$$\bar{g}_{ab} = \psi^4 \tilde{g}_{ab}. \quad (1)$$

A representative three - metric of the chosen conformal three-geometry will be written as $\tilde{g}_{ab}$ where it can be assumed that $\tilde{g}$ is one.

It turns out (see later) that the scale factor is essentially the Hamiltonian. Thus the time will be extrinsic: the York time, τ , is defined^(19IV) by

$$\tau = \frac{2}{3} \sqrt{\bar{g}} \pi = \frac{4}{3} K, \quad (2)$$

where K is the extrinsic curvature scalar for the space-like hypersurface (the three-geometry). This implies that the York time is a scalar. It will be taken to be a constant (because for this case the momentum and Hamiltonian constraints decouple, as will be shown below).

With the $\tilde{g}_{ab}$ metric, an arbitrary transverse, traceless tensor density

$$\tilde{\pi}^{ab}_{TT} = \tilde{\sigma}^{ab} \quad (3)$$

(this equation is just notational) can be constructed. This is discussed in detail by York^(19IV). If the definition

$$\tilde{\pi}^{ab} = \tilde{\sigma}^{ab} + \frac{1}{2} \sqrt{\tilde{g}} \tilde{g}^{ab} \tau \quad (4)$$

is made, then the equation

$$\tilde{\nabla}_b \tilde{\pi}^{ab} = 0 \quad (5)$$

follows.

The mathematical objects $\tilde{g}_{ab}$ and $\tilde{\sigma}_{ab}$ may be specified freely at some initial time, τ . York now defines a conformal transformation to the physical variables by

$$g_{ab} = \varphi^4 \tilde{g}_{ab}, \quad \sigma^{ab} = \varphi^{-4} \tilde{\sigma}^{ab} \quad (6)$$

and shows^(19IV) that σ^{ab} remains transverse and traceless. Thus the actual superspace momenta, defined as

$$\pi^{ab} = \sigma^{ab} + \frac{1}{2} \sqrt{g} g^{ab} \tau, \quad (7)$$

automatically obey the momentum constraints:

$$\nabla_b \pi^{ab} = 0. \quad (8)$$

The Hamiltonian constraint remains to be solved and is now in the form of a quasi-linear elliptic equation which determines the scale factor, φ :

$$(-8 \tilde{\nabla}^2 + {}^3\tilde{R}) \varphi = \tilde{M} \varphi^{-7} - \frac{3}{8} \tau^2 \varphi^5 \quad (9)$$

where

$$\tilde{\nabla}^2 = \tilde{g}^{ab} \tilde{\nabla}_a \tilde{\nabla}_b, \quad (10)$$

and

$$\tilde{M} = \tilde{g}_{ac} \tilde{g}_{bd} \tilde{\sigma}^{ab} \tilde{\sigma}^{cd}. \quad (11)$$

($\tilde{M}$ is obviously unchanged by the conformal scaling).

It is easy to show that the A.D.M. action can be rewritten as

$$I = \int (\sigma^{ab} dg_{ab} - \sqrt{g} d\tau) \sigma^1 \wedge \sigma^2 \wedge \sigma^3 \quad (12)$$

where the σ^i are the basis forms for the three-geometry. Thus the Hamiltonian density conjugate to York time is

$$H = \sqrt{g} = \varphi^6 \quad (13)$$

The theory described here has only been used so far to point out that a conformal superspace of all the possible conformal three-geometries forms the configuration space for sourceless general relativity^(19III) and to examine existence and uniqueness theorems⁽²⁰⁾.

If a source is present, the constraints are modified, giving

$$\bar{C}^i = C^i - 2\kappa S^i = 0 \quad (14)$$

$$\bar{C}^0 = C^0 - 2\kappa \sqrt{g} T_0^0 = 0, \quad (15)$$

where S^i is the current density of the sources (which is a linear combination⁽²⁶⁾ of the T_0^i) and $-T_0^0$ is the energy per unit proper volume. For York's analysis of the structure of the initial value equations to remain valid, the S^i and T_0^0 must scale in a definite way under conformal transformations. York and Murchadha⁽²⁰⁾ claim that this is a feature of sources in general (which is almost certainly false, as will be discussed in the next section). Their claim is based on the fact that the charge-free electromagnetic field does scale.

With the charge-free electromagnetic field and gravity, the momentum constraints remain independent of the Hamiltonian constraint. The energy scales as

$$T_0^0 = \varphi^{-8} \tilde{T}_0^0. \quad (16)$$

Used in (9) and (15), this gives

$$\varepsilon \tilde{\nabla}^2 \varphi = {}^3\tilde{R} \varphi - \tilde{M} \varphi^{-7} + \frac{3}{8} \tilde{\chi}^2 \varphi^5 + 2\kappa \tilde{T}_0^0 \varphi^{-3}. \quad (17)$$

It was shown that there are very strong existence and uniqueness results for $\gamma \neq 0$, while the non-"generic" case of $\gamma = 0$ is not a good one for a study of the initial value problem.

York^(19IV) points out that the earlier work of Choquet-Bruhat⁽⁹²⁾ treated only the $\gamma = 0$ case with the energy density completely fixed (and the $T_0^i = 0$) and so tried to specify more data than that which is consistent with the physics.

5.2 York Time, Homogeneity and Sources

York time will now be discussed in the context of homogeneous models, possibly with a source of scalar "pions". In this case, from AIII(22),

$$-T_0^0 = \frac{1}{2} \frac{\dot{\phi}^2}{N^2} + \frac{1}{2} m^2 \phi^2 \quad (1)$$

$$= \frac{1}{2} \frac{\pi_\phi^2}{g} + \frac{1}{2} m^2 \phi^2, \quad (2)$$

with an equation of motion, AIII(26),

$$\dot{\pi}_\phi + N \sqrt{g} m^2 \phi = 0, \quad (3)$$

and $\phi = \phi(t)$ only. Since T_0^0 is not a function of the space coordinates, and enters the constraint equation multiplied by $\sqrt{g}$, then the usual form basis (expressed naturally in terms of the duals of the generators of the homogeneity Lie group if it acts ^{Simply} transitively) may be used⁽⁵¹⁾. This means that the space integration may be performed, giving a multiplicative factor for the action which does not affect the field equations. Thus this factor will be dropped, as it was in the Friedmann model supported by massless "pions". In a consistent notation, set

$$\sqrt{g} = Y = R^3 = \varphi^6. \quad (4)$$

Equations (2) and (3) remain unchanged, and show that, for $m = 0$

$$\pi_\phi = C \quad (5)$$

$$T_o^o = \varphi^{-12} \tilde{T}_o^o \quad (6)$$

and

$$-\tilde{T}_o^o = \frac{1}{2} C^2. \quad (7)$$

Since AIII(12) shows that the momentum constraints are unchanged (even if $m \neq 0$), a massless scalar source does obey the York criteria (although with a different scalar factor).

However it is clear, from (2), that the massive case will be quite different because of the naked ϕ term. It seems inconceivable that if a solution exists, it will scale in any definite manner (Consider for example the form of $\phi = \phi(R)$ for $m = 0$ in 3.2(32).) Similarly, an examination of the equations AIII(II), AIII(12), AIII(7) and AIII show that for the inhomogeneous case (with m arbitrary) that there are naked $\partial_j \phi$ terms in all the constraints which almost certainly do not simply scale under York's conformal transformations. We therefore conjecture that the only quantum field sources that can be analysed à la York is the source-free electromagnetic field and a homogeneous massless scalar field.

It is interesting to note that the usual dust source does scale, even for the inhomogeneous case because of the equation (given by Liang⁽³⁹⁾)

$$-T_o^o = \frac{\mu(x)}{\sqrt{g}} \quad (8)$$

where μ is a fixed function of space. Thus

$$T_o^o = \varphi^{-6} \tilde{T}_o^o \quad (9)$$

and

$$8 \tilde{\nabla}^2 \varphi = ({}^3\tilde{R} + \tilde{T}_o^o) \varphi - \tilde{M} \varphi^{-7} + \frac{3}{8} \chi^2 \varphi^5. \quad (10)$$

So York and Murchadha's existence and uniqueness theorems can be trivially extended to cover universes with dust sources.

For homogeneous universes with a source of massless "pions", the Hamiltonian constraint becomes (using (6) and 5.1(17))

$$0 = {}^3\tilde{R}\psi - (\tilde{M} - 2\kappa\tilde{T}_0^0)\psi^{-7} + \frac{3}{8}\tau^2\psi^5 \quad (11)$$

where (19IV)(20)

$$\tilde{M} \geq 0 \quad (12)$$

and

$$-\tilde{T}_0^0 \geq 0. \quad (13)$$

Setting $\kappa = 1/2$ (as previously) and using (4), gives

$$0 = {}^3\tilde{R} Y^{4/3} - (\tilde{M} - \tilde{T}_0^0) + \frac{3}{8}\tau^2 Y^2 \quad (14)$$

where Y is the Hamiltonian appropriate for a choice of the York time, τ .

Unfortunately this Hamiltonian is a little complicated for use in models, although it can be viewed as cubic equation in $Y^{2/3}$ and so an explicit expression can be found (which will involve cubic roots). Quantization may proceed in exactly the same way as before, in spite of the complicated form of Y : this will just mean that explicit integrations and wave packet construction will be even more difficult.

It is important to note that, as before, the spectrum of Y will be just the classical spectrum and so quantization (with the Hamiltonian as some power of the radius of the universe) does not (naively) prevent a classical collapse. These considerations should also apply to the inhomogeneous models, so that if York time is a "canonical" choice of time, then the main hope for the relevance of the quantum theory to the collapse problem must be that something new comes from using quantized matter sources which have no classical analogue. For example, it may be that near the singularity, all the spins can line up (in some mysterious way) and so produce an expansion

such as that produced by Trautmann's⁽⁹³⁾ torsion model. Isham and Nelson⁽⁷⁵⁾ are at present considering such a possibility.

It is easy to see (from the action principle) that if the Hamiltonian is taken to be the radius

$$H = R = \varphi^2 \quad (15)$$

then the appropriate extrinsic time is

$$\tau = \frac{1}{3} g^{-\frac{1}{2}} \tau = \frac{1}{3} \varphi^{-4} \tau. \quad (16)$$

(Homogeneity of the models ensures that τ is a scalar.) In this case the constraint equation (11) simplifies to a quadratic equation in H^2 :

$$0 = -(\tilde{M} - \tilde{T}_0^0) + {}^3\tilde{R} H^4 + \frac{1}{24} \tau^2 H^2. \quad (17)$$

Although these models are covered by the work of York and Murchadha⁽¹⁹⁾⁽²⁰⁾, we have shown that the existence condition is now very simply that the quadratic equation above should have a positive real solution. For non zero curvature

$$H^2 = \frac{-\frac{\tau^2}{24} + \sqrt{\left(\frac{\tau^2}{24}\right)^2 + 4(\tilde{M} - \tilde{T}_0^0) \cdot {}^3\tilde{R}}}{2 \cdot {}^3\tilde{R}} \quad (18)$$

The existence condition is that the curvature must be positive and both $\tilde{M}$ and $\tilde{T}_0^0$ may not be zero. For zero curvature, then again $\tilde{M}$ and $\tilde{T}_0^0$ cannot both be zero.

So for homogeneous models with a possible source of a massless scalar field, the existence theorems are very simple: the curvature may not be negative and $\tilde{M}$ and $\tilde{T}_0^0$ may not both be zero.

In particular, all the Bianchi models⁽⁵¹⁾ may be extended. Consider for example the Bianchi types I and IX, used by Misner⁽³⁶⁾. In these cases (with factors which may be absorbed),

$$\tilde{M} = p_+^2 + p_-^2 \quad (19)$$

where the $\beta_{\pm}$ are the anisotropy momenta (discussed in the next section). Thus, using (7) and (19),

$$\tilde{M} - \tilde{T}_0^0 = \dot{P}_+^2 + \dot{P}_-^2 + \frac{1}{2}\pi\dot{\phi}^2, \quad (20)$$

and it's clear that for all these homogeneous models, the source behaves mathematically in the Hamiltonian just like an extra anisotropy parameter. Of course, the physical interpretation is very different!

Specifically, the homogeneous Friedmann model with massless "pions" is equivalent to the Kantowski-Sachs⁽⁵²⁾ model (after using a canonical transformation. This was first noticed by Kuchař⁽⁹⁴⁾.) An attempt to quantize the Kantowski-Sachs model was made earlier by Fishbone⁽⁵¹⁾, but this suffers from the technical deficiencies, discussed earlier, in that the incorrect Klein-Gordon approach is used, ignoring the complications of a time dependent Hamiltonian. However it is important to note that classical models which are related by a canonical transformation lead, in general, to unitarily inequivalent quantum models.

5.3 Extended Configuration Space

It is interesting to consider the configuration space for the wave function. This could be called the "reduced superspace" because, as was noted previously, the superspace philosophy seems to be inappropriate for the quantum theory: the time must be extracted, leaving only the configuration variables.

Consider now the Mixmaster universe in the new language. The configuration variables are $\beta_{\pm}$, which are the variables which specify the conformal three geometry, ${}^3\tilde{g}$. So in this sourceless case, the "reduced superspace" is just the "conformal superspace" of York⁽¹⁹⁾.

If β_+ and β_- are considered as components of an anisotropy vector, $\underline{\beta}$, which makes an angle, K , with the β_+ axis, then it can be shown⁽⁹⁵⁾ that each possible

conformal three-geometry is represented once by one 60° wedge emanating from the origin of the β plane. Thus the configuration space can be taken to be the wedge defined, for example, by $0 \leq K \leq 60^\circ$.

However it is important to realize that any 60° wedge could be chosen because the only difference between these conformal geometries would be the orientation of their coordinate systems. If the whole β plane is considered, then $\beta = 0$ represents the isotropic case, $K = 0^\circ, \pm 120^\circ$ represent the "oblate" axially isotropic case and $K = 180^\circ, \pm 60^\circ$ are the "prolate" axially isotropic cases.

Now in a simple conformal superspace, those conformal three-geometries with larger symmetry groups have different neighbourhood structures than those with smaller symmetry groups. This means that conformal superspace is not a manifold but has strata, in exactly the same way as in the superspace considerations⁽³⁴⁾. It is clear that the $0 \leq K \leq 60^\circ$ wedge has this structure: the strata given by $K = 0$ and $K = 60^\circ$ but with $\beta \neq 0$ have each point with only half a neighbourhood, and within the $K = 0$ stratum, the origin has only half a neighbourhood.

DeWitt⁽²²⁾ has proposed that a manifold be constructed by joining many copies of a simple superspace along their strata. In this case, extended conformal superspace is just the whole β plane where the isotropic conformal three-geometry is represented once, the axially isotropic conformal three-geometries are represented three times and there are six copies of all the other conformal three-geometries.

There is a good dynamical reason for using the extended configuration space, besides the obvious appeal of using a simpler mathematical object. This is that the classical trajectories of the conformal three-geometries in the extended space are smooth, whereas they generally execute a non differentiable reflection in the simple configuration space⁽²²⁾. For this reason, all the work on these models and the Mixmaster model in particular, have used the extended conformal superspace.

In the quantum theory there are compelling reasons why the extended conformal superspace must be used. Consider the "momentum" operators, $\hat{p}_{\pm}$, which are conjugate to the $\beta_{\pm}$ and so have the usual canonical commutation relations. On the wedge $0 \leq \kappa \leq 60^\circ$, boundary conditions have to be imposed so that the wave function is reflected at the edges of the wedge.

It is clear that these boundary conditions would place restrictions on the spectra of the momenta. However the boundaries are artificial in that a change of coordinates, which is considered to be unphysical, can rotate the wedge in the $\beta_{\pm}$ plane, thus producing new boundary conditions and so probably new restrictions on the momenta.

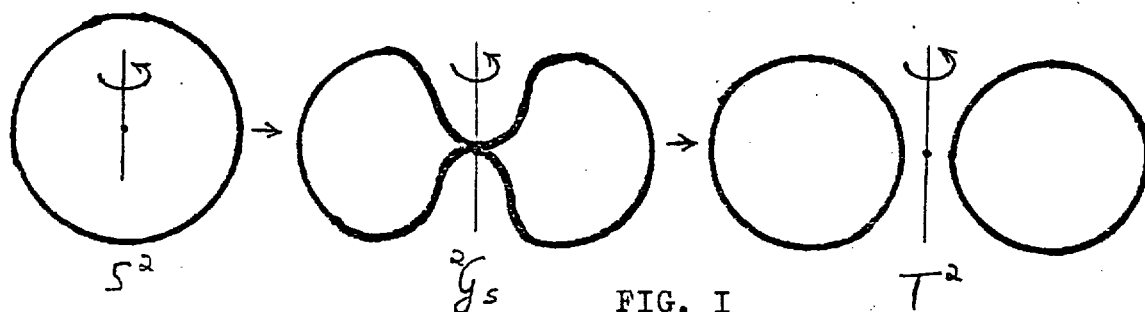
So the quantum theory requires that unphysical boundaries (due to the choice of coordinates) should be ignored, which finds a natural solution by using extended configuration space.

CHAPTER 6. TOPOLOGY CHANGE?

6.1. Introduction

Einstein stressed on many occasions that his field equations do not single out any particular topology on spacetime. A number of people, culminating with Geroch⁽⁹⁶⁾, showed that if the general theory of relativity and causality are taken seriously to arbitrarily small distances (which can clearly have no observational support) then the classical theory will not permit a change in the topology of an intrinsic three-geometry. As Penrose points out this is hardly surprising, since it is obvious that a change in the topology is acausal. (This point will be returned to later.)

Wheeler⁽⁸⁾ has argued that quantization produces fluctuations in the geometry and that, on the scale of the Planck length, these fluctuations can become so large that a quantum transition of topology (somehow) occurs. This change in topology is envisaged as typically occurring as follows. Consider the sphere in two dimensions, S^2 , being deformed continuously until a singular geometry, ${}^2\mathcal{G}_s$, is obtained. This is now torn at the singularity and continuously deformed into the torus, T^2 . This can be represented pictorially by drawing the cross-sections:



(which have to be rotated to get the geometry).

This type of singular geometry has been described as having a "conical singularity". This is an apt description because the underlying structure is not a manifold: most of the points of the space have the usual neighbourhoods that are homeomorphic to open sets in some fixed n -dimensional Euclidean space. However one point has neighbourhoods that are mapped into an n -dimensional

cone (that is imbedded in a Euclidean space of $n+1$ dimensions). Reynolds⁽⁹⁷⁾ has studied these singularity manifolds mathematically.

On the basis of the (limited) classical success "mass without mass" and "charge without charge" models⁽⁹⁸⁾ using wormholes Wheeler proposed that the "acceptable topologies" were S^3 , $W_1 = S^1 \times S^2$ and the W_n (which are the sphere with n "handles" or wormholes)⁽⁸⁾. Fisher⁽³⁴⁾ analysed the mathematical structure of the "stratified manifold", $S^{(n)}$, that is obtained as the superspace of all intrinsic three-geometries for a fixed topology. Komorowski⁽²³⁾, in a largely unknown mathematical paper, showed how a topology may be given to the superspaces on S^3 and $S^1 \times S^2$ so that it is possible to pass continuously (in a technical sense) from one superspace to the other.

It is clear that the question of topology change should be examined using some such "grand superspace" which combines superspaces on different topologies. This is an extremely difficult problem and has to be tackled directly: it is clear from the discussion in chapter 5, section 3 that Brill's⁽⁹⁾ comment "Extended superspace is interesting for topology change because many of the problems it raises - for example, allowed boundary values of the wave functional at the boundary between two copies of $S^{(n)}$ - are analogous to problems in the more complicated grand superspace." is substantially incorrect.

Gowdy⁽⁹⁹⁾ has constructed some anisotropic and inhomogeneous models which can describe S^3 or the disjoint union of $S^1 \times S^2$ and S^3 . The topology change here would be rather drastic since part of space would effectively cease to exist. Gowdy has shown that here there is a "classical barrier" to a topology change which is analogous to the usual potential barrier of quantum mechanics.

However for a topology change to be able to occur quantum mechanically, at least two things seem to be essential. Firstly, the topology change must be described by some dynamical parameter. For example a description

of different topologies by traditional algebraic techniques is inadequate unless Betti numbers, etc. are analogous to spin, and this appears to be extremely unlikely. (For speculations on "spin without spin", using spin manifolds, see Wheeler⁽⁸⁾.)

Secondly, it remains to be shown even then that the quantization will give a larger spectrum for the parameter describing the topology change than the values allowed classically. Classically, the topology change is completely forbidden, whilst the familiar barrier penetration of quantum mechanics occurs for potential barriers where the region on the other side of the barrier can be reached by a classical trajectory with higher energy.

An indication that it may be possible for quantum mechanics to have an "extended spectrum" was given (admittedly in just a model) in chapter 4, section 3. It was found there that transitions occur between a Friedmann universe filled with massless scalars to a (non classical) empty Friedmann universe.

Thus we attempted to construct suitable models with transitions between S^3 and $S^1 \times S^2$. These will be described next.

6.2 Some Macroscopic Topology Change Models

The torus, T^2 , may be imbedded in Euclidean three-space to give the familiar doughnut. This may be obtained as a surface of revolution of a circle of radius R , at a distance z from the origin, and parametrized by ϕ, ψ , as illustrated

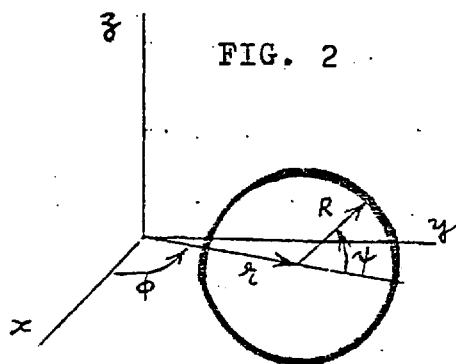


FIG. 2

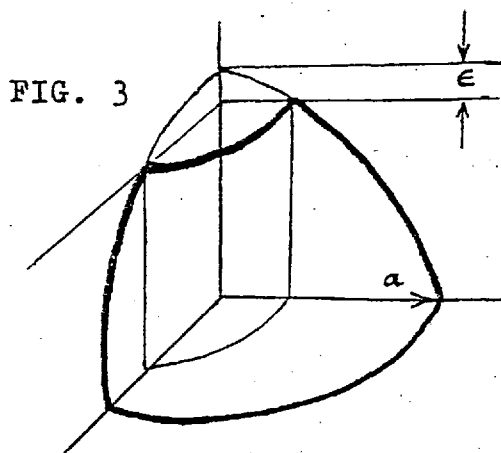


FIG. 3

in figure 2. For $\lambda > R \neq 0$, the doughnut inherits a smooth geometry from $\mathbb{R}^3$ and both ϕ and ψ range between 0 and 2π . For $\lambda = R$, the singular geometry 2G_s is obtained with the conical singularity that is discussed in section 1 occurring at the origin, while for $R > \lambda \neq 0$ the geometry isn't smooth at the two points above the origin where there are "cusps". Finally, for $\lambda = 0$, the smooth sphere S^2 is obtained and the coordinate ψ must be restricted to lie between $-\pi/2$ and $\pi/2$ so that the sphere is not covered twice.

The doughnut may also be constructed by cutting out antipodal discs, defined by $|a-z| < \epsilon$ for $\epsilon > 0$, from the sphere, S^2 , with radius, a , in $\mathbb{R}^3$. This is illustrated for $x, y, z > 0$ in figure 3. The "rims", $|a-z| = \epsilon$, are then identified by pulling what is left of the sphere into the shape of the doughnut.

The important relations between the co-ordinates used are

$$\left. \begin{aligned} \sqrt{x^2 + y^2} &= \lambda + R \cos \psi, \\ z &= R \sin \psi. \end{aligned} \right\} \quad (1)$$

For $\lambda = 0$, the geometry is that of the usual isotropic sphere which remains invariant under rotations about any axis passing through the origin. However for λ non zero, only rotations about the z axis leave the geometry invariant. Thus the isometries of the geometry are reduced by the introduction of a non zero λ parameter.

Topologically, the pierced sphere W_1 is $S^1 \times S^2(100)$ and this can be given a geometrical structure in exactly the same way as in the previous discussion in which S^2 was pierced to give $T^2 = S^1 \times S^1$. Consider the usual sphere in $\mathbb{R}^4$ (which is a fictional imbedding space and not spacetime) which is pierced and parametrized by

$$\left. \begin{aligned} x &= (\lambda + R \cos \psi) \sin \theta \cos \phi \\ y &= (\lambda + R \cos \psi) \sin \theta \sin \phi \\ z &= (\lambda + R \cos \psi) \cos \theta \\ w &= R \sin \psi \end{aligned} \right\} \quad (2)$$

which give the obvious generalization of (1). The natural metric on $S' \times S^3$ is inherited from $\mathbb{R}^4$ and is

$$\begin{aligned} ds^2 &= (dx^2 + dy^2 + dz^2 + d\omega^2)|_{S' \times S^3} \\ &= R^2 \left\{ d\psi^2 + \left(\frac{r}{R} + \cos\psi \right)^2 (d\theta^2 + \sin^2\theta d\phi^2) \right\} \end{aligned} \quad (3)$$

Setting

$$R = \frac{r}{R} \quad (4)$$

it is clear that for R equal to zero, the isotropic three sphere is obtained⁽⁵⁵⁾ in which case ψ must be restricted to the range of $-\frac{\pi}{2}$ to $\frac{\pi}{2}$, instead of its range over 2π which is necessary for the smooth $S' \times S^3$ geometries given when R is greater than one.

The field equations can now be obtained by the straight forward type of calculation given in appendix II for the Friedmann case, which corresponds to R equal to zero. Not unexpectedly, the equations are more complicated than for the Friedmann case. For example, the space curvature is given by

$${}^3R = \frac{6\cos^2\psi + 4R\cos\psi}{R^2(R + \cos\psi)^2} \quad (5)$$

This can be partially checked by observing that for $R=0$, it agrees with the Friedmann $k=1$ result, given in AII(23).

Unfortunately it is found that R is not a dynamical variable. This result is obtained from the requirement that the Ricci tensor must vanish for empty universes. In particular since

$$R_0' = \frac{2\sin\psi}{R^2(R + \cos\psi)^2} \frac{d}{dt} R, \quad (6)$$

$$\dot{R} = 0. \quad (7)$$

In fact, it turns out that there are no empty space solutions.

One conceivable way to get out of this difficulty is to introduce anisotropy and so consider some $S' \times S^2$ as a generalization of the Misner⁽³⁶⁾ Mixmaster universe. This is easier said than done because the Bianchi type models have a beautiful group theoretical structure which permitted Bianchi to introduce anisotropy very simply.

This is not possible for the $S^1 \times S^2$ geometry introduced in this section and our efforts to force it in various ways have failed. Another possible way is to try to introduce a scalar field as a source. This can be done by inserting the equations AIII(33) - (34) - (35) into the Ricci tensor. This looks more hopefull because (6) becomes

$$\frac{2 \sin \psi}{R^2 (R + \cos \psi)^2} \dot{R} = \dot{\phi} \partial^i \phi. \quad (8)$$

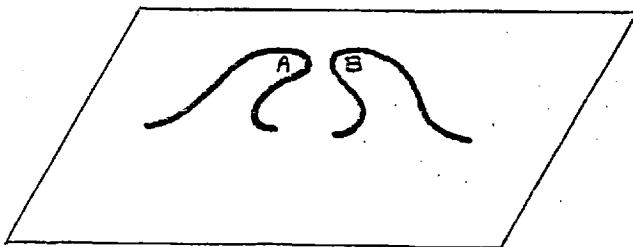
Unfortunately, once again the field equations do not permit a solution (even for m non zero) unless R is zero.

Thus, since it appears that this simple model cannot produce a dynamical R , quantization of it cannot excite this geometry.

6.3 Causality and Pair Production

Had the topology change just proposed occurred, it would have been an acausal process. (This is explained below.) Therefore, to be in accord with experiment, it should only have occurred for small R . (The adjective small is left deliberately vague because it is not clear whether it should mean "with respect to the Planck length" - which is the natural length of gravity - or "with respect to hadron sizes" - which is about the minium size for which causality can be demanded on observational grounds.) Thus consider essentially the same process as studied in the last section of topology change occurring on a small scale with some background geometry which, on the scale of the wormhole, looks flat (figure 4).

FIG. 4



The classical causality problem is clear: points A and B are separated on a space-like hypersurface. The topology changes as points A and B meet and the manifold

is torn at $A = B$ to provide a wormhole. The identification of the two space-like separated points is a violation of causality.

So if this wormhole is to be formed, the whole process must be "sufficiently microscopic": that is, be part of the foamlike structure⁽⁸⁾. However, since this process is analogous to particle pair production⁽⁸⁾, it would seem that processes that look acausal classically should not be rejected out of hand.

It is well known⁽¹⁰¹⁾ that a classical description of pair production in an electromagnetic field is acausal. Also, it is easy to see that if the Klein-Gordon equation for pions is treated as a square root Hamiltonian (so that the observables are represented by self-adjoint operators - see chapter 2, section 2), this Hamiltonian looks acausal:

$$i\hbar \frac{\partial \psi(\underline{x}, t)}{\partial t} = \int d^3x' K(\underline{x} - \underline{x}') \psi(\underline{x}', t) \quad (1)$$

where the kernel

$$K(\underline{x} - \underline{x}') = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\mathbf{p} \cdot (\underline{x} - \underline{x}')/\hbar} c \sqrt{\mathbf{p} \cdot \mathbf{p} + m^2 c^2} \quad (2)$$

has non-zero contributions of importance only for $|\underline{x}' - \underline{x}| \leq \hbar/mc$ which is the Compton wavelength. This acausality reflects the pair production that is obligatory in a quantum theory of fields. However, when discussed within the context of the quantum theory of fields, the direct analogue of (13), causality to arbitrarily small distances (microcausality) is maintained.

Returning to the "pair" production illustrated by figure 4 evolving into figure 5, it is

FIG. 5



interesting to note that the conical singularity through which this geometry passes is foreign to the whole

rationale of Einstein's "complete field equations" approach where particles would be described everywhere as singularity-free solutions⁽¹⁰²⁾.

This can be seen by now filling the wormhole (figure 5) with sourcefree electric lines of force⁽⁷⁾ which emerge from one end of the tube and so this end of the wormhole appears to be a source of positive charge. At the other end of the wormhole, the lines of force disappear and so this looks like a source of negative charge. It has been shown⁽⁷⁾, classically that the flux through each wormhole may not change.

But if the wormhole is (quantum mechanically) allowed to pinch, then it is clear that A and B (of figure 4) become genuine sources! We suggest that a more reasonable possibility is that the whole wormhole scales down as the mouths become closer (viewed from the background) and that the wormhole is never pinched. Instead, the metric on the wormhole part becomes, in the limit, degenerate and this is interpreted as annihilation of the "pair". Of course, if the metric is degenerate, then this is a classical singularity, even if it is (effectively) at only one point of the background space.

This process is not completely whimsical. Misner⁽¹⁰³⁾ has solved the initial value equations for a wormhole (with the correct wormhole topology) in empty space (with no electromagnetic fields). Misner's wormhole behaves like two neutral concentrations of mass energy. It is expected that a singularity will develop, but its nature is not known because the time development is very complicated. Misner has suggested that near each mouth there will develop a Schwarzschild-like singularity. However it is conceivable that for a small wormhole, this could provide a model for pair annihilation, producing radiation. Clarification on this issue would be of great interest.

With wormholes collapsing to a point, causality would be maintained. Perhaps quantization would allow transitions from a smooth background to one with a non

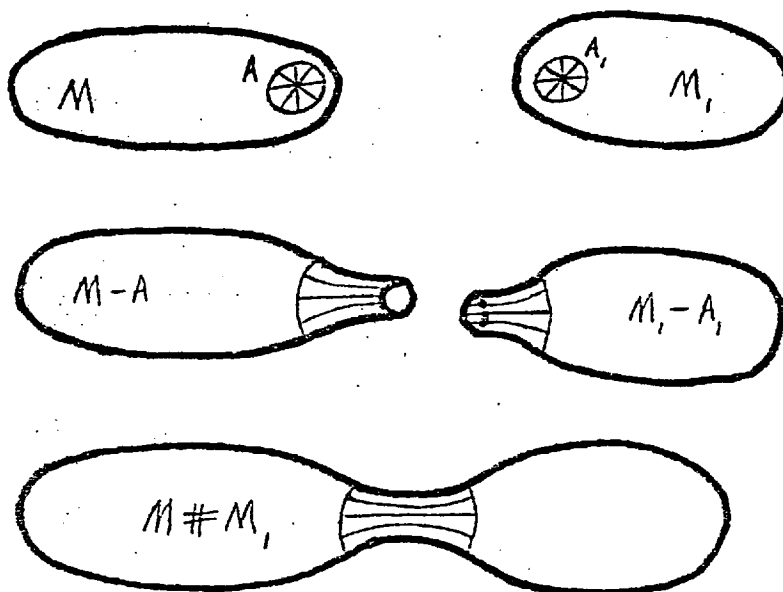
degenerate wormhole thus avoiding the degenerate metric in a natural way, and looking very much like the process of (real) pair production where the particles just appear spontaneously at space-like separated points.

6.4 The Foam

We attempted to provide some analysis of this foam-like structure by considering either small Friedmann spheres or wormholes added to a background. The background manifold, M , was taken in practice to be the torus, T^3 , and the metric tensor, G_M , was taken to be the usual (flat) one.

The idea was to put a suitable metric on the topological connected sum ⁽¹⁰⁴⁾ $M \# M_1$ of the two manifolds M, M_1 . The topological connected sum can be obtained simply by choosing points $A \in M$ and $A_1 \in M_1$. Polar co-ordinates are imposed in open balls around A and A_1 . Now an identification is made on these balls by inverting the radial coordinate in A_1 , and then identifying this new coordinate (suitably scaled) in A_1 with the radial coordinate in A . This can be illustrated pictorially by removing the points A, A_1 , flaring out the balls into collars, and identifying the collars by fitting them over each other with the neck of one fitted to the base of the other. (see figure 6).

FIG. 6



Now some sort of addition of the metrics has to be defined. First, some more notation is needed. Let the radial coordinate in the ball, B_{r_0} , around A be r with the range

$$0 < r < r_0$$

where A is given by setting r equal to zero (and similarly for B_{R_0} around A₁). If the metrics were just added, then the resultant "metric" on $M \# M_1$ would be discontinuous at $r=0$ and $r=r_0$.

Alternatively, define the new metric as a smoothed addition,

$$G_{M \# M_1} = f G_M + (1-f) G_{M_1}, \quad (1)$$

where f is some smooth function such that it is identically one on $G_M - B_{r_0}$ and identically zero on $G_{M_1} - B_{R_0}$.

It is well known that such a function must exist, and can be constructed explicitly⁽¹⁰⁵⁾, as follows. Consider the C^∞ function

$$g(r) = \begin{cases} \exp\left(\frac{1}{r-r_0} - \frac{1}{r}\right) & \text{if } 0 < r < r_0 \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

This is a bump function (see figure 7). The smoothing function is defined as

$$f(r) = \frac{\int_0^r g(s) ds}{\int_0^{r_0} g(s) ds} \quad (3)$$

and its graph is drawn in figure 8.

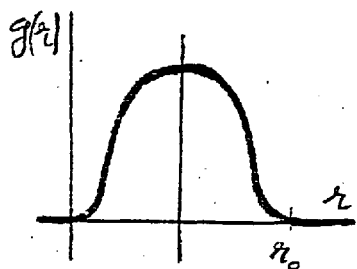


FIG. 7

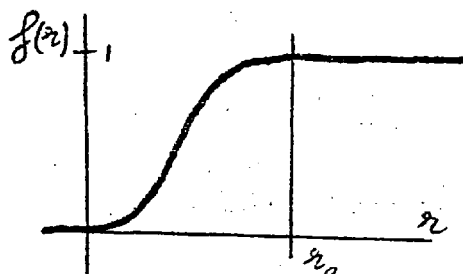


FIG. 8

Now it is easy to fix r_0 as a function of a scale parameter (R , say) of M_1 , such that when $R = 0$ (that is, $G_{M_1} = 0$ which means that M_1 has disappeared), $r_0 = 0$. So the "metric" on $M \# M_1$ becomes

$$G_{M \# M_1} = G_M, \quad (4)$$

which is highly degenerate and is "like a step function" at the "points" A . This is then to be reinterpreted physically as just the perfectly smooth background ${}^3\mathcal{G}(M)$.

Unfortunately the approach proposed here has a very serious drawback: even if the classical field equations can be solved with a dynamical parameter describing the "size" of ${}^3\mathcal{G}(M)$, the smoothing function appears explicitly in the equations. Thus even the constraint equations become very complicated for the simplest of models.

For example, consider the anisotropic ${}^3\mathcal{G}(T^3)$ with just a "bump", radius R_0 .

$$g_{ij} = f R^2 B_i S_{ij} + (1-f) R^2 \delta_{ij}. \quad (5)$$

Set

$$A_i = R^2 B_i - R^2, \quad (6)$$

and

$$R^2 = x'^2 + x^2 + x^3{}^2. \quad (7)$$

The Ricci curvature scalar is given by

$$\begin{aligned} {}^3R = & \sum_i \sum_{h \neq i} \left\{ -2 \left[f'' \frac{x_h^2}{2R^2} + f' \frac{R^2 - x_h^2}{2R^3} \right] A_i g^{hh} g^{ii} \right. \\ & + g^{ii} \frac{f'^2}{4R^2} \left[2x_i^2 g^{ii} g^{hh} A_i A_h + x_i^2 (g^{hh} A_h)^2 - x_h^2 g^{hh} g^{ll} A_i A_l \right. \\ & \left. \left. + x_h^2 (g^{ii} A_i)^2 \right] \right\}. \end{aligned}$$

A quantum equation of motion would contain this expression and the possibility of solving such an equation seems remote.

Finally, it is worth noting that we have found that this idea (viz using a family of metrics such that the degenerate metric in (4) is reinterpreted as the smooth background metric) is essentially the same as that used by Komorowski⁽²³⁾ for his "point addition" defined on purely mathematical grounds. However the deliberations of this chapter provide physical reasons for considering this type of topology change and a direct way in which it could be parametrized in model calculations.

6.5 Conclusion

It is clear that a treatment of changing topology is still a long way off. However it does seem certain that quantum gravity requires some objects which are not just smooth three-geometries.

To see this, consider the situation in ordinary quantum field theory⁽¹²⁾⁽¹⁰⁶⁾. This is usually presented in a Fock space, $\mathcal{F}$, representation because this gives immediate access to the particle description. Alternatively, the field aspect can be emphasized by using an L^2 space of state functionals (analogous to the usual quantum mechanical representation). It has been shown that Fock space is unitarily equivalent to an L^2 space defined on a certain space, S' , with a certain measure. Besides all the obvious field configurations, the space S' also contains the distributions such as the Dirac delta - "functions" and the step "functions".

Now even free field theories with an infinite number of degrees of freedom require distributions in order to be able to support a representation of the canonical commutation relations in the usual functional form.

For gravity, what are the "extra" elements of the appropriate domain space for the wave function? Are these "distribution valued conformal three-geometries"? In particular, does the quantum theory require the consideration of conical singularities (cf delta functions) and degenerate metrics (cf step functions) as idealizations that must nevertheless be included in the structure of the theory?

APPENDIX I

Notations, Definitions and A.D.M. Decomposition

The standard notation of Greek indices $\mu, \nu, \dots$ running from 0 to 3 for four dimensional space-time objects, and latin indices $i, j, \dots$ running from 1 to 3 is used, as well as the standard definition of the Christoffel symbols (of the second kind):

$$\Gamma_{\mu\nu}^{\alpha} = \frac{1}{2} g^{\alpha\beta} (g_{\mu\beta,\nu} + g_{\nu\beta,\mu} - g_{\mu\nu,\beta}). \quad (1)$$

The signature is chosen to be $-, +, +, +$, and the Ricci tensor is defined to be

$$R_{\mu\nu} = \Gamma_{\mu\nu,\alpha}^{\alpha} - \Gamma_{\mu\alpha,\nu}^{\alpha} + \Gamma_{\mu\nu}^{\alpha} \Gamma_{\alpha\beta}^{\beta} - \Gamma_{\mu\beta}^{\alpha} \Gamma_{\nu\alpha}^{\beta}, \quad (2)$$

following the conventions of A.D.M.⁽²⁴⁾. Their 3 + 1 decomposition of space-time is also followed. This involves decomposing the metric tensor as

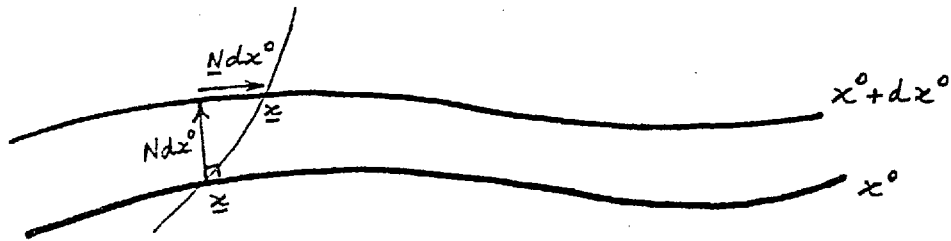
$${}^4g_{\mu\nu} = \begin{pmatrix} -N^2 + N^i N_i & N_j \\ N_i & g_{ij} \end{pmatrix} \quad (3)$$

$${}^4g^{\mu\nu} = \begin{pmatrix} -\frac{1}{N^2} & \frac{N^j}{N^2} \\ \frac{N^i}{N^2} & g^{ij} - \frac{N^i N^j}{N^2} \end{pmatrix} \quad (4)$$

where a presuperscript 4 indicates that the appropriate tensor is defined on space-time, and $g_{ij}(x, x^0)$ is the natural metric tensor defined on the space-like hypersurface defined by the value of the time co-ordinate, x^0 . The inverse of this three-metric is written as g^{ij} and its relation to ${}^4g^{ij}$ can be read from (4). This three-metric is used to define

$$N^i = g^{ij} N_j. \quad (5)$$

The proper time between two surfaces labelled with the parameters x^0 and $x^0 + dx^0$ is $N dx^0$ and so N is usually called the lapse function. Similarly the quantities N^i are known as the shift functions because the tip of a normal vector, whose base is at the point, $\underline{x}$, with co-ordinates x^i in the first hypersurface, can be connected by a vector (lying in the second hypersurface with the same spatial co-ordinates x^i) whose components are $N^i dx^0$:



The intrinsic curvature of the hypersurface labelled by x^0 is described by the Ricci curvature scalar, ${}^3R(x, x^0)$, of the three-geometry. The extrinsic curvature of the hypersurface (which describes how it is imbedded in space-time) is given by

$$K_{ij} = \frac{1}{2N} (N_{i|j} + N_{j|i} - g_{ij,0}) \quad (6)$$

where the $|$ symbol means covariant differentiation using the three-metric.

It is convenient to describe the extrinsic curvature by the three-tensor density

$$\pi^{ij} = -\sqrt{g} (K^{ij} - g^{ij} K_{kl} g^{kl}) \quad (7)$$

where g is the determinant of the three-metric.

The action for the free gravitational field is defined as

$$I_G = \frac{1}{2K} \int {}^4R \sqrt{-g} d^4x \quad (8)$$

where the coupling constant is set equal to zero in this thesis

$$K = \frac{8\pi G}{c^4} = \frac{1}{2}. \quad (9)$$

By means of the A.D.M. decomposition and discarding a four-divergence, the gravitational Lagrangian density can be written in canonical form (with constraints) as follows:

$$\mathcal{L}_G = \pi^{ij} \dot{g}_{ij} - N_\mu C^\mu \quad (10)$$

where

$$C^0 = \frac{1}{\sqrt{g}} \left[\pi^{ij} \pi_{ij} - \frac{1}{2} (\pi^k_k)^2 \right] - \sqrt{g} {}^3R \quad (11)$$

and

$$C^i = -2\pi^{ij}{}_{|j} . \quad (12)$$

It turns out that the N_μ are just Lagrange multipliers and their variation give the constraint equations

$$C^\mu(\pi^{ij}, g_{kl}) = 0 . \quad (13)$$

These are just the initial value equations.

The C^μ can be written as

$$C^i = 2\sqrt{g} N \cdot {}^4G^{oi} \quad (14)$$

and

$$C^0 = -2\sqrt{g} N^2 \cdot {}^4G^{00} , \quad (15)$$

where the Einstein-tensor is defined as

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} \cdot {}^4R g_{\mu\nu} . \quad (16)$$

If matter is included, then the action (if it exists!) is defined as

$$\mathbb{I} = \mathbb{I}_G + \mathbb{I}_M \quad (17)$$

where

$$\begin{aligned} \delta \mathbb{I}_M &= -\frac{1}{2} \int T_{\mu\nu} \delta g^{\mu\nu} \sqrt{-{}^4g} d^4x , \\ &= \frac{1}{2} \int T^{\mu\nu} \delta g_{\mu\nu} \sqrt{-{}^4g} d^4x \end{aligned} \quad (18)$$

using

$$\delta g^{\rho\sigma} = -g^{\rho\mu} g^{\sigma\nu} \delta g_{\mu\nu} \quad (19)$$

which can be derived from

$$g^{\rho\sigma} g_{\sigma\lambda} = \delta_\lambda^\rho .$$

Another relation which is useful when considering these variational principles is

$$\delta \sqrt{-{}^4g} = \frac{1}{2} \sqrt{-{}^4g} g^{\mu\nu} \delta g_{\mu\nu} . \quad (20)$$

Variation of (17) gives the Einstein field equations

$$G_{\mu\nu} = K T_{\mu\nu}. \quad (21)$$

Finally, a dot is used to denote differentiation with respect to time, and a dash is used to denote differentiation of any function with respect to its argument: that is

$$\frac{d}{dx} f(x) = f'(x).$$

Equations are numbered for each section. If an equation from another chapter or section is required, it is denoted by a sequence such as 4.2(3) which refers to equation(3) of chapter 4, section 2. Equations which are given in the appendices are referred to as AII(3) in an obvious notation.

APPENDIX IICalculations for Friedmann Metrics

Choose

$$ds^2 = -N(t)^2 dt^2 + R(t)^2 g_{ij} dx^i dx^j \quad (1)$$

i.e.

$$N_i = 0, \quad g_{ij} = R^2(t) \delta_{ij}$$

Now

$${}^4g_{00} = -N^2 \quad {}^4g^{00} = -\frac{1}{N^2} \quad (2)$$

$${}^4g_{0i} = N_i = 0 \quad {}^4g^{0i} = \frac{N^i}{N^2} = 0$$

$${}^4g^{ij} = g^{ij} - \frac{N^i N^j}{N^2} = g^{ij} = \frac{\delta^{ij}}{R^2} \quad (3)$$

Also

$$\sqrt{-{}^4g} = N \sqrt{g}$$

The Christoffel symbols are

$$\Gamma_{00}^0 = \frac{1}{2} g^{00} g_{00,0} = \frac{\dot{N}}{N} \quad (4)$$

$$\begin{aligned} \Gamma_{0i}^0 &= \frac{1}{2} g^{0\beta} (g_{0\beta,i} + g_{i\beta,0} - g_{0i,\beta}) \\ &= \frac{1}{2} g^{00} (g_{00,i} + g_{i0,0} - g_{0i,0}) + \frac{1}{2} g^{0j} (g_{0j,i} + g_{ij,0} - g_{0i,j}) \\ &= 0 \end{aligned} \quad (5)$$

$$\begin{aligned} \Gamma_{00}^i &= \frac{1}{2} g^{i\beta} (g_{0\beta,0} + g_{0\beta,0} - g_{00,\beta}) \\ &= 0 \end{aligned} \quad (6)$$

$$\begin{aligned} \Gamma_{ij}^0 &= \frac{1}{2} g^{0\beta} (g_{i\beta,j} + g_{j\beta,i} - g_{ij,\beta}) \\ &= \frac{1}{2} g^{00} (-g_{ij,0}) \\ &= -\frac{R\dot{R}}{N^2} \delta_{ij} \end{aligned} \quad (7)$$

$$\begin{aligned} \Gamma_{0j}^i &= \frac{1}{2} g^{i\beta} (g_{0\beta,j} + g_{j\beta,0} - g_{0j,\beta}) \\ &= \frac{1}{2} g^{ik} (g_{jk,0}) \\ &= \frac{1}{2} \frac{\delta^{ik}}{R^2} \cdot 2R\dot{R} \delta_{jk} \\ &= \frac{\dot{R}}{R} \delta_{ij} \end{aligned} \quad (8)$$

$$\begin{aligned}
 \Gamma_{jh}^i &= \frac{1}{2} g^{i\beta} (g_{j\beta,h} + g_{h\beta,j} - g_{jh,\beta}) \\
 &= S_{jh}^i
 \end{aligned} \tag{9}$$

which is defined as the Christoffel symbol for $R = 1$

The Ricci tensor is

$$\begin{aligned}
 R_{00} &= \Gamma_{00,\alpha}^\alpha - \Gamma_{0\alpha,0}^\alpha + \Gamma_{00}^\alpha \Gamma_{\alpha\beta}^\beta - \Gamma_{0\beta}^\alpha \Gamma_{0\alpha}^\beta \\
 &= \Gamma_{00,0}^0 - \Gamma_{00,0}^0 - \Gamma_{0i,0}^i + \Gamma_{00}^0 \Gamma_{00}^0 + \Gamma_{00}^0 \Gamma_{0i}^i - \Gamma_{00}^0 \Gamma_{00}^0 - \Gamma_{0j}^i \Gamma_{0i}^j \\
 &= -3 \frac{d}{dt} \frac{\dot{R}}{R} + \frac{\dot{N}}{N} 3 \frac{\dot{R}}{R} - 3 \frac{\dot{R}^2}{R^2}
 \end{aligned} \tag{10}$$

$$\begin{aligned}
 R_{0i} &= \Gamma_{0i,\alpha}^\alpha - \Gamma_{0\alpha,i}^\alpha + \Gamma_{0i}^\alpha \Gamma_{\alpha\beta}^\beta - \Gamma_{0\beta}^\alpha \Gamma_{i\alpha}^\beta \\
 &= \Gamma_{0i,j}^j - \Gamma_{00,i}^0 - \Gamma_{0j,i}^j + \Gamma_{0i}^j \Gamma_{jh}^h - \Gamma_{0h}^j \Gamma_{ij}^h \\
 &= \frac{\dot{R}}{R} (\Gamma_{ih}^h - \Gamma_{ih}^h) \\
 &= 0
 \end{aligned} \tag{11}$$

$$\begin{aligned}
 R_{ij} &= \Gamma_{ij,\alpha}^\alpha - \Gamma_{i\alpha,j}^\alpha + \Gamma_{ij}^\alpha \Gamma_{\alpha\beta}^\beta - \Gamma_{i\beta}^\alpha \Gamma_{j\alpha}^\beta \\
 &= \Gamma_{ij,0}^0 + \Gamma_{ij,h}^h - \Gamma_{ih,j}^h + \Gamma_{ij}^0 \Gamma_{00}^0 + \Gamma_{ij}^0 \Gamma_{0h}^h + \Gamma_{ij}^h \Gamma_{h0}^0 \\
 &\quad - \Gamma_{ih}^0 \Gamma_{j0}^h - \Gamma_{i0}^h \Gamma_{jh}^0 - \Gamma_{ia}^h \Gamma_{ja}^h \\
 &= \frac{d}{dt} \left(\frac{R\dot{R}}{N^2} \right) S_{ij} + \frac{\dot{N}}{N} \frac{R\dot{R}}{N^2} S_{ij} + 3 \frac{\dot{R}}{R} \frac{R\dot{R}}{N^2} S_{ij} \\
 &\quad - 2 \frac{\dot{R}}{R} \frac{R\dot{R}}{N^2} S_{ij} + R_{ij}
 \end{aligned}$$

where R_{ij} is the Ricci tensor formed from the S_{ij}^h .

$$\begin{aligned}
 \text{i.e. } R_{ij} &= R_{ij} + \left\{ \frac{1}{N^2} (\dot{R}^2 + R\ddot{R}) - \frac{2R\dot{R}\dot{N}}{N^3} + \frac{\dot{N}R\dot{R}}{N^3} + \frac{\dot{R}^2}{N^2} \right\} S_{ij} \\
 &= R_{ij} + \left\{ \frac{R\ddot{R}}{N^3} + \frac{2\dot{R}^2}{N^2} - \frac{\dot{N}R\dot{R}}{N^3} \right\} S_{ij}
 \end{aligned} \tag{12}$$

$$R_{00} = -3 \frac{\ddot{R}}{R} + 3 \frac{\dot{N}\dot{R}}{NR} \tag{13}$$

The curvature scalar is given by

$$\begin{aligned}
 {}^4R &= R_{\mu\nu} g^{\mu\nu} = -\frac{R_{00}}{N^2} + g^{ij} R_{ij} \\
 &= -\frac{R_{00}}{N^2} + \frac{1}{R^2} \delta^{ij} R_{ij} \\
 &= \frac{R}{R^2} + \frac{6\ddot{R}}{N^2 R} + \frac{6\dot{R}^2}{N^2 R^2} - \frac{6\dot{N}\dot{R}}{N^3 R}, \quad (14)
 \end{aligned}$$

where

$$R = \delta^{ij} R_{ij}.$$

The Einstein tensor is

$$\begin{aligned}
 G_{00} &= R_{00} + \frac{1}{2} N^2 {}^4R \\
 &= R_{00} - \frac{1}{2} R_{00} + \frac{3N^2}{2R^2} \left\{ \frac{R\ddot{R}}{N^2} + \frac{2\dot{R}^2}{N^2} - \frac{\dot{N}R\dot{R}}{N^3} \right\} + \frac{N^2 R}{2R^2} \\
 &= \frac{3}{2} \left(-\frac{\ddot{R}}{R} + \frac{\dot{N}\dot{R}}{N R} + \frac{\ddot{R}}{R} + \frac{2\dot{R}^2}{R^2} - \frac{\dot{N}\dot{R}}{N R} \right) + \frac{N^2 R}{2R^2} \\
 &= \frac{3\dot{R}^2}{R^2} + \frac{N^2 R}{2R^2} \quad (15)
 \end{aligned}$$

$$\begin{aligned}
 G_0^0 &= -\frac{G_{00}}{N^2} \\
 &= -\frac{3\dot{R}^2}{N^2 R^2} - \frac{R}{2R^2} \quad (16)
 \end{aligned}$$

$$\begin{aligned}
 G_{ij} &= R_{ij} + \left\{ \frac{R\ddot{R}}{N^2} + \frac{2\dot{R}^2}{N^2} - \frac{\dot{N}R\dot{R}}{N^3} \right\} \delta_{ij} \\
 &\quad - \frac{1}{2} R^2 \delta_{ij} \left(-\frac{R_{00}}{N^2} + \frac{3}{R^2} \left\{ \frac{R\ddot{R}}{N^2} + \frac{2\dot{R}^2}{N^2} - \frac{\dot{N}R\dot{R}}{N^3} \right\} + \frac{R}{R^2} \right) \\
 &= R_{ij} + \left(-\frac{3}{2} \frac{R\ddot{R}}{N^2} + \frac{3}{2} \frac{\dot{N}R\dot{R}}{N^3} - \frac{R\ddot{R}}{2N^2} - \frac{\dot{R}^2}{N^2} + \frac{\dot{N}R\dot{R}}{2N^3} - \frac{R}{2} \right) \delta_{ij} \\
 &= R_{ij} + \left(-\frac{2R\ddot{R}}{N^2} + \frac{2\dot{N}R\dot{R}}{N^3} - \frac{\dot{R}^2}{N^2} - \frac{R}{2} \right) \delta_{ij} \quad (17)
 \end{aligned}$$

$$\begin{aligned}
 G_i^j &= \frac{\delta^{jk}}{R^2} G_{ik} \\
 &= \frac{R_i^j}{R^2} + \left(-\frac{2\ddot{R}}{N^2 R} + \frac{2\dot{N}\dot{R}}{N^3 R} - \frac{\dot{R}^2}{N^2 R^2} - \frac{R}{2R^2} \right) \delta_i^j \quad (18)
 \end{aligned}$$

Since the Friedmann constant curvature spaces are Einstein spaces⁽⁵⁵⁾,

$$R_{ij} = 2h S_{ij} \quad (19)$$

i.e.

$$R = 6h \quad (20)$$

Thus the Einstein tensor can be rewritten as

$$G_i^j = \left(-\frac{2R\ddot{R} + \dot{R}^2}{N^2 R^2} + \frac{2\dot{N}\dot{R}}{N^3 R} - \frac{h}{R^2} \right) \delta_i^j \quad (21)$$

$$G_o^o = -3 \frac{\dot{R}^2/N^2 + h}{R^2} \quad (22)$$

Another useful relation is

$${}^3R = \frac{{}^3R}{R^2} = \frac{6h}{R^2} \quad (23)$$

An extremely useful relation between G_o^o and the G_i^j is now derived:

$$\begin{aligned} \frac{d}{dt} (R^3 G_o^o) &= -\frac{d}{dt} \left[3 \left(h + \frac{\dot{R}^2}{N^2} \right) R \right] \\ &= -3 \left(h + \frac{\dot{R}^2}{N^2} \right) \dot{R} - 3R \left(-\frac{2\dot{N}\dot{R}}{N^3} + \frac{2\dot{R}\ddot{R}}{N^2} \right) \\ &= 3\dot{R}R^2 \left(-\frac{h}{R^2} - \frac{\dot{R}^2}{N^2 R^2} + \frac{2\dot{N}\dot{R}}{N^3 R} - \frac{2\dot{R}\ddot{R}}{N^2 R} \right) \\ &= \frac{dR^3}{dt} G_i^i, \quad \nabla_i \quad (24) \end{aligned}$$

The gravitational Lagrangian density for a Friedmann geometry is easily obtained. From (3), (14) and (20), with $K = \frac{1}{2}$,

$$\begin{aligned} \mathcal{L}_G &= N\sqrt{g} \cdot {}^4R \\ &= \sqrt{g} N R^3 \left[\frac{6h}{R^2} + \frac{6\ddot{R}}{N^2 R} + \frac{6\dot{R}^2}{N^2 R^2} - \frac{6\dot{N}\dot{R}}{N^3 R} \right] \end{aligned}$$

$$\mathcal{L}_G = \sqrt{8} \left[6 \hbar N R + \frac{d}{dt} \frac{R^2 \dot{R}}{N} - \frac{R \dot{R}^2}{N} \right].$$

Since a total time derivative can be discarded from the action principle, the Lagrangian density written as

$$\mathcal{L}_G = \sqrt{8} \left(6 \hbar N R - 6 \frac{R \dot{R}^2}{N} \right). \quad (25)$$

By factoring out the $\int \sqrt{8} d^3x$ from the action (since a constant does not affect the field equations) then Lagrangian is

$$L_G = 6 \hbar N R - 6 \frac{R \dot{R}^2}{N} \quad (26)$$

The momentum, π_R , conjugate to the radius, R , is defined as

$$\pi_R = \frac{\partial L_G}{\partial \dot{R}} \quad (27)$$

$$= - \frac{12 R \dot{R}}{N}. \quad (28)$$

Thus

$$\begin{aligned} L_G &= \frac{\pi_R \dot{R}}{2} + 6 \hbar N R \\ &= \pi_R \dot{R} - \frac{\dot{R}}{2 \pi_R} \pi_R^2 + 6 \hbar N R \\ &= \pi_R \dot{R} + N \left(6 \hbar R + \frac{\pi_R^2}{24 R} \right). \end{aligned} \quad (29)$$

Another form of interest is obtained by setting

$$R = R_0 e^{\pm x}. \quad (30)$$

This gives

$$L_G = 6 \hbar N R_0 e^{\pm x} - \frac{6 R_0^3 e^{\pm 3x} \dot{x}^2}{N}. \quad (31)$$

With

$$\pi_x = \frac{\partial L_G}{\partial \dot{x}} \quad (32)$$

$$= - \frac{12 R_0^3 e^{\pm 3x} \dot{x}}{N}, \quad (33)$$

The Lagrangian becomes

$$\begin{aligned}
 L_G &= \frac{\pi_x \dot{x}}{2} + 6\hbar N R_0 e^{\pm x} \\
 &= \pi_x \dot{x} - \frac{\dot{x}}{2\pi_x} \pi_x^2 + 6\hbar N R_0 e^{\pm x} \\
 &= \pi_x \dot{x} + N \left(6\hbar R_0 e^{\pm x} + \frac{\pi_x^2}{24 R_0^3 e^{\pm 3x}} \right) \quad (34)
 \end{aligned}$$

This can be summarized by noting that

$$N R^2 \pi_R^2 + \pi_R \dot{R} = N \pi_x^2 + \pi_x \dot{x} \quad (35)$$

Also of interest is the "York form" where

$$Y = R^3 \quad (36)$$

becomes the Hamiltonian. From (26),

$$\pi_Y = \frac{\partial L_G}{\partial \dot{Y}} \quad (37)$$

$$\begin{aligned}
 &= \frac{\partial}{\partial \dot{Y}} \left(6\hbar N Y^{Y_3} - \frac{2 \dot{Y}^2}{3 N Y} \right) \\
 &= -\frac{4}{3} \frac{\dot{Y}}{N Y} \quad (38)
 \end{aligned}$$

so

$$\begin{aligned}
 L_G &= \frac{\pi_Y \dot{Y}}{2} + 6\hbar N Y^{Y_3} \\
 &= \pi_Y \dot{Y} - \frac{\dot{Y}}{2\pi_Y} \pi_Y^2 + 6\hbar N Y^{Y_3} \\
 &= \pi_Y \dot{Y} + N \left(6\hbar Y^{Y_3} + \frac{3}{8} Y \pi_Y^2 \right) \quad (39)
 \end{aligned}$$

$$= \frac{d}{dt} (\pi_Y \dot{Y}) - Y \ddot{Y} + N \left(6\hbar Y^{Y_3} + \frac{3}{8} Y \pi_Y^2 \right) \quad (40)$$

APPENDIX III

The Scalar Field

The matter Lagrangian (density) is defined to be the usual one for the scalar field (but written covariantly with opposite signature):

$$\mathcal{L}_M = -\frac{1}{2} \sqrt{-g} (g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi + m^2 \phi^2), \quad (1)$$

which gives the stress-energy tensor (using AI(18))

$$T_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi + g_{\mu\nu} \mathcal{L}, \quad (2)$$

where

$$\mathcal{L} = \frac{\mathcal{L}_M}{\sqrt{-g}} = -\frac{1}{2} (g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi + m^2 \phi^2). \quad (3)$$

Use of the Euler-Lagrange equations gives the covariant generalization of the Klein-Gordon equation

$$\nabla_\mu \nabla^\mu \phi - m^2 \phi = 0, \quad (4)$$

where the ∇_μ denotes the covariant derivative. This may be rewritten, using $\sqrt{-g} = N \sqrt{g}$, as

$$+ \partial_\mu (N \sqrt{g} g^{\mu\nu} \partial_\nu \phi) - N \sqrt{g} m^2 \phi = 0. \quad (5)$$

In order to achieve canonical form, the momentum canonical to ϕ is defined as

$$\pi_\phi = \frac{\partial \mathcal{L}_M}{\partial \dot{\phi}}, \quad (6)$$

that is, by using (1),

$$\begin{aligned} \pi_\phi &= -\sqrt{-g} g^{0\mu} \partial_\mu \phi \\ &= \frac{\sqrt{g}}{N} \dot{\phi} - \frac{\sqrt{g}}{N} N^i \partial_i \phi. \end{aligned} \quad (7)$$

Now the Lagrangian density is rewritten as

$$\begin{aligned} \mathcal{L}_M &= -\frac{1}{2} N \sqrt{g} \left[-\frac{1}{N^2} \dot{\phi}^2 + \left(g^{ij} - \frac{N^i N^j}{N^2} \right) \partial_i \phi \partial_j \phi \right. \\ &\quad \left. + 2 \frac{N^i}{N^2} \dot{\phi} \partial_i \phi + m^2 \phi^2 \right] \end{aligned}$$

$$\begin{aligned}
\mathcal{L}_m &= \frac{1}{2} \frac{\sqrt{g}}{N} \dot{\phi}^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi + \frac{1}{2} \frac{\sqrt{g}}{N} N^i N^j \partial_i \phi \partial_j \phi \\
&\quad - \sqrt{g} \frac{N^i}{N} \phi \partial_i \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \quad (8) \\
&= \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \pi_\phi (\dot{\phi} - N^i \partial_i \phi) - \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi \\
&\quad - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \pi_\phi \dot{\phi} - N \left(\frac{1}{2} \frac{\pi_\phi^2}{\sqrt{g}} + \frac{\sqrt{g}}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{\sqrt{g}}{2} m^2 \phi^2 \right) \\
&\quad - N^i \pi_\phi \partial_i \phi. \quad (9)
\end{aligned}$$

This is precisely of the form required so that when added to the gravitational Lagrangian density, the structure is maintained, viz. a canonical pair of dynamical variables is added and extra terms are added to the Hamiltonian and momentum constraints (see Ryan⁽⁵¹⁾ for general remarks and Deser and Higbie⁽⁷⁶⁾ for this Lagrangian density with mass zero as a special case of their considerations). Thus

$$2K\mathcal{L} = -\dot{\pi}^{ij} g_{ij} + \pi_\phi \dot{\phi} - N_\mu \bar{C}^\mu + \mathcal{D} \quad (10)$$

where

$$\begin{aligned}
\bar{C}^0 &= -\sqrt{g} {}^3R + \frac{1}{\sqrt{g}} \left(\pi^{ij} \pi_{ij} - \frac{1}{2} (\pi^k_k)^2 \right) \\
&\quad + 2K \left(\frac{1}{2} \frac{\pi_\phi^2}{\sqrt{g}} + \frac{\sqrt{g}}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{\sqrt{g}}{2} m^2 \phi^2 \right) \quad (11)
\end{aligned}$$

$$\begin{aligned}
\mathcal{L}_m &= \frac{1}{2} \frac{\sqrt{g}}{N} \dot{\phi}^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi + \frac{1}{2} \frac{\sqrt{g}}{N} N^i N^j \partial_i \phi \partial_j \phi \\
&\quad - \sqrt{g} \frac{N^i}{N} \phi \cdot \partial_i \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \quad (8) \\
&= \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \pi_\phi (\dot{\phi} - N^i \partial_i \phi) - \frac{1}{2} \frac{N}{\sqrt{g}} \pi_\phi^2 - \frac{1}{2} N \sqrt{g} g^{ij} \partial_i \phi \partial_j \phi \\
&\quad - \frac{1}{2} N \sqrt{g} m^2 \phi^2 \\
&= \pi_\phi \dot{\phi} - N \left(\frac{1}{2} \frac{\pi_\phi^2}{\sqrt{g}} + \frac{\sqrt{g}}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{\sqrt{g}}{2} m^2 \phi^2 \right) \\
&\quad - N^i \pi_\phi \partial_i \phi. \quad (9)
\end{aligned}$$

This is precisely of the form required so that when added to the gravitational Lagrangian density, the structure is maintained, viz. a canonical pair of dynamical variables is added and extra terms are added to the Hamiltonian and momentum constraints (see Ryan⁽⁵¹⁾ for general remarks and Deser and Higbie⁽⁷⁶⁾ for this Lagrangian density with mass zero as a special case of their considerations). Thus

$$2\kappa \mathcal{L} = -\dot{\pi}^{ij} g_{ij} + \pi_\phi \dot{\phi} - N_\mu \bar{\mathcal{C}}^\mu + \mathcal{D} \quad (10)$$

where

$$\begin{aligned}
\bar{\mathcal{C}}^0 &= -\sqrt{g} \cdot {}^3R + \frac{1}{\sqrt{g}} \left(\pi^{ij} \pi_{ij} - \frac{1}{2} (\pi^k_k)^2 \right) \\
&\quad + 2\kappa \left(\frac{1}{2} \frac{\pi_\phi^2}{\sqrt{g}} + \frac{\sqrt{g}}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{\sqrt{g}}{2} m^2 \phi^2 \right) \quad (11)
\end{aligned}$$

$$\bar{C}^i = -2\pi^{ij}{}_{|j} + 2\kappa \pi_\phi g^{ij} \partial_j \phi, \quad (12)$$

and

$$\mathcal{D} = -2 \left(\pi^{ij} N_j - \frac{1}{2} \pi_j^j N^i + \sqrt{g} g^{ij} N_{,j} \right)_{,i}.$$

The divergence $\mathcal{D}$ is discarded, as before in the purely gravitational case. Also, the Einstein coupling constant is set equal to a half so that the 2κ factors disappear. This is equivalent to rescaling the ϕ (π_ϕ) by $\sqrt{2\kappa}$.

For convenience, the stress-energy tensor is re-expressed in various forms here:

$$T_\mu{}^\nu = g^{\rho\nu} \partial_\mu \phi \partial_\rho \phi + \delta_\mu{}^\nu L \quad (13)$$

and

$$T^{\mu\nu} = g^{\sigma\mu} g^{\rho\nu} \partial_\sigma \phi \partial_\rho \phi + g^{\mu\nu} L. \quad (14)$$

Now

$$\begin{aligned} L = & \frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{1}{2} \frac{N^i N^j}{N^2} \partial_i \phi \partial_j \phi \\ & - \frac{N^i}{N^2} \dot{\phi} \partial_i \phi - \frac{1}{2} m^2 \phi^2, \end{aligned} \quad (15)$$

So

$$\begin{aligned} T_0{}^0 = & -\frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} g^{ij} \partial_i \phi \partial_j \phi + \frac{1}{2} \frac{N^i N^j}{N^2} \partial_i \phi \partial_j \phi \\ & - \frac{N^i}{N^2} \dot{\phi} \partial_i \phi - \frac{1}{2} m^2 \phi^2 \end{aligned} \quad (16)$$

$$\begin{aligned} T_0{}^i = & g^{0i} \dot{\phi} \partial_0 \phi + g^{ij} \dot{\phi} \partial_j \phi \\ = & N^i \frac{\dot{\phi}^2}{N^2} + g^{ij} \dot{\phi} \partial_j \phi - \frac{N^i N^j}{N^2} \dot{\phi} \partial_j \phi \end{aligned} \quad (17)$$

$$\begin{aligned}
 T_i^j &= 4 g^{\rho j} \partial_i \phi \partial_\rho \phi + \delta_i^j L \\
 &= N^j \dot{\phi} \partial_i \phi + g^{kj} \partial_i \phi \partial_k \phi - \frac{N^k N^j}{N^2} \partial_i \phi \partial_k \phi + \delta_i^j L \quad (18)
 \end{aligned}$$

In the special case of a homogeneous scalar field, $\phi = \phi(t)$
i.e $\partial_i \phi$, then

$$\mathcal{L}_m = \pi_\phi \dot{\phi} - N \left(\frac{1}{2} \frac{\pi_\phi^2}{\sqrt{g}} + \frac{\sqrt{g}}{2} m^2 \phi^2 \right) \quad (19)$$

where

$$\pi_\phi = \frac{\sqrt{g}}{N} \dot{\phi} \quad (20)$$

Also

$$L = \frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} m^2 \phi^2, \quad (21)$$

$$T_0^0 = -\frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} m^2 \phi^2, \quad (22)$$

$$T_0^i = N^i \frac{\dot{\phi}^2}{N^2}, \quad (23)$$

and

$$T_i^j = \delta_i^j \left(\frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} m^2 \phi^2 \right). \quad (24)$$

The covariant Klein-Gordon equation, (5), becomes

$$\partial_\mu (N \sqrt{g} g^{\mu 0} \dot{\phi}) - N \sqrt{g} m^2 \phi = 0$$

i.e.

$$\partial_0 \left(-\frac{\sqrt{g}}{N} \dot{\phi} \right) + \dot{\phi} \partial_i (N \sqrt{g} N^i) - N \sqrt{g} m^2 \phi = 0, \quad (25)$$

which is

$$\frac{d}{dt} \left(\frac{\sqrt{g}}{N} \dot{\phi} \right) + N \sqrt{g} m^2 \phi = 0 \quad (26)$$

if

$$\partial_i (N \sqrt{g} N^i) = 0. \quad (27)$$

For a general scalar field with the choice of $N_i = 0$, equations (16), (17), (18) become

$$T_o^o = -\frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} g^{ij} \partial_i \phi \partial_j \phi - \frac{1}{2} m^2 \phi^2 \quad (28)$$

$$T_o^i = g^{ij} \dot{\phi} \partial_j \phi \quad (29)$$

$${}^4T_i{}^j = g^{hj} \partial_i \phi \partial_h \phi + \delta_i^j \left\{ \frac{1}{2} \frac{\dot{\phi}^2}{N^2} - \frac{1}{2} g^{rs} \partial_r \phi \partial_s \phi - \frac{1}{2} m^2 \phi^2 \right\} \quad (30)$$

$${}^4T = {}^4T_\mu{}^\mu = \frac{\dot{\phi}^2}{N^2} - g^{ij} \partial_i \phi \partial_j \phi - 2m^2 \phi^2 \quad (31)$$

Now

$$G_\mu{}^\nu = R_\mu{}^\nu - \frac{1}{2} \delta_\mu{}^\nu {}^4T = K T_\mu{}^\nu$$

gives

$$-{}^4R = K {}^4T,$$

$$R_\mu{}^\nu = K \left(T_\mu{}^\nu - \frac{1}{2} \delta_\mu{}^\nu {}^4T \right) = K J_\mu{}^\nu, \quad (32)$$

so the $J_\mu{}^\nu$ are of interest and are given by

$$J_o^o = -\frac{\dot{\phi}^2}{N^2} + \frac{1}{2} m^2 \phi^2 \quad (33)$$

$$J_o^i = g^{ij} \dot{\phi} \partial_j \phi \quad (34)$$

$$J_i{}^j = g^{hj} \partial_i \phi \partial_h \phi + \delta_i^j \cdot \frac{1}{2} m^2 \phi^2 \quad (35)$$

APPENDIX IVTime Dependent Hamiltonians

The time dependent Schrödinger equation is⁽³²⁾

$$\hat{H}(\hat{x}, \hat{p}, t) \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \quad (1)$$

Thus

$$\hat{H}^2 \psi = i\hbar \hat{H} \frac{\partial \psi}{\partial t} = i\hbar \frac{\partial}{\partial t} (\hat{H} \psi) - i\hbar \dot{\hat{H}} \psi$$

$$\text{i.e.} \quad \hat{H}^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial t^2} - i\hbar \dot{\hat{H}} \psi \quad (2)$$

Now

$$\psi_s(t) = T e^{-i \int_0^t \hat{H}(s) ds / \hbar} \psi_s(0) \quad (3)$$

where T denotes time ordering, gives back

$$i\hbar \frac{\partial \psi_s(x, t)}{\partial t} = \hat{H}(t) \psi_s(x, t). \quad (4)$$

The time ordering may be omitted
provided that $[\hat{H}(t), \hat{H}(t')] = 0$.

If it is assumed that $\psi_E(x, t)$ is such that

$$\hat{H} \psi_E(x, t) = E(t) \psi_E(x, t) \quad (5)$$

which is interpreted as a continuously changing eigenvalue equation, then

$$\hat{H}^2 \psi_E(x, t) = E^2 \psi_E(x, t) \quad (6)$$

Now from the time derivative of (4)

$$\dot{\hat{H}} \psi_E + \hat{H} \dot{\psi}_E = \dot{E} \psi_E + E \dot{\psi}_E,$$

which gives

$$\dot{\hat{H}} \psi_E = \dot{E}(t) \psi_E(x, t) \quad (7)$$

Thus, from (2), (5), (6)

$$E^2(t) \psi_E + \hbar^2 \frac{\partial^2}{\partial t^2} \psi_E + i \hbar \dot{E}(t) \psi = 0. \quad (8)$$

This is the "Klein-Gordon" equation and the Schrödinger equation is

$$i \hbar \frac{\partial \psi_E(x,t)}{\partial t} = E(t) \psi_E(x,t). \quad (9)$$

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