Quantum Cosmology

and the

Decoherent Histories Approach
to
Quantum Theory

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ABSTRACT

In the canonical approach to quantum cosmology the wave function of the universe is annihilated by the total Hamiltonian constraint due to the diffeomorphism invariance of general relativity (or reparametrization invariance for simpler models). Such a system does not possess a uniquely defined time parameter and all physical questions about it must be posed without reference to time. We therefore consider the question: What is the quantum probability that the system enters a region $\Delta$ without any reference to time at all? We use the decoherent histories approach to quantum theory to obtain this probability. The decoherence functional is constructed using path integral methods with initial states attached using the (positive definite) “induced” inner product between solutions to the constraint equation. The construction is complicated by the fact that the amplitudes (class operators) calculated using a path integral typically do not satisfy the constraint equation everywhere, but we show how they may be systematically modified in such a way that they do satisfy the constraint.

A first testing ground is the relativistic particle where we choose $\Delta$ to be a section of a spacelike hypersurface. Different possible results for the probabilities are obtained, depending on how the relativistic particle is quantized (using the Klein-Gordon equation, or its square root, with the associated Newton-Wigner states). We compare and find agreement with the results obtained using operators which commute with the constraint (the “evolving constants” method).

We then consider a more general reparametrization invariant system and
a general region $\Delta$. We first analyze the classical case, where the answer has a variety of forms in terms of a phase space probability distribution function. In the quantum case, when the histories are decoherent, the probabilities approximately coincide with the classical case, with the phase space probability distribution replaced by the Wigner function of the quantum state. For most initial states, decoherence requires an environment, and we compute the required influence functional and examine some of its properties. Special attention is given again to the construction of class operators describing the histories, and also to the extent to which reparametrization invariance is respected. The results support, for simple models, the usual heuristic proposals for the probability distribution function associated with a semiclassical wave function satisfying the Wheeler-DeWitt equation.

Finally we derive a master equation for the reduced density matrix of a quantum cosmological model in a semiclassical approximation. We investigate the effect of the different terms and compare with the standard master equation for Quantum Brownian motion. We reproduce and extend the result that in quantum cosmology a different term is responsible for decoherence. We also compare with the results obtained by using the decoherent histories approach.
For Rabea

who decided to endure a theoretical physicist

For My Parents
Preface

The work presented in this thesis was carried out in the Theoretical Physics Group, Imperial College, London between January 1999 and May 2002. The supervisor was Dr. Jonathan J. Halliwell.

The results presented in Chapter 2 and Chapter 3 were published in collaboration with Jonathan Halliwell in Physical Review D, Refs. [43] and [44]. We are grateful to Jim Hartle, John Klauder and Don Marolf for useful discussions and conversations.

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Contents

Abstract 2

Preface 5

Conventions and Abbreviations 9

List of Figures and Tables 10

1 Introduction 11

1.1 The Problem: How Can We Observe the Wave Function of the Universe? . 11

1.1.1 Overview of the Thesis . . . . . . . . . . . . . . . . . . . . . . . . . . 16

1.2 The Ingredients . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 18

1.2.1 Properties and Observables of Reparametrization Invariant Systems 18

1.2.2 Quantization of Reparametrization Invariant Systems – the Rieffel induced inner product . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 20

1.2.3 The Decoherent Histories Approach to Quantum Theory . . . . . . . . 23

1.3 Our Approach . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 26

1.3.1 The Decoherence Functional For Reparametrization Invariant Models 26

1.4 Relation to other work . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 28


2 Decoherent Histories Analysis of the Relativistic Particle 30

2.1 Introduction ......................................................... 30

2.1.1 Summary of this Chapter .......................... 34

2.2 The Parametrized Non-Relativistic Particle ................. 35

2.3 Green Functions of the Klein-Gordon equation ............. 39

2.4 An Operator Approach for the Klein-Gordon Equation .......... 42

2.5 Decoherent Histories Analysis in the Klein-Gordon Quantization .... 46

2.5.1 The Class Operator for Not Crossing a Spacelike Surface ... 46

2.5.2 Crossing Propagators and the Path Decomposition Expansion .... 50

2.5.3 First and Last Crossing Relativistic Propagators ............ 51

2.5.4 General Prescription for Constructing Modified Class Operators .... 54

2.5.5 A Multiple Crossings Decomposition? .................. 56

2.6 The Newton-Wigner Case .............................................. 58

2.7 Summary and Discussion ........................................... 60

3 Life in an Energy Eigenstate:

Decoherent Histories Analysis of a Model Timeless Universe 63

3.1 Introduction ............................................................... 63

3.2 The Classical Case ................................................... 65

3.2.1 Normalization of the classical phase space distribution function ... 70

3.3 The Quantum Case ...................................................... 72

3.3.1 Construction of the Decoherence Functional .................... 72

3.3.2 Modified Class Operators ...................................... 74

3.4 The Semiclassical Approximation to the Decoherence Functional and Probabilities .............................................. 75
CONTENTS

3.5 Systems of Harmonic Oscillators ........................................ 79
3.6 Decoherence Through an Environment .................................. 84
  3.6.1 Semiclassical Approximation to the Decoherence Functional with Environment ........................................ 84
  3.6.2 Calculation of the Influence Functional ................................. 86
  3.6.3 Reparametrization Invariance in the Influence Functional .......... 88
  3.6.4 Decoherence and the Evaluation of the $v$ Integral .................. 90
3.7 Superposition States ............................................................ 92
3.8 Summary and Discussion ....................................................... 94

4 The Master Equation in Quantum Cosmology ................................ 96
  4.1 Introduction ........................................................................ 96
  4.2 The Master Equation for Quantum Brownian Motion .................... 98
  4.3 The Master Equation for a Quantum Cosmological Model ............... 100
    4.3.1 The Semiclassical Reduced Density Matrix and the Corresponding Wigner Function ........................................ 101
    4.3.2 The Derivation of the Master Equation for $\rho_{\text{red}}$ .................. 102
    4.3.3 Discussion of the Derived Master Equation .......................... 103
    4.3.4 Relation to Other Work .................................................. 106
  4.4 Conclusions and Discussion .................................................. 107

5 Summary and Outlook ............................................................. 108

Figures ....................................................................................... 112

Bibliography .............................................................................. 121
Conventions and Abbreviations

When not explicitly written out, natural units are used: $\hbar = c = 1$.

$\langle \mid A \rangle, \langle \mid I \rangle, \langle \mid KG \rangle$ and $\langle \mid S \rangle$ are the auxiliary, induced, Klein-Gordon and Schrödinger inner product.

$\Delta (\Delta')$ is used as the symbol for the history of entering (not entering) the region $\Delta$.

$g_\Delta(x_f, t_f|x_0, t_0)$ is the restricted propagator representing the history of entering the region $\Delta$.

$g_{\Delta'}(x_f, t_f|x_0, t_0)$ is the restricted propagator representing the history of not entering the region $\Delta$.

The signature of the spacetime metric used in Chapter 2 is $(+,−,−,−)$ following [42].

We use the following summation convention: two identical indices are summed over.

In Chapter 2 Greek indices run from 0 to 3, Latin indices from 1 to 3.

Figures are all at the end of the thesis, starting on page 112.

Abbreviations

PDX : path decomposition expansion, explained on page 50
List of Figures and Tables

Table 1: The different class operators used in Section 2.5 . . . . . . . . 47

Figure 1 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 112
Figure 2 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 113
Figure 3 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 114
Figure 4 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 115
Figure 5 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 115
Figure 6 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 116
Figure 7 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 116
Figure 8 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 117
Figure 9 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 117
Figure 10 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 118
Figure 11 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 119
Figure 12 . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 120
Chapter 1

Introduction

1.1 The Problem: How Can We Observe the Wave Function of the Universe?

Or to formulate the problem in more technical terms:

What are appropriate mathematical objects to derive probabilities for physical properties in canonical quantum cosmology?

Quantum cosmology attempts to regard the whole Universe as a quantum system. Some may say that this is a futile enterprise, since quantum effects on such large scales have never been measured. But there are several good reasons for undertaking it. First of all, all physical experiments show that our world is fundamentally quantum, so it is valid to assume that this is also true for the whole universe. Secondly, since the universe is expanding, it once has been smaller and general relativity predicts that it was created in a Big Bang. For times just after the Big Bang, the scales were such that quantum gravitational effects have to be taken into account. Thirdly, general relativity sees the Big Bang as a singularity and hence breaks down there. It cannot say anything about initial conditions for the evolution of the universe and an important part of quantum cosmology is to find such initial conditions.
But from the outset quantum cosmology has certain difficulties to deal with. First of all, in a quantum universe there is nothing classical left over (especially there is no approximately classical laboratory outside the universe). Even space and time are somehow quantized. But since our minds tend to use classical objects, there is a tension between the mind and the physical theory. For another, the evolution of the universe is dominated by gravity, and so quantum cosmology needs a quantum theory of gravity. Up to now, a fully consistent theory of quantum gravity does not exist. There are several suggestions how to find one, for example from string theory or a path integral formulation. In this thesis we will work in the canonical approach to quantum gravity. None of these approaches is yet fully conclusive although some of them have got quite far and make interesting predictions. If one tries to do quantum cosmology, one is testing these approaches. So one may sum up the immediate difficulty in quantum cosmology as follows: One tries to describe something far beyond daily experience in a language one does not know yet or is not very sure about. Maybe this is the reason that the search for a fundamental theory of quantum gravity has been going on now for nearly seventy years.

As already mentioned, we are using the canonical approach to quantum gravity in this thesis. This approach starts by rewriting general relativity in Hamiltonian form. Since diffeomorphism invariance is the symmetry of general relativity, general relativity is a constrained system. The total Hamiltonian is a sum of constraints. In the Dirac quantization procedure \[18, 57\] the classical constraints become operators that annihilate the physical wave functions of the quantum system. In general relativity the important constraint is the Hamiltonian constraint which gives the famous Wheeler-DeWitt equation
\[
\hat{H}(h_{ab}, \phi)\Psi[h_{ab}, \phi] = 0 ,
\]
first developed and investigated by Wheeler and DeWitt in the 60s \[17, 109\].

\(h_{ab}\) is the Riemannian metric on a three dimensional hypersurface and \(\phi\) represents some matter fields. Classically the time evolution of \(h_{ab}\) corresponds to the evolution of the induced metric on a spacelike hypersurface which is pulled through spacetime. If we apply this equation to the whole Universe, we enter the area of quantum cosmology and \(\Psi\) is then called the ‘wave function of the Universe’\[52\].

Although written above in a simple way, the Wheeler-DeWitt equation has several
severe mathematical and conceptual problems. The mathematical problems have to do with the fact that one is dealing with a quantum field theory. One has to use the correct representation for the above equation. One also has to renormalize various operators correctly and then identify the space of physical states $\Psi_{\text{phys}}$ that obey the Wheeler-DeWitt equation (1.1.1). A very successful approach has used the so-called loop variables (for a nice review see [103]). These problems will not be of direct relevance to the work presented in this thesis.

Related to these problems is the choice of the inner product on the space of the physical states $\Psi_{\text{phys}}$. This is of importance for us as we want to calculate probabilities using scalar products of state vectors. We are going to use the Rieffel induced inner product, also known as refined algebraic quantization or group averaging [2, 19, 27, 28, 51, 58, 78]. The procedure to get this inner product has been successfully used for quantum cosmological models as well as for the loop variable approach. More on this product will be said in Section 1.2.2.

The problem we are considering in this thesis is how to understand and interpret the Wheeler-DeWitt equation from a conceptual point of view. For one thing the universe is a genuinely closed system and one has to consider the quantum theory of closed systems. But the most significant feature of the Wheeler-DeWitt equation is that it contains absolutely no reference to time whatsoever. There is nothing analogous to the time dependent Schrödinger equation in quantum gravity. This is not surprising since spacetime itself is the object of quantization. In normal quantum field theory spacetime still provides the background for the quantum fields to propagate on. In quantum gravity this background is lost.

It is usually argued that “time”, or more precisely, the physical systems that we use to measure time, are contained already in the gravitational and matter fields [13, 61, 75–77]. While this is very plausible it leaves us with the question as to how to extract interesting physical predictions from this wave function, given the absence of the time coordinate that plays a central role in standard quantum theory.

To separate some of the mathematical problems from the conceptual ones, one often uses simplified models. One can impose additional symmetries on the degrees of freedom
to get the so-called minisuperspace models. For example, one starts from the Robertson-Walker metric with the scale factor \( a \) of the Universe as the only gravitational degree of freedom. If one minimally couples a homogenous scalar field \( \phi \) and quantizes this model, the Wheeler-DeWitt equation has the form (assuming a closed universe)

\[
\hat{H}\Psi(a, \phi) = \left( \frac{1}{2Ma} \frac{\partial^2}{\partial a^2} - \frac{M}{2} a - \frac{1}{2a^3} \frac{\partial^2}{\partial \phi^2} + a^3 V(\phi) \right) \Psi(a, \phi) = 0 .
\] (1.1.2)

where \( M \) is proportional to the square of the Plank mass (see [11] for a reduced phase space quantization of this model). The remnant of the diffeomorphism invariance of full general relativity is the reparametrization invariance of these kinds of models (the action is invariant under reparametrizations of its time label). More on systems obeying this invariance will be said in Section 1.2.1. In this thesis we will only confine ourselves to these kinds of models.

With these kinds of models, heuristic methods (mainly the “WKB interpretation”) have been used to extract useful predictions [36] for quantum cosmological questions like the initial conditions of the universe. What we are concerned with in this thesis is how such heuristic ideas may be incorporated in a properly defined interpretational framework for the quantum theory of timeless models.

An open question is how far the simple models capture properties of the full theory. Although the simple minisuperspace models are unlikely to be reasonable physical approximations to a full quantum gravity theory, it does seem likely that a quantum theory of gravity will center around a timeless equation of the form (1.1.1) (the loop variable approach, for example, involves such an equation), hence it remains important to understand the quantization and interpretation of such systems at an elementary level.

Explicitly we want to investigate how to define probabilities for certain properties of reparametrization invariant systems like the quantum cosmological minisuperspace models. Inspired by ideas formulated by Barbour about timeless theories [5–7] we are going to look at timeless properties for these systems, that means properties that do not involve time or the notion of an instant in time at all. But the crucial hurdle is how to mathematically formulate such a type of question in the case of quantum systems. There is a variety of interesting physical situations in which our classical view of the world inspires us to ask questions that quantum theory does not easily answer. For example, classical mechanics
CHAPTER 1. INTRODUCTION

concerns simultaneously specified values of coordinates and momenta while quantum theory has to go through some contortions to say what this means operationally. Another important class of problems of this type involve time in a non-trivial way. The arrival time problem and tunnelling time problem, for example, have been the subject of considerable recent interest [1].

Furthermore one can formulate questions that do not involve time at all. These kinds of questions are not unnatural in physics. Consider for example the following case. Suppose we have a system of particles in a state of fixed total energy. It could, for example, be a light particle orbiting a massive particle. Then classically, we can ask whether the light particle passes through a certain region of configuration space at any stage during its orbit. Or we can ask which of the possible classical orbits the light particle follows (For an example see Fig. 1). The important point here is that these sorts of questions do not involve time explicitly. Much experimental and observation data is in fact of this type. For example, astronomical observations yield planetary orbits, and particle physics experiments often yield a photograph of a track in a bubble chamber. So for example, suppose the coordinates of the system are \( x = (x_1, x_2, \cdots x_n) \), we can ask: What is the probability distribution of, say, \( x_2, \cdots x_n \), given the value of \( x_1 \)?

In this thesis we will be mainly concerned with the following of these kind of questions: Given that the system is in an energy eigenstate or obeys a Wheeler-DeWitt type equation, what is the probability that it enters a certain region \( \Delta \) of configuration space, irrespective of time?

Classically, this question may be answered reasonably easily. We look for all the phase space initial data points whose classical trajectories pass through \( \Delta \), and then the desired probability for entering \( \Delta \) is the probability measure on this subset of phase space. As we shall see in more detail, the question is considerably more complicated in quantum theory.

One significant approach to this kind of problem that is currently being pursued involves constructing quantum operators corresponding to the classical observables representing the mentioned questions. An important feature of these operators is that they have to commute with the constraints to be gauge invariant “quantum observables” [16, 80–82, 84, 99–102]. Since in the case of reparametrization invariant systems the Hamiltonian
itself is the constraint, these observables cannot show any time evolution and are therefore also known as “evolving constants”. We will say some more about them in Sections 1.2.1 and 1.2.2.

However, the timeless aspects of quantum cosmology outlined above suggest that a particularly useful approach to quantization is the decoherent histories approach [22–24, 29–31, 38, 48, 89–95][For further developments in the decoherent histories approach, particularly adapted to the problem of spacetime coarse grainings, see [62–64]). This is because it deals directly with entire trajectories and does not obviously require a time coordinate. One aim of this thesis is to show that the decoherent histories approach can be used to calculate probabilities for histories in configuration space in simple timeless models. In particular, we shall show in Chapter 3 that in the classical limit, the decoherent histories approach produces a set of classical trajectories with a probability measure on that set. A comparison with the “evolving constants” approach mentioned above will be made in Chapter 2 for the relativistic particle.

1.1.1 Overview of the Thesis

Let us now give a brief overview of the contents of this thesis.

The remaining sections of this chapter will be introductory. In Section 1.2 we will give a short introduction to reparametrization invariant models and how one quantizes them. The second part will be a short review of the decoherent histories approach to quantum theory.

In Section 1.3 we apply the decoherent histories approach to reparametrization invariant systems and suggest an expression for the probability of the system entering a certain region in configuration space, irrespective of time. This is the main question that will be followed throughout the thesis.

In Section 1.4 we describe the relation of the research presented in this thesis to the work of other researchers.

In Chapter 2 we apply our formalism to the relativistic particle. As our region \( \Delta \) we choose a subset of the spacelike hypersurface \( x^0 = \tau \). We consider the Newton-Wigner and
Klein-Gordon quantization of the relativistic particle and construct operators corresponding to crossing $x^0 = \tau$. With these operators we will get expressions for crossing $\Delta$ in the operator approach. The second part of this chapter is then devoted to the decoherent history analysis of crossing this region. A problem will be the correct definition of the class operators corresponding to the history of crossing or not crossing $\Delta$. After solving this, we obtain expressions for the probabilities that agree with those obtained in the operator approach.

In Chapter 3 we now consider a more general reparametrization invariant model and a general region $\Delta$ (which for some calculations has to be open). We discuss the classical case and find a phase space distribution that is the classical observable for entering $\Delta$. It also leads to the standard heuristic interpretation of WKB wave functions for quantum cosmological models.

In Section 3.3 we start to set up the decoherence functional for the quantum case. We find that we have to modify the class operators again, so that they obey the constraint. We manage to find them in a semiclassical approximation. If one has decoherence, the decoherence functional reduces to the classical result. For a harmonic oscillator we use timeless coherent states to discuss the probability of entering a series of regions $\Delta$ that lie along a classical path. Finally we introduce an environment. We show that this environment leads to decoherence for single and superpositions of initial WKB states and that the influence functional respects the reparametrization invariance.

These results motivate us to derive the master equation for a semiclassical quantum cosmological density matrix in Chapter 4. The master equation has proven to be a useful tool to study decoherence for quantum mechanical models. We reproduce and extend a previous quantum cosmological master equation and compare it with the results using the decoherent histories approach.

Finally we summarize the main results of this thesis in Chapter 5 and mention open questions which the research for this thesis has raised.
1.2 The Ingredients

1.2.1 Properties and Observables of Reparametrization Invariant Systems

The characterizing property of reparametrization invariant systems is that the form of their action \( S = \int_0^\lambda d\lambda' \mathcal{L}(q, \dot{q}) \) is invariant under reparametrizations of the time label \( \lambda' \). Hence time reparametrizations (which are of the form \( \lambda' \rightarrow f(\lambda') \)) are a gauge symmetry for this kind of system. One has a free choice of the parameter \( \lambda \) to describe the evolution of the system (up to some minor restrictions concerning the functions \( f \) like them being monotonic).

Examples are the relativistic particle or actions for cosmological models that are derived by implementing symmetries in the full Einstein action. One can also transform any standard theory where time \( t \) is a physical parameter into this form by turning \( t \) into a canonical variable. One example for this procedure (called parametrization) is the parametrized non-relativistic particle.

If \( q \) and its conjugate momentum \( p \) transform as scalars under the reparametrizations, the Hamiltonian analysis gives an action of the form

\[
S = \int_0^\lambda d\lambda' \left( p \frac{dq}{d\lambda'} - NH(q, p) \right)
\]

(1.2.1)

where \( N \) is a Lagrange multiplier. Variation of this action leads to the fact that the Hamiltonian \( H \) itself is a constraint of a system. For the actual evolution \( q(\lambda), p(\lambda) \) of the system we have

\[
H(q, p) = 0
\]

(1.2.2)

For example, the Hamiltonian analysis of the relativistic particle gives the constraint \( p^\mu p_\mu - m^2 = 0 \): the mass shell condition for relativistic particles.

What are the physical consequences if the time label of the action is not a physical parameter anymore? In a standard non-relativistic particle theory, the variables of interest are, for example, positions at a fixed moment of time \( x(t) \). In this case, the time \( t \) is regarded as an observable physical parameter. In a theory without time, by contrast, the quantities of interest are curves in configuration space \( x(\lambda) \) (or more generally, in
phase space). Here, $\lambda$ is not a physically measurable time, but is simply a parameter labelling the points along the curve, and the curves are parameterized in this way for mathematical convenience. Furthermore, one of the characteristic features of genuinely timeless theories is that none of the components of $x$ is monotonic in $\lambda$. This means that it is not possible to use one of the components of $x$ as a “time” parameter, except for local sections of the curve. Despite these features, such classical theories are well-defined and predictive. Indeed, many classical cosmological models are of this type. For example, in the massive scalar field cosmological model (for a positive curvature Friedman-Robertson-Walker metric) [54], the classical solutions go backwards and forwards in both the scale factor $a$ and the scalar field $\phi$. Therefore, the most general such classical theory is one in which there is a probability distribution on the set of classical trajectories, and this is also well-defined (subject to careful normalization) as we shall see in Chapter 3. Such probability distributions are of particular interest for predicting, for example, the likelihood of the initial conditions for inflation [55, 56].

A closely related issue is the fact that reparametrization invariance is essentially the freedom to redefine the parameter $\lambda$ labelling points along a trajectory. Individual phase space points are not reparametrization-invariant, since they are moved along the classical trajectories by a reparametrization. But a useful invariant quantity is the entire classical trajectory, as we shall see later in more detail. This simple observation turns out to be an especially useful focal point for what we do in Chapter 3.

This also means that the physical observables $O(q,p)$ for reparametrization invariant systems should not distinguish points along trajectories. Or to formulate it in terms of a gauge theory; the observables have to be invariant under gauge transformations generated by the constraint $H$, which means that they must have a vanishing Poisson bracket with the constraint. So a physical observable has to obey $\{O, H\} = 0$. They will be constant along the trajectories and show no dynamics.

For a free particle in two dimensions, for example, the classical trajectories with initial conditions $\tilde{x}_i$, $\tilde{p}_i$ have the form,

$$x_1(t) = \tilde{x}_1 + \frac{\tilde{p}_1}{m} t, \quad x_2(t) = \tilde{x}_2 + \frac{\tilde{p}_2}{m} t$$  \hspace{1cm} (1.2.3)
and we may eliminate $t$ between them to write,

$$x_1 = \tilde{x}_1 + \frac{\tilde{p}_1}{\tilde{p}_2} (x_2 - \tilde{x}_2) \quad (1.2.4)$$

This is the classical answer to the question “What is the value of $x_1$ at a given value of $x_2$?” which does not refer to a external time parameter.

More details about these systems and their properties can be found in Chapter 4 of Ref. [57].

### 1.2.2 Quantization of Reparametrization Invariant Systems – the Rieffel induced inner product

If one applies the Dirac quantization procedure [18, 57] to quantize reparametrization invariant systems, one represents the constraint $H$ as a constraint operator $\hat{H}$ on a auxiliary Hilbert space with an inner product like

$$\langle \Psi | \Phi \rangle_A = \int d^n x \ \Psi^*(x) \Phi(x) \quad (1.2.5)$$

The physical states $\Psi_{\text{phys}}$ have to be annihilated by $\hat{H}$, i.e.

$$\hat{H}(x) \Psi_{\text{phys}}(x) = 0 \quad (1.2.6)$$

so that they are invariant under the gauge transformations $e^{i \varepsilon \hat{H}}$.

Thus one obtains the vector space of physical states. But if the constraint operator $\hat{H}$ has a continuous spectrum around zero, this leads to the fact that the physical states are not normalizable in the auxiliary Hilbert space inner product.

The Rieffel induction scheme [2, 27, 28, 51, 58, 78] gives a valid inner product on the vector space of physical states so that it can be turned into a Hilbert space. This scheme has been rediscovered several times since its first formulation in the sixties. It is also known as refined algebraic quantization or group averaging. A short review is given in [19]. For us the application of the scheme to the Hilbert space for minisuperspace models is most important and was achieved by Marolf, given in [79, 81–84].

In this section we are only giving a very heuristic derivation of this scheme and only as far as we need it for our investigations in the following chapters. For an exact mathematical
CHAPTER 1. INTRODUCTION

formulation the physical states have to be elements of a dual space to the auxiliary Hilbert space. This and further mathematical properties are for example discussed in Ref. [27, 28].

One way to implement this scheme is to consider eigenstates of the constraint

$$\hat{H}\psi_{\lambda k} = \lambda \psi_{\lambda k}$$

(1.2.7)

where $k$ is a degeneracy label. These are normalizable in the auxiliary inner product via

$$\langle \psi_{\lambda k}, \psi_{\lambda' k'} \rangle_A = \delta(\lambda - \lambda')\delta(k - k')$$

(1.2.8)

The induced inner product between solutions to the constraint then consists of dropping the $\delta(\lambda - \lambda')$ term on the right and taking the limit $\lambda, \lambda' \to 0$. This produces a well-defined positive definite inner product on the solutions $|\psi_{\text{phys}}\rangle$ to the constraint.

Another way of incorporating this scheme is to define a kind of ‘$\delta$-function’ operator involving the constraint $\hat{H}$ by

$$\delta(\hat{H}) := \int_{-\infty}^{+\infty} \frac{d\lambda}{2\pi} e^{i\lambda \hat{H}}$$

(1.2.9)

Since $\hat{H}\delta(\hat{H}) = 0$ we can find physical solutions to the constraint by acting with $\delta(\hat{H})$ on an auxiliary state,

$$|\psi_{\text{phys}}\rangle = \delta(\hat{H})|\psi_{\text{aux}}\rangle.$$ 

(1.2.10)

The inner product in the auxiliary Hilbert space between two physical states $|\psi_{\text{phys}}\rangle$ and $|\psi'_{\text{phys}}\rangle$ is now

$$\langle \psi_{\text{phys}}|\psi'_{\text{phys}} \rangle_A = \langle \psi_{\text{aux}}|\delta^2(\hat{H})|\psi'_{\text{aux}} \rangle_A = \delta(0)\langle \psi_{\text{aux}}|\delta(\hat{H})|\psi'_{\text{aux}} \rangle_A$$

(1.2.11)

which is again infinite. However we can delete $\delta(0)$ to obtain the induced inner product

$$\langle \psi_{\text{phys}}|\psi'_{\text{phys}} \rangle_I := \langle \psi_{\text{aux}}|\delta(\hat{H})|\psi'_{\text{aux}} \rangle_A.$$ 

(1.2.12)

It turns that this product is equivalent to the one given above. $\delta(\hat{H})$ effectively behaves as an projection operator (which it clearly is in the case of a discrete spectrum), since we essentially are allowed to replace $[\delta(\hat{H})]^2$ with $\delta(\hat{H})$.

Using this scheme one can define an inner product for the solutions to the Klein-Gordon equation which is positive definite. As is generally known, the standard Klein-Gordon
inner product does not have this property. Regarding the Wheeler-DeWitt equation one is able to create solutions (at least formally) and to define an inner product for them. For minisuperspace models this can be done explicitly (see the papers by Marolf [79, 81–84]).

What are quantum operators that represent physical observables with which we can calculate expectation values and probabilities for these kind of systems?

It is generally believed that the interesting dynamical variables are again those that respect reparametrization invariance [16, 80–82, 84, 99–102]. The condition $\{ O, H \} = 0$ for the classical observable translates into $[ \hat{O}, \hat{H} ] = 0$. The quantum observables have to commute with the constraint operator $\hat{H}$. This also ensures that $\hat{O}|\Psi_{\text{phys}}\rangle$ is again a physical state, since we have

$$[ \hat{O}, \hat{H} ] = 0 \implies \hat{H}\hat{O}|\Psi_{\text{phys}}\rangle = 0 \quad (1.2.13)$$

In the following chapters we will use quantum operators derived from the decoherent histories approach and encounter the problem that they lead out of the physical state space.

Because the constraint equation (1.2.6) is not of the Schrödinger type, it does not have an external time variable, so we cannot talk about the value of a variable at a particular “time”. Instead, “time” is somehow encoded in the variables already present in the wave equation. In the Klein-Gordon equation, for example, we might be interested in the value of the spatial coordinate $x$ at given $x^0$. We might equally be interested in the value of $x^0$, say, at given $x^1$. We need operators commuting with $H$ which express these quantities.

Suppose we are interested in the operator corresponding to the value of $A$ when $B$ takes the value $\tau$. The appropriate operator is

$$[A]_{B=\tau} = \int_{-\infty}^{\infty} ds \ A(s) \ \frac{dB(s)}{ds} \ \delta (B(s) - \tau) \quad (1.2.14)$$

where $A(s) = e^{iHs}Ae^{-iHs}$, and similarly for $B(s)$ [80–82, 84]. (We assume a suitable operator ordering is chosen in this expression, although note that it is not always possible to make it self-adjoint). It is readily verified that this operator commutes with $H$ and hence is a quantum observable. The study of operators of this type is the basis of the operator approach (sometimes known as the “evolving constants” method). From the computation
of the spectrum of this operator Eq. (1.2.14) one may compute a projection operator $P_\alpha$ say, onto a range of the spectrum. The associated probability is then of the form $\text{Tr}(P_\alpha \rho)$.

Any other approach ought to make some kind of contact with the operator approach described above at some stage, and in particular, the decoherent histories approach must contain some notion corresponding to the notion of an observable in the operator approach. (See also Refs. [46, 47] for some much earlier approaches to these issues). In this thesis our main emphasis will be on expressions for probabilities derived from a decoherent history analysis, but especially in Chapter 2 we will compare the two approaches.

1.2.3 The Decoherent Histories Approach to Quantum Theory

The central ingredient for our investigations is the decoherent histories approach to quantum theory which we aim to adapt to the timeless situation of quantum cosmological models.

The decoherent (or consistent) histories approach to quantum theory aims to allow you to make statements about closed quantum systems without referring to the notion of measurement or classicality. It was developed by Griffiths [29–31], Omnès [89–95] and, especially in the context of quantum cosmology, by Gell-Mann and Hartle [22–25, 49, 50]. A particular adaption to the problem of spacetime coarse graining was developed by Isham and Linden [62–64].

The important idea is to investigate whether one can consistently assign probabilities to possible histories of a quantum system.

Propositions about quantum systems are represented by projectors $P$ in the corresponding Hilbert space. We select a set of projection operators $\{P_\beta\}$ that is exhaustive and mutually exclusive:

$$\sum_\beta P_\beta = 1 \quad P_\beta P_\gamma = \delta_{\beta \gamma} P_\beta$$

(1.2.15)

A history $\alpha = (\alpha_1, \cdots, \alpha_k)$ of the system is represented by a chain of projection operators at different times $\{t_k\}$

$$C_\alpha = P_{\alpha_1}(t_1) \cdots P_{\alpha_k}(t_n)$$

(1.2.16)
CHAPTER 1. INTRODUCTION

The $C_\alpha$ are called class or history operators and satisfy

$$\sum_\alpha C_\alpha = 1 \quad (1.2.17)$$

due to the exhaustiveness of the projection operators. If the projectors project onto one-dimensional subspaces of the underlying Hilbert-space, the history is called fine-grained, otherwise it is coarse-grained.

An important functional on the set of histories is the *decoherence functional* which is defined for two histories, $\alpha$ and $\alpha'$, and an initial density matrix $\rho$ for the quantum system. It is given by

$$D(\alpha, \alpha') = \text{Tr} \left( C_\alpha \rho C_{\alpha'}^\dagger \right) \quad (1.2.18)$$

and is a measure of the quantum interference of the two histories.

The candidate probability $p(\alpha)$ for a history $\alpha$ is $D(\alpha, \alpha)$. The key point is that $p(\alpha)$ obeys the sum rules for probabilities if and only if

$$\text{Re} \, D(\alpha, \alpha') = 0 \quad \text{for all } \alpha \neq \alpha' \quad (1.2.19)$$

A family of histories, consisting of the set of all possible $\alpha$ for times $t_k$, is called consistent, or weakly decoherent, if it obeys this condition. Only then is $p(\alpha)$ a probability measure on this family of histories. A family for which the imaginary part vanishes as well, so that $D(\alpha, \alpha') = 0$, is a *family of decoherent histories* and obeys the (medium) decoherence condition. For a pure initial state $\rho = |\psi\rangle \langle \psi|$ this condition is equivalent to the existence of so-called generalized records. These records are orthogonal projectors $R_\alpha$ such that $R_\alpha |\psi\rangle = C_\alpha |\psi\rangle$ for all $\alpha$ [22–24, 39].

Note also that when there is decoherence, using (1.2.17), the probabilities may be written as

$$p(\alpha) = \text{Tr} \left( C_\alpha \rho \right) \quad (1.2.20)$$

and for pure initial states as $p(\alpha) = \text{Tr} \left( R_\alpha \rho \right)$.

The decoherence condition is generally only satisfied for coarse-grained histories. The fulfilment also depends strongly on the initial state $\rho$. Often the condition is only approximately satisfied. This is often achieved when the system undergoes the physical process
of decoherence where interference effects of the system are diminished through interaction with an environment (for an extensive review see Ref. [26]).

The decoherent histories approach is, however, more general and we will exploit this generality [50]. We can include the possibility of both an initial state \( \rho \) and a final state \( \rho_f \) (normally taken to be proportional to the identity), and we therefore have to include the normalization factor \( N = (\text{Tr}(\rho_f \rho))^{-1} \). In this case the decoherence functional takes the form

\[
D(\alpha, \alpha') = \frac{1}{N} \text{Tr} \left( \rho_f C_\alpha \rho C_{\alpha'}^\dagger \right)
\]

In its application to the reparametrization invariant systems considered in this thesis, we will attach the initial and final states to the class operators using the induced inner product scheme [51] described in the previous section. So for pure initial and final states, the decoherence functional is

\[
D(\alpha, \alpha') = \frac{1}{N} (\Psi_f \circ I C_\alpha \circ I \Psi) (\Psi_f \circ I C_{\alpha'} \circ I \Psi)^* \tag{1.2.22}
\]

where \( \circ I \) here denotes the induced inner product. (We may of course sum over initial or final pure states to get mixed ones.)

One can also generalize the class operators \( C_\alpha \) representing histories. The \( C_\alpha \) can be written as restricted path integrals which sum up to the quantum mechanical propagator \( g(x_f, t_f | x_0, t_0) \), and one can turn this around and define histories by splitting the propagator into a sum of restricted propagators \( g_\alpha(x_f, t_f | x_0, t_0) \),

\[
g(x_f, t_f | x_0, t_0) = \sum_\alpha g_\alpha(x_f, t_f | x_0, t_0) \tag{1.2.23}
\]

The restricted propagators \( g_\alpha(x_f, t_f | x_0, t_0) \) are defined as the path integral running over paths obeying the condition \( \alpha \) and weighted with the amplitude \( e^{iS} \). One can now talk of histories defined by the condition \( \alpha \).

Yamada and Tagaki [111–114] have used this generalization to examine the probability of a particle entering a spacetime region in normal quantum mechanics (the square \( \Sigma \) in Fig. 2). They define the restricted propagator \( g_\Sigma(x_f, t_f | x_0, t_0) \) for entering the spacetime region \( \Sigma \) as being the path integral of paths entering \( \Sigma \) (e.g the dotted path in Figure 2). This is a generalization of the history operator (1.2.16), since this operator cannot
be written a chain of projection operators. On the other hand \( g_{\Sigma}(x_f, t_f|x_0, t_0) \), which is defined as the restricted propagator of the paths never entering the region \( \Sigma \), is such a chain of projection operators (a chain with an infinite number of projectors, since the time label \( t_k \) is now continuous). The candidate probability for the particle entering \( \Sigma \) is given by

\[
p(\Sigma) = D(\Sigma, \Sigma) = \int dz \int dx \int dy \, g_{\Sigma}(z, t_f|y, t_0) \rho(y, x, t_0) g_{\Sigma}^*(z, t_f|x, t_0) .
\] (1.2.24)

If we only consider the two member family of histories that the particle enters the region \( \Sigma \) or not, represented by \( g_{\Sigma} \) and \( g_{\bar{\Sigma}} \), we have the consistency condition

\[
0 = \text{Re}D(\Sigma, \bar{\Sigma}) = \text{Re} \int dz \int dx \int dy \, g_{\Sigma}(z, t_f|y, t_0) \rho(y, x, t_0) g_{\bar{\Sigma}}^*(z, t_f|x, t_0) .
\] (1.2.25)

The investigations of Yamada and Tagaki show that this condition can only satisfied for very restricted initial states \( \rho(y, x, t_0) \). If one introduces an environment, the restrictions can be weakened.

1.3 Our Approach

We now apply (and adapt on the way) the decoherent histories approach to reparametrization invariant systems like quantum cosmological models.

In particular we want to find an expression for the quantum probability of a particle entering a certain region in configuration space irrespective of time. We do not refer to a certain time to reflect the timeless character of the Wheeler-DeWitt equation. By solving this problem and then selecting special kinds of regions one could for example arrive at an answer to the question about the probability that the system follows some kind of orbit (see Figure 1 for the case of a central potential).

1.3.1 The Decoherence Functional For Reparametrization Invariant Models

The systems we are interested in have the property that the central equation is a constraint equation of the Hamiltonian operator on the wave function

\[
(\hat{H} - E_0)\Psi = 0
\] (1.3.1)
There is no time evolution. Hence we want to find an expression for the probability that some region in configuration space is entered at all. This expression will be in the form of a decoherence functional. We then can check the decoherence condition to prove that our candidate probability is a valid probability.

We found that we can use $\delta(\hat{H} - E_0)$ to generate solutions to (1.3.1). We can rewrite this in terms of propagators by calculating (switching the sign in the $\lambda$ integration)

$$G_{E_0}(x, y) = \langle x | \delta(\hat{H} - E_0) | y \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \ e^{iE_0\lambda} \langle x | e^{-i\lambda\hat{H}} | y \rangle = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \ e^{iE_0\lambda} g(x, \lambda | y, 0)$$

(1.3.2)

Solutions to the constraint equation can now be generated by $\int dy \ G_{E_0}(x, y) \Psi_{\text{aux}}(y)$. We additionally require $\delta(\hat{H} - E_0)\delta(\hat{H} - E_0) = \delta(\hat{H} - E_0)$ in the sense of the induced inner product, so that $G(x, y)$ propagates solutions into the same solution again. We now want to find a representation for the history that the particle enters a region $\Delta$ in configuration space. For this we replace $g(x, \lambda | y, 0)$ in equation (1.3.2) by the restricted propagator $g_{\Delta}(x, \lambda | y, 0)$. This restricted operator is defined by being the path integral over all paths with time parameter “length” $\lambda$ between $y$ and $x$ that enter the configuration space region $\Delta$ (see Figure 3). This is a special case of the restricted propagators used by Yamada and Tagaki. It corresponds to choosing their region $\Sigma$ to be $\Delta \times [0, \lambda]$.

Following [50, 51] we now define the history operator for entering $\Delta$ for our reparametrization invariant system to be

$$C_{E_0}^{\Delta}(x, y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\lambda \ e^{iE_0\lambda} g_{\Delta}(x, \lambda | y, 0)$$

(1.3.3)

A problem with this definition is that these class operators do not necessarily obey the constraints and hence will lead out of the Hilbert space of physical states. This problem was already recognized in [51]. The following solution was suggested: One has to identify appropriate boundary conditions for the class operator $C_{\Delta}$ and then replace it with a propagator $C_{\Delta}'$ that obeys these boundary conditions and the constraint. Dealing with this problem will be a crucial part of our investigations in the following chapters.

Assuming that we have a class operator $C_{E_0}^{\Delta}$ that obeys the constraint, we can set up
the probability of entering $\Delta$ for an initial state $|\Psi_{E_0}\rangle$ to be

$$p(\Delta) = D(\Delta, \Delta) = \text{Tr}_{\text{ind}} \left[ C_{E_0}^{E_0} |\Psi_{E_0}\rangle\langle \Psi_{E_0}| C_{E_0}^{E_0} \right], \quad (1.3.4)$$

where the subscript “ind” reminds us that we have to take the trace using the induced inner product. The best way to implement the inner product is to select different energies for the class operators and the wave functions at the beginning. Afterwards one sets the energies equal to value $E_0$ and deletes the $\delta$-functions involving zero.

Using and inserting the definition of $C_{E_0}^{E_0}$, we obtain

$$p_{\text{aux}}(\Delta) = \text{Tr} \left[ C_{E_1}^{E_1} |\Psi_{E_2}\rangle\langle \Psi_{E_3}| C_{E_4}^{E_4} \right]$$

$$= \frac{1}{(2\pi)^2} \int dq_f \int \int d\lambda d\lambda' e^{i(E_1\lambda - E_4\lambda')} \int dq_0 dq'_0$$

$$g_{\Delta}(q_f, \lambda|q_0, 0)\Psi_{E_2}(q_0)\Psi_{E_3}^*(q'_0)g_{\Delta}^*(q_f, \lambda|q'_0, 0) \quad (1.3.5)$$

As a check, we can now calculate the probability for the particle entering the whole configuration space, for which $g_{\Delta}(x, \lambda|y, 0) = g(x, \lambda|y, 0)$. We get

$$p_{\text{aux}}(\mathbb{R}^2) = \delta(E_1 - E_2)\delta(E_3 - E_4)\langle \Psi_{E_3}| \Psi_{E_2}\rangle . \quad (1.3.6)$$

Setting all energies equal to $E_0$ gives $\delta(0)^3$ which in the induced inner product scheme leads to the probability $p(\mathbb{R}^2) = 1$. This is the result we expect.

The decoherence functional $D(\Delta, \Delta)$ can be set up in the same way. We will discuss it and the expression for the probabilities in the following two chapters, first for the relativistic particle, then for a more general quantum cosmological model.

### 1.4 Relation to other work

Finally, we outline the relationship of this thesis to other works in the field. This thesis is part of a programme to apply the decoherent histories approach to quantum cosmology, or models of the type used in quantum cosmology, and ultimately to quantum gravity more generally. The decoherent histories approach generally and its applications to quantum cosmology have been set out at length by Hartle in his 1992 Les Houches Lectures [50],
and more recent relevant aspects of this were discussed by Hartle and Marolf [51]. The formalism has been applied to particular reparametrization invariant models in two other places besides this thesis. Whelan [110] has used the formalism to compute probabilities on timelike surfaces for the relativistic particle. Also, Craig and Hartle [15] have applied the formalism to a Bianchi IX quantum cosmological model. The last two papers use the Klein-Gordon inner product whereas we use the positive-definite induced inner product to construct the decoherence functional.

There is also some connection with the work on probabilities for non-trivial spacetime coarse grainings in non-relativistic quantum mechanics [45, 49, 85, 111–114]. In recent years there has been much interest in constructing observables corresponding to questions involving time. A lot of effort has been made to find so-called time-of-arrival operators, the quantum version of measuring the time at which a particle enters a certain region [1]. Related observables ask the question if a particle enters a certain spatial region during a certain time interval. The calculations of Yamada and Tagaki [111–114] using decoherent histories try to answer this question. The problem is that in normal quantum mechanics measurements are always chosen to be at a certain instant of time. But the mentioned observables consider measurements stretched over an amount of time. This work is of interest to us because we stretch the amount of time to infinity since we ask the question whether the system enters the region $\Delta$ at all.

This thesis is also very much in the spirit of [40], which attempts to interpret the Wheeler-DeWitt equation in terms of emergent trajectories by introducing model detectors into the Hamiltonian. This was in turn inspired by Barbour’s observations [5] on the similarity between the Wheeler-DeWitt equation and Mott’s calculation showing the emergence of a straight line track from a spherical wave in alpha decay [87] (See also [10, 12] for further discussions of the Mott calculation.), together with some of Barbour’s more general observations about the Wheeler-DeWitt equation and timeless theories [5–7].

Regarding the work presented in Chapter 4, the reduced density matrix for quantum cosmological models has often been discussed [35, 65, 86, 96], but a master equation which it obeys has to our knowledge only been calculated once [66].
Chapter 2

Decoherent Histories Analysis of the Relativistic Particle

2.1 Introduction

A simple but important example of a reparametrization invariant system is the relativistic particle with the constraint equation \( p^\mu p_\mu - m^2 = 0 \).\(^1\) Quantization leads to the Klein-Gordon equation

\[
(\Box + m^2) \phi(x) = (\partial^\mu \partial_\mu + m^2) \phi(x) = 0
\]

Understanding this equation is also of direct relevance to quantum cosmology since the Wheeler-DeWitt equation for simple models has the form of a Klein-Gordon equation in a general curved spacetime background with a spacetime dependent mass term. Traditional approaches to relativistic quantum theory note the various difficulties of interpreting the Klein-Gordon equation and then pass quickly on to quantum field theory. The Wheeler-DeWitt equation, however, in its full form, already represents a second-quantized field theory. To work with the Wheeler-DeWitt equation we must therefore return to wave equations of the Klein-Gordon type and understand how to overcome their difficulties without resorting to second quantization.

\(^1\)In this chapter Greek indices run from 0 to 3, Latin indices from 1 to 3.
We begin by briefly reviewing how the various aspects of the our formalism mentioned in Chapter 1 can be applied to the relativistic particle.

The inner product traditionally associated with the Klein–Gordon and similar equations is the Klein-Gordon inner product,

\[ \psi^* \phi_{KG} = \langle \psi | \phi \rangle_{KG} = i \int_{\Sigma} d^3x \, \psi^* \partial_0 \phi \]

(2.1.2)

It is evaluated on a spacelike surface \( \Sigma \), and is independent of the choice of such surface if \( \psi \) and \( \phi \) are solutions to the Klein-Gordon equation. This inner product is, however, not positive definite. When a separation into positive and negative frequencies is possible, written as \( \psi = \psi^+ + \psi^- \), it is positive on the positive frequency sector and negative on the negative frequency sector.

The induced inner product coincides with the Klein-Gordon inner product but with the sign of the negative frequency sector changed so as to make the product positive:

\[ \psi^* \phi_{I} = \langle \psi | \phi \rangle_{I} = \langle \psi^+ | \phi^+ \rangle_{KG} - \langle \psi^- | \phi^- \rangle_{KG} \]

(2.1.3)

For the free relativistic particle, we could quite simply have defined an inner product by the object on the right, and this is well-defined since the positive and negative frequency sectors do not interact in this case. The advantage of the induced inner product, however, is that it provides a good inner product even when the split into positive and negative frequencies is not possible. This is the case for quantum cosmological models. (See Refs.[2, 19, 27, 28, 51, 58, 78] for more details).

Regarding the “timeless” properties we want to investigate, this chapter will focus on the following question: given a solution to the Klein-Gordon, what is the probability of finding the particle in a spatial region \( \Delta \) of a spacelike surface?

The question is clearly a simple one, but it turns out to expose some subtle aspects of the decoherent histories approach applied to reparametrization invariant systems, and is an important test of the formalism in a familiar situation. Furthermore, it may also be regarded as a preparatory exercise for the treatment of more complicated quantum cosmological models.
To answer this question in the operator ("evolving constants") approach we are going to use a quantum operator like (1.2.14). This is the operator for the observable corresponding to the value of $A$ when $B$ takes the value $\tau$. It is of the form

$$[A]_{B=\tau} = \int_{-\infty}^{\infty} ds \ A(s) \frac{dB(s)}{ds} \delta (B(s) - \tau)$$  \hspace{1cm} (2.1.4)

where $A(s) = e^{iHs}Ae^{-iHs}$, and similarly for $B(s)$ [80–82, 84]. (We assume a suitable operator ordering is chosen in this expression, although note that it is not always possible to make it self-adjoint). It is readily verified that this operator commutes with $H$ and hence is a quantum observable. After the spectrum of this operator Eq(2.1.4) is computed one may compute a projection operator $P_\alpha$ say, onto a range of the spectrum. The associated probability is then of the form $\text{Tr}(P_\alpha \rho)$.

As already mentioned, the decoherent histories approach to quantum theory provides a second method of calculating the probability we are interested in. On the face of it this method is quite different to the operator method outlined above, and there is no particular reason to assume that the methods are equivalent.

In the application of the decoherent histories approach to the relativistic particle we attach the initial and final states to the class operators $C_\alpha$ using the induced inner product (2.1.3) for the Klein-Gordon equation. So for pure initial and final states, the decoherence functional is

$$D(\alpha, \alpha') = \frac{1}{N} \langle \psi_f \circ_I C_\alpha \circ_I \psi \rangle \langle \psi_f \circ_I C_{\alpha'} \circ_I \psi \rangle^*$$  \hspace{1cm} (2.1.5)

where $\circ_I$ here denotes the induced inner product. This is different to Refs. [15, 110] where the Klein-Gordon product was used. The key problem is then the construction of the class operators $C_\alpha$ corresponding to the question of the particle entering the spatial region $\Delta$. This is the step analogous to the construction of operators above in Eq.(2.1.4), and therefore the class operators must somehow incorporate reparametrization invariance. It should be stated at this stage that there does not at present seem to be a completely clear and unambiguous prescription for constructing the class operators, and part of the aim of this Chapter is therefore to explore possible constructions and examine their properties.

The stated question concerning the spacelike region $\Delta$ is a question about a configuration region, since the configuration space of the relativistic particle is spacetime itself.
Therefore the natural approach to calculating the class operators is to use the configuration path integrals for reparametrization invariant systems developed in Section 1.3.1 (following Refs. [50, 51]). For the relativistic particle these have the form

\[ C_\alpha(x'', x') = \int dT \, g_\alpha(x'', T|x', 0) \]  \hspace{1cm} (2.1.6)

where

\[ g_\alpha(x'', T|x', 0) = \int_\alpha Dx^\mu \exp \left( -i \int_0^T ds \left[ \eta_{\mu\nu} \dot{x}^\mu \dot{x}^\nu \frac{\eta_{\mu\nu}}{4} + m^2 \right] \right) \]  \hspace{1cm} (2.1.7)

The path integral for \( g \) has the form of a non-relativistic propagator. The sum is over paths from spacetime points \( x' \) to \( x'' \) where the paths are restricted in some way defined by the coarse-graining \( \alpha \). For example, we might be interested in the probability that the particle passes through some region of spacetime, or not. More details about the construction of this object, including the specification of the range of the \( T \) integration, will be given below.

An issue which arises with this definition is that these class operators often do not everywhere satisfy the constraint equation with respect to their end-points. As we shall see in particular examples, they satisfy the constraint except on the boundaries of the regions defining the coarse grainings. This is an issue because the induced inner product is only defined between solutions to the constraint. The auxiliary inner product is still defined, but in operating with such a class operator on the initial state, we are stepping out of the physical state space. Fortunately, we will find in particular examples that the problem is easily fixed by a small amount of intuitively sensible doctoring on the class operators, guided by the requirement that path integral methods agree with operator methods. In particular, we will follow the suggestion of Hartle and Marolf, which, loosely speaking, is to replace \( C_\alpha \) by a new object \( C'_\alpha \) which satisfies the constraint equation everywhere, and satisfies the same essential boundary conditions as the path integral-defined object \( C_\alpha \) [51].

It is easily seen that the operator and decoherent histories approaches are different, with no guarantee of their equivalence in general. They both deal with objects which are compatible with the constraint (the operator (2.1.4) and the class operators \( C'_\alpha \)), but the operator method looks at a projection operator onto ranges of the spectrum of (2.1.4), whilst the decoherent histories approach works with the class operators \( C_\alpha \) and
DECOHERENT HISTORIES ANALYSIS OF THE REL. PARTICLE

the decoherence functional (2.1.5). The class operators are not projections in general, and in some sense are generalizations of projections to non-commuting alternatives, so the two formalisms are quite different. However, it is known that when there is exact decoherence in the decoherent histories approach, the probabilities for a history $\alpha$ and a pure state $\rho$ may be written in the form $\text{Tr}(R_\alpha \rho)$ where $R_\alpha$ is a projection operator [22–24, 39]. This corresponds to the existence records mentioned in Section 1.2.3.

2.1.1 Summary of this Chapter

As stated, the main aim of this chapter is to derive expressions for the probability of crossing a spacelike surface in relativistic quantum mechanics, using the decoherent histories approach, and the similar operator approaches.

To get a feel for the formalism for reparametrization-invariant systems, we start in Section 2.2 by applying the formalism to the non-relativistic particle in parametrized form. To prepare the way for the study of the Klein-Gordon equation, we then briefly review some useful aspects of relativistic quantum mechanics in Section 2.3.

Our main results are described in Sections 2.4 and 2.5 where we apply the formalism outlined above to the relativistic particle. In Section 2.4, we construct a position operator which commutes with the constraint. Its eigenstates are the Newton-Wigner states, and in fact the operator is essentially the same as the Newton-Wigner operator [88]. The associated probabilities on spacelike surfaces are those one would anticipate on the basis of the Schrödinger equation, which is the square root of the Klein-Gordon equation. Another, different, candidate expression for the probability associated with a section of spacelike surface is the flux of the Klein-Gordon current (with the sign of the negative frequency part changed, as in Eq.(2.1.3)). This probability is related to a different set of position states which are non-orthogonal but relativistically invariant. There are, therefore, even at this simple level of canonical quantization, two distinct quantizations of the relativistic particle, which are not equivalent (corresponding loosely speaking to “quantize then constrain” versus “constrain then quantize”). We shall refer to them as the Klein-Gordon (KG) and Newton-Wigner (NW) quantizations.

In Section 2.5 we consider the decoherent histories analysis of the system in the KG
quantization. We compute the decoherence functional for histories which cross a surface of constant $x^0$ in a spatial region $\Delta$ (or in its complement $\bar{\Delta}$). Since the paths move backwards and forwards in time, the notion of crossing is ambiguous and needs to be carefully defined. We show that the essentially unique notions of crossing associated with the KG quantization are first and last crossing. We thus obtain probabilities associated with the spacelike surface of the form of a Klein-Gordon inner product (with a sign change in the negative frequency sector like the induced inner product (2.1.3)). However, the histories are only approximately decoherent (with the off-diagonal terms proportional to the overlap of the relativistically invariant position states).

The computation of the crossing probabilities hinges on resolving a subtle point: the path integral representation of the class operator for not crossing suggests that there is a non-zero amplitude that the particle will never cross a spacelike surface, contrary to intuition. This issue turns out in fact to be related to the problem of class operators which do not satisfy the constraint mentioned above. An important part of the analysis of Section 2.5 is a demonstration of how the class operators may be modified in a sensible way so that they do satisfy the constraint. The properly modified class operator for not crossing a spacelike surface then turns out to be zero, in agreement with physical intuition.

In Section 2.6, we consider the decoherent histories analysis in the NW quantization. This is much simpler, being very similar in form to non-relativistic quantum mechanics. Decoherence is exact and the expected NW probability expressions are easily recovered.

We summarize and conclude in Section 2.7.

2.2 The Parametrized Non-Relativistic Particle

The very first testing ground for ideas about the quantization of reparametrization invariant systems is the parametrized non-relativistic particle. This is the usual non-relativistic particle but with the time coordinate $t$ raised to the status of a dynamical variable, with conjugate momentum $p_t$. Its action in Hamiltonian form is

$$S = \int ds \left( p_x \dot{x} + p_t \dot{t} - NH \right)$$

(2.2.1)
where a dot denotes differentiation with respect to the parameter $s$. $N$ is a Lagrange multiplier enforcing the constraint

$$H = p_t + h = 0$$  \hspace{1cm} (2.2.2)

where $h$ is the usual Hamiltonian $h = p_x^2/2m$. Canonical quantization leads to the Schrödinger equation,

$$H \psi = (p_t + h) \psi(x, t) = \left(-i \frac{\partial}{\partial t} + h\right) \psi(x, t) = 0$$  \hspace{1cm} (2.2.3)

In terms of dynamics nothing new is gained at this stage. But the interesting question is to see what the usual expressions for probabilities look like in the language introduced in Chapter 1.

Following the general scheme, we normalize solutions to the constraint by first considering eigenstates of $H$, as in Eq. (1.2.7) They are normalized using the auxiliary inner product according to

$$\langle \Psi_{\lambda k} | \Psi_{\lambda' k'} \rangle_A = \int dt dx \Psi_{\lambda k}^*(x, t) \Psi_{\lambda' k'}(x, t) = \delta(\lambda - \lambda')\delta(k - k')$$  \hspace{1cm} (2.2.4)

Since $H = p_t + h$, the solutions to the eigenvalue equation may be written

$$\Psi_{\lambda k}(x, t) = \frac{1}{\sqrt{2\pi}} e^{i\lambda t} \psi_k(x, t)$$  \hspace{1cm} (2.2.5)

where $\psi_k(x, t)$ satisfies the Schrödinger equation. It follows that

$$\frac{1}{2\pi} \int dt \int dx \ e^{-i\lambda t+i\lambda' t} \psi_k^*(x, t) \psi_{k'}(x, t) = \delta(\lambda - \lambda')\delta(k - k')$$  \hspace{1cm} (2.2.6)

The integral contains within it the usual inner product

$$\langle \psi_k | \psi_{k'} \rangle_S = \int dx \ \psi_k^*(x, t) \psi_{k'}(x, t)$$  \hspace{1cm} (2.2.7)

This has the important property that it is independent of time when the states obey the Schrödinger equation, so the time integral may be done in Eq.(2.2.6), pulling down a delta function $\delta(\lambda - \lambda')$, and it follows that

$$\langle \psi_k | \psi_{k'} \rangle_S = \delta(k - k')$$  \hspace{1cm} (2.2.8)

This means that the expected Schrödinger inner product on surfaces of constant $t$ follows from the induced inner product defined on the whole of spacetime.
We may now ask for the probabilities in various situations of interest. Perhaps the simplest is the probability of finding the particle in the spatial region $\Delta$ at time $t_0$. In the usual approach it is of course

$$p_\Delta = \int_\Delta dx \, |\psi(x, t_0)|^2$$

To express this in the language of Section 1.2.2, we seek an operator which commutes with the constraint $H$ and corresponds to the answer to “the value of $x$ when $t = t_0$.” Following the general scheme this is

$$X = \int_{-\infty}^{\infty} ds \, \frac{dt(s)}{ds} \, x(s) \, \delta(t(s) - t_0)$$

where $x(s)$ and $t(s)$ are the evolution of $x$ and $t$ using the constraint $H$ as a Hamiltonian:

$$x(s) = e^{iHs}xe^{-iHs}, \quad t(s) = e^{iHs}te^{-iHs}$$

Since $H = p_t + h$ this is

$$x(s) = e^{ihs}xe^{-ihs} = x + \frac{ps}{m}$$

$$t(s) = e^{ip_t s}te^{-ip_t s} = t + s$$

The integral over $s$ may be done in Eq.(2.2.10) with the result

$$X = x - \frac{p(t - t_0)}{m}$$

It is easy to confirm that this commutes with $H$.

Since $H$ and $X$ commute, they possess a joint set of eigenstates $u_{\lambda \bar{x}}$. The eigenvalue equation for $X$ is

$$X u_{\lambda \bar{x}}(x, t) = \bar{x} u_{\lambda \bar{x}}(x, t)$$

with solutions

$$u_{\lambda \bar{x}}(x, t) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\lambda \bar{g}(x, t|\bar{x}, t_0)}$$

where $g$ is the non-relativistic propagator. In the auxiliary inner product these are normalized according to

$$\langle u_{\lambda \bar{x}} | u_{\lambda' \bar{x}'}, A \rangle = \delta(\lambda - \lambda') \, \delta(\bar{x} - \bar{x}')$$
The amplitude for an eigenstate of the constraint of the form
\[ \Psi_{\lambda'}(x, t) = \frac{1}{(2\pi)^{3/2}} e^{i\lambda t} \psi(x, t) \] (2.2.18)
to be in an eigenstate of \( X \) is
\[ \langle u_{\lambda} \bar{x} | \Psi_{\lambda'} \rangle_A = \frac{1}{(2\pi)^{3/2}} \int dt dx \ e^{it(\lambda - \lambda')} g^*(x, t|\bar{x}, t_0) \psi(x, t) \]
\[ = \delta(\lambda - \lambda') \psi(\bar{x}, t_0) \] (2.2.19)
The probability is then computed from the expression
\[ \int_\Delta d\bar{x} \langle \Psi_{\lambda''} | u_{\lambda \bar{x}} \rangle_A \langle u_{\lambda \bar{x}} | \Psi_{\lambda'} \rangle_A = \delta(\lambda'' - \lambda)\delta(\lambda - \lambda') \int_\Delta d\bar{x} |\psi(\bar{x}, t_0)|^2 \] (2.2.20)
Following the induced inner product prescription, we drop the delta-functions on the right, thereby obtaining the expect result for the probability, Eq.(2.2.9).

The operator formalism with Eq.(2.1.4) (respectively Eq. (1.2.14)) allows one to ask a richer variety of questions than those normally considered in non-relativistic quantum mechanics. We may consider, for example, the question, “What is the value of \( t \) at a given value of \( x \)?” The associated operator is
\[ T = t_0 + \frac{m(x - x_0)}{p} \] (2.2.21)
A suitable operator ordering must be chosen, but the presence of the \( 1/p \) factor makes it difficult to turn this into a self-adjoint operator (see for example Ref.[32]). This operator arises in relation to the arrival time problem in non-relativistic quantum mechanics, an issue that has attracted a lot of recent attention in the literature [1].

Both of the above questions in non-relativistic quantum mechanics may also be analyzed using the decoherent histories approach. We will not go into the details here, except to make some simple observations that are related to the relativistic particle case we consider later.

In the decoherent histories approach, the probability Eq.(2.2.9) may also be obtained using a standard non-relativistic path integral, in which one sums over paths which cross the surface \( t = t_0 \) in the spatial range \( \Delta \). It is a property of this path integral that the paths cross this surface once and only once, and as a consequence of this, the histories
are exactly decoherent. As described in Section 1.2.3, exact decoherence of histories for a pure initial state $\rho$ implies that records exist [22–24, 39], or in other words, that the probability may be written in the form $\text{Tr}(R_\alpha \rho)$ for some projection operator $R_\alpha$. This is thoroughly consistent with the existence of the self-adjoint operator (2.2.14) from which the probabilities Eq.(2.2.9) are derived in the operator approach.

But now consider, by contrast, the probability for crossing a surface of constant $x$. In the decoherent histories analysis of this question (which is rather non-trivial [45, 49, 85, 111–114]), the paths may cross the surface many times. Furthermore, it is found that the histories are typically not decoherent (unless an environment to produce decoherence is included, but we do not consider that case here), and this appears to be related to the multiple crossings. We cannot therefore deduce the existence of records and a probability of the form $\text{Tr}(R_\alpha \rho)$. There would be an inconsistency with the operator approach here if there was a self-adjoint operator corresponding to this question. But interestingly, as we have seen, the corresponding operator Eq.(2.2.21) is not self-adjoint. The point therefore, is that multiple surface crossings and the associated lack of decoherence in the decoherent histories approach appear to be related to the absence of a self-adjoint operator in the operator approach. We will see more evidence of this in the case of the relativistic particle in Sections 2.5 and 2.7.

### 2.3 Green Functions of the Klein-Gordon equation

The Klein-Gordon equation has a variety of associated Green functions and it will be useful to briefly summarize them here. In order to agree with the notation of Ref.[42] (which we follow very closely), we use particle physics convention in which the signature of the metric is $(+−−−)$. The positive and negative frequency Wightman functions $G^\pm$ are defined by

$$G^\pm(x, y) = \frac{1}{(2\pi)^3} \int_{k_0 = \pm \omega_k} \frac{d^3k}{2\omega_k} e^{-ik \cdot (x-y)}$$  \hspace{1cm} (2.3.1)

where $\omega_k = \sqrt{k^2 + m^2}$. They satisfy the composition laws

$$G^\pm = \pm G^\pm \circ_{KG} G^\mp, \quad G^\pm \circ_{KG} G^\mp = 0$$  \hspace{1cm} (2.3.2)
where $\circ_{KG}$ denotes the Klein-Gordon inner product. The causal Green function is defined by

$$iG(x, y) = G^+(x, y) - G^-(x, y) \quad (2.3.3)$$

Its main property is that it propagates all solutions to the Klein-Gordon equation

$$\phi = iG \circ_{KG} \phi \quad (2.3.4)$$

It also obeys the composition law

$$G = iG \circ_{KG} G \quad (2.3.5)$$

The Hadamard function is defined by

$$G^{(1)}(x, y) = G^+(x, y) + G^-(x, y) \quad (2.3.6)$$

and obeys the composition laws,

$$G^{(1)} = iG \circ_{KG} G^{(1)} = iG^{(1)} \circ_{KG} G, \quad G = -iG^{(1)} \circ_{KG} G^{(1)} \quad (2.3.7)$$

All of the above are solutions to the Klein-Gordon equation.

The Feynman Green function is

$$iG_F(x, y) = \theta(x^0 - y^0)G^+(x, y) + \theta(y^0 - x^0)G^-(x, y) \quad (2.3.8)$$

and satisfies

$$\left(\Box + m^2\right) G_F(x, y) = -\delta^{(4)}(x - y) \quad (2.3.9)$$

It obeys the composition laws

$$G_F = iG_F \circ_{KG} G_F \quad (2.3.10)$$

Also of interest is the Newton-Wigner propagator

$$G_{NW}(x, x^0, y, y^0) = \frac{1}{(2\pi)^3} \int_{k_0 = \omega_k} d^3k \ e^{-ik \cdot (x-y)} \quad (2.3.11)$$

which is the propagator associated with the positive square root of the Klein-Gordon equation

$$i \frac{\partial \phi}{\partial x^0} = h\phi \quad (2.3.12)$$
where $h = \sqrt{-\nabla^2 + m^2}$. It is also useful to define a negative frequency Newton-Wigner propagator, given by (2.3.11) but with $k_0 = -\omega_k$, and this will be denoted $\tilde{G}_{NW}$. It is easily seen that the Newton-Wigner propagator is related to the Wightman function by

$$G_{NW}(x, y) = 2i \frac{\partial}{\partial x^0} G^+(x, y) = -2i \frac{\partial}{\partial y^0} G^+(x, y)$$

(2.3.13)

Some of these Green functions can be obtained from a path integral of the form (2.1.6), (2.1.7). An unrestricted sum with $T$ integrated over an infinite range yields the Hadamard function $G^{(1)}$. (See Fig. 4). A half-infinite range, $0 \leq T < \infty$, yields $iG_F$, where $G_F$ is the Feynman Green function. (See, for example, Ref.[34]). The Newton-Wigner propagator can also be obtained from (2.1.6), (2.1.7) by summing over all paths from $y$ to $x$ which never cross the surface of constant $x^0$, except when they end at the point $x$. (See Fig. 5). More details of this construction are discussed in Sections 2.5 and 2.6. (See also Ref.[42]).

From the path integral representations, one can see that $G^{(1)}$ corresponds to the operator $\delta(H)$, which is essentially the identity on the constraint subspace (and so we effectively have $\delta(H)|\phi\rangle = |\phi\rangle$ for solutions to the constraint). This is perhaps confusing since $G^{(1)}$ does not in fact propagate positive and negative frequency solutions to the Klein-Gordon equation (it is the causal Green function $G$ that does this job, via Eq.(2.3.4)). The resolution of this is the choice of inner product. $G^{(1)}$ does in fact propagate all solutions if they are attached with the induced inner product (2.1.3). For suppose we have a solution $\phi = \phi^+ + \phi^-$. Then

$$G^{(1)} \circ_I \phi = (G^+ + G^-) \circ_I (\phi^+ + \phi^-)$$

$$= G^+ \circ_{KG} \phi^+ - G^- \circ_{KG} \phi^-$$

$$= (G^+ - G^-) \circ_{KG} (\phi^+ + \phi^-)$$

$$= iG \circ_{KG} \phi$$

(2.3.14)

In this sense, $G^{(1)}$ is effectively equivalent to $G$.

It is also interesting note in this connection that it was claimed in Ref.[42] that there is no path integral of the form (2.1.6), (2.1.7) that will yield the causal propagator $G$ directly. Whilst this is still in some sense true, one can see that it depends on how the initial states are attached: the path integral for $G^{(1)}$ but with initial states attached using the induced inner product does in fact effectively give the causal propagator $G$. 
We may now consider the form of the decoherence functional for the Klein-Gordon equation (we follow the construction of Ref. [51]). We take it to be of the form (2.1.5). We take a fixed pure initial state and sum over a complete set of final states. This gives

\[ D(\alpha, \alpha') = \sum_{\psi_f} (\psi_f \circ_I C_{\alpha} \circ_I \psi)(\psi_f \circ_I C_{\alpha'} \circ_I \psi)^* \]  

(2.3.15)

where note here that we use the induced inner product. (The normalization factor is unity in this case). Since \( \psi_f \) denotes a complete set of positive and negative frequency solutions, it is easy to show that

\[ \sum_{\psi_f} \psi_f^*(x) \psi_f(y) = G^{(1)}(x, y) \]  

(2.3.16)

Furthermore, since \( C_{\alpha} \) are solutions to the constraints, the action of \( G^{(1)} \) changes nothing, \( G^{(1)} \circ_I C_{\alpha} = C_{\alpha} \), so we have

\[ D(\alpha, \alpha') = \psi^* \circ_I C_{\alpha'}^\dagger \circ_I C_{\alpha} \circ_I \psi \]  

(2.3.17)

Finally, when there is exact decoherence, \( D(\alpha, \alpha') = 0 \) for \( \alpha \neq \alpha' \), the probabilities are

\[ p(\alpha) = D(\alpha, \alpha') = \sum_{\alpha'} D(\alpha, \alpha') = \psi^* \circ_I C_{\alpha} \circ_I \psi \]  

(2.3.18)

In the KG quantization, the induced inner product becomes the modified KG inner product (2.1.3), with initial states normalized in this inner product. In the NW quantization, states obey the Schrödinger equation, they are normalized in a Schrödinger inner product and \( \circ \) is taken to be that inner product in the decoherence functional.

### 2.4 An Operator Approach for the Klein-Gordon Equation

We now describe the use of operator methods to obtain probabilities associated with the Klein-Gordon equation. The relativistic particle is described by the constraint

\[ H = p_0^2 - p^2 - m^2 = 0 \]  

(2.4.1)

where the canonical variables \( x^\mu, p^\nu \) obey the commutation relations

\[ [x^\mu, p^\nu] = -i\eta^{\mu\nu} \]  

(2.4.2)
We are interested in the question, “What is the value of $x^k$ when $x^0 = \tau$?” As indicated already, there are potentially many ways of formulating and answering this question. We will first use the operator methods of Section 1.2.2. Following Eq.(2.1.4), the operator expressing this question is

$$X^k = \int_{-\infty}^{\infty} ds \frac{1}{2} \{ \frac{dx^0(s)}{ds}, \delta(x^0(s) - \tau) \} x^k(s)$$

(2.4.3)

where $\{ , \}$ denotes the anticommutator, and we have

$$x^0(s) = x^0(0) + p^0 s$$

(2.4.4)

$$x^i(s) = x^i(0) + p^i s$$

(2.4.5)

The object of interest is therefore given by

$$X^k = x^k - \frac{p^k}{2} \{ \frac{1}{p^0}, (x^0 - \tau) \}$$

(2.4.6)

and it is easily seen that this commutes with $H$. One might anticipate that the $1/p^0$ factor may present problems in turning this into a self-adjoint operator, but this problem does not arise since we are looking for eigenstates of $X^i$ which also satisfy the constraint, and this bounds $p_0$ away from zero. (Essentially the same operator was also considered by Marolf [82]).

We choose a momentum representation, in which

$$x^k \to -i \frac{\partial}{\partial p_k}, \quad x^0 \to -i \frac{\partial}{\partial p^0}$$

(2.4.7)

and $X^k$ is

$$X^k = \left( -i \frac{\partial}{\partial p_k} + i \frac{p^k}{p^0} \frac{\partial}{\partial p^0} - i \frac{p^k \tau}{2(p^0)^2} + \frac{p^k \tau}{p^0} \right)$$

(2.4.8)

(recalling that $p^k = -p_k$ with our choice of signature). This is self-adjoint in the momentum space version of the auxiliary inner product

$$\langle \phi|\psi \rangle_A = \int d^4 p \ \phi^*(p) \psi(p)$$

(2.4.9)

The eigenstates of $X^k$ are the functions

$$f(p) = \frac{1}{(2\pi)^{3/2} (2p^0)^{1/2}} e^{ip^0(\tau - \tau_0)} g(p \cdot \xi)$$

(2.4.10)
where \( g \) is any function of \( p \cdot p \), and the eigenvalue is \( x^k \). For these to be eigenstates of the constraint we also need to choose \( g = \delta(p \cdot p - m^2) \). Introducing the eigenstates \(|p\rangle\) of \( p^\mu \), (where \( \langle p|p'\rangle_A = \delta^{(4)}(p - p') \)), the eigenstates of \( X^i \) may be written

\[
|x, \tau\rangle = \frac{1}{(2\pi)^{3/2}} \int d^4p \left(2p^0\right)^{1/2} e^{ip^0\tau - ip \cdot x} \delta(p^2 - m^2) |p\rangle
\]

\[
= \frac{1}{(2\pi)^{3/2}} \int \frac{d^3p}{(2\omega_p)^{1/2}} e^{i\omega_p\tau - ip \cdot x} |p+\rangle + \frac{i}{(2\pi)^{3/2}} \int \frac{d^3p}{(2\omega_p)^{1/2}} e^{-i\omega_p\tau - ip \cdot x} |p-\rangle
\]

\[
= |x, \tau+\rangle + i|x, \tau-\rangle
\]

(2.4.11)

(The factor of \( i \) in the negative frequency term, not present in other definitions of these states [42, 53], does not in fact make any difference.) Here, we have introduced the momentum states \(|p\pm\rangle\) on the positive and negative frequency sectors which are normalized in the induced inner product as

\[
\langle p\pm|p\mp\rangle_I = 2\omega_p \delta(p - p')
\]

and also \( \langle p\pm|p\mp\rangle_I = 0 \). The states \(|x, \tau\rangle\) are the Newton-Wigner states [88]. They are orthogonal at equal times, and satisfy the completeness relation

\[
1 = \int d^3x \langle x, \tau+\rangle \langle x, \tau+\rangle + \int d^3x \langle x, \tau-\rangle \langle x, \tau-\rangle
\]

(2.4.13)

The probability of entering a spacelike region \( \Delta \) at time \( \tau \) is given by

\[
p_\Delta = \int_\Delta d^3x \ |\langle x, \tau+|\psi\rangle_I|^2 + \int_\Delta d^3x \ |\langle x, \tau-|\psi\rangle_I|^2
\]

(2.4.14)

where the states \( \psi_{\pm}(x, \tau) = \langle x, \tau|\pm\rangle_I \) obey the Klein-Gordon equation and its positive/negative square root. They are normalized in a Schrödinger inner product which is related to the induced inner product by

\[
\langle \psi|\phi\rangle_I = \int_{\mathbb{R}^3} d^3x \ [\psi_+^*(x, \tau)\phi_+(x, \tau) + \psi_-^*(x, \tau)\phi_-(x, \tau)]
\]

(2.4.15)

The Newton-Wigner states could also have been obtained by solving the constraint classically and then considering the eigenstates of the operators

\[
X^k = x^k \pm \frac{p^k \tau}{\sqrt{p^2 + m^2}}
\]

(2.4.16)
The Newton-Wigner states therefore correspond to “constraining before quantization”. It is also important to compare with the position operator introduced by Newton and Wigner [88], which is, on the surface $x^0 = 0$, in the momentum representation

$$X_{NW}^k = -i \frac{\partial}{\partial p_k} - \frac{p_k}{2\omega_p^2}$$  \hspace{1cm} (2.4.17)

This is in fact the same as the operator

$$\int d^3x \langle x, \tau^+ | x^k \langle x, \tau^+ |$$  \hspace{1cm} (2.4.18)

with $\tau = 0$, in terms of the Newton-Wigner states above. Eq.(2.4.17) is not the same as (2.4.6), since the constraint holds in Eq.(2.4.17), but has not yet been imposed in Eq.(2.4.6). Eq.(2.4.17) is, however, the same as Eq.(2.4.16), with $\tau = 0$, once one recognizes that the inner product structure (2.4.12) requires the replacement

$$x^k \to -(2\omega_p)^{\frac{1}{2}} i \frac{\partial}{\partial p_k} \frac{1}{(2\omega_p)^{\frac{1}{2}}} = -i \frac{\partial}{\partial p_k} - \frac{p_k}{2\omega_p^2}$$  \hspace{1cm} (2.4.19)

There is therefore agreement with the earlier work of Newton and Wigner.

An alternative way of defining position states is to first consider eigenstates of the position operator $\hat{x}^\mu$ on the auxiliary Hilbert space, and then project onto the constraint subspace using $\delta(H)$. This corresponds to quantizing before constraining, and yields

$$|x\rangle = \frac{1}{(2\pi)^{3/2}} \int_{p_0=\omega_p} \frac{d^3p}{2\omega_p} e^{ip\cdot x} |p^+\rangle + \frac{1}{(2\pi)^{3/2}} \int_{p_0=-\omega_p} \frac{d^3p}{2\omega_p} e^{ip\cdot x} |p^-\rangle$$  \hspace{1cm} (2.4.20)

$$= |x^+\rangle + |x^-\rangle$$

Unlike the Newton-Wigner states, these states are Lorenz-invariant. Furthermore, they not orthogonal, since

$$\langle x|y \rangle_I = G^{(1)}(x, y)$$  \hspace{1cm} (2.4.21)

although they are approximately orthogonal in the sense that $G^{(1)}(x, y)$ decays when $x$ and $y$ are separated by more than the Compton wavelength $m^{-1}$. They also obey a completeness relation

$$1 = i \int d^3x \left( |x^+\rangle \overline{\partial_0}\langle x^+ | - |x^-\rangle \overline{\partial_0}\langle x^- | \right)$$  \hspace{1cm} (2.4.22)

These properties of the states $|x\rangle$ are reminiscent of the coherent states, and suggest that the probability for crossing a spacelike surface $x^0 = \tau$ in the region $\Delta$ may be taken to be

$$p_\Delta = i \int_{\Delta} d^3x \left( \phi^*_+ \overline{\partial_0}\phi_+ - \phi^*_- \overline{\partial_0}\phi_- \right)$$  \hspace{1cm} (2.4.23)
The states $\phi_{\pm}(x) = (x \pm |\phi\rangle$ are positive/negative frequency solutions to the Klein-Gordon equation. The minus sign in the second term ensures that the expression is positive, and in the limit $\Delta = \mathbb{R}^3$ this expression becomes the norm of $\phi$ in the induced inner product, as required.

### 2.5 Decoherent Histories Analysis in the Klein-Gordon Quantization

We now come to the main point of this Chapter which is to use the decoherent histories approach to compute the answer to the question, “What is the probability that the particle is found in the spatial region $\Delta$ at time $x^0 = \tau$?”. In this Section, we consider the KG quantization, with the aim of obtaining Eq.(2.4.23), and we consider the NW quantization and Eq.(2.4.14) in Section 2.6.

The decoherence functional is given by Eq.(2.3.17). We take a pure initial state, and we sum over a complete set of positive and negative solutions in the final state.

The main issue is to compute the class operators $C_\alpha(x'', x')$ corresponding to crossing $x^0 = \tau$ either inside the region $\Delta$ or outside it, in its complement $\bar{\Delta}$. We expect that these operators can be obtained by a sum over paths which either cross or do not cross the region (in a sense to be made more precise below). As mentioned in the introduction to this chapter, one important subtlety will be to find the class operators that obey the constraint.

For an overview of the various class operators we use in this section, see Table 1 on page 47 for their defining equation number, if they obey the constraint and some additional remarks.

#### 2.5.1 The Class Operator for Not Crossing a Spacelike Surface

In computing a class operator of the form $C_\alpha(x'', x')$ we sum over paths from $x'$ to $x''$ satisfying some condition specified by the coarse graining $\alpha$. However, this construction appears to allow for the possibility of defining a coarse graining consisting of paths from
Table 1: The different class operators used in Section 2.5

<table>
<thead>
<tr>
<th>Class operator</th>
<th>Defining Eq.</th>
<th>Obeys constraint?</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{NC}(x'', x')$</td>
<td>(2.5.1)</td>
<td>No (class operator for not crossing $x^0 = \tau$)</td>
</tr>
<tr>
<td>$C_{C}(x'', x')$</td>
<td>(2.5.4)</td>
<td>No (class operator for crossing $x^0 = \tau$)</td>
</tr>
<tr>
<td>$C'_{NC}(x'', x')$</td>
<td>(2.5.5)</td>
<td>Yes (modified noncrossing class operator)</td>
</tr>
<tr>
<td>$C'_{\Delta}(x'', x')$</td>
<td>(2.5.12),(2.5.13)</td>
<td>No (class operator for the first crossing of $x^0 = \tau$ in $\Delta$)</td>
</tr>
<tr>
<td>$C''_{\Delta}(x'', x')$</td>
<td>(2.5.14)</td>
<td>No (class operator for the last crossing of $x^0 = \tau$ in $\Delta$)</td>
</tr>
<tr>
<td>$\tilde{C}_{\Delta}(x'', x')$</td>
<td>(2.5.16)</td>
<td>“Yes” (the average of $C'<em>{\Delta}(x'', x')$ and $C''</em>{\Delta}(x'', x')$ for $x^{0''}$ and $x^{0'}$ on opposite sides of $x^0 = \tau$)</td>
</tr>
<tr>
<td>$C'<em>{\Delta}(x'', x') = \tilde{C}</em>{\Delta}(x'', x')$ for all $x'', x'$</td>
<td></td>
<td>Yes (modified class operator for crossing $\Delta$)</td>
</tr>
<tr>
<td>$C'<em>{\Delta}(x'', x') = G^{(1)}(x'', x') - C'</em>{\Delta}(x'', x')$</td>
<td></td>
<td>Yes (modified class operator for not crossing $\Delta$)</td>
</tr>
<tr>
<td>$C''_{\Delta}(x'', x')$</td>
<td>(2.5.16),(2.5.18)</td>
<td>Yes (modified class operator for crossing $\Delta$; equal to $C'_{\Delta}(x'', x')$)</td>
</tr>
</tbody>
</table>
DECOHERENT HISTORIES ANALYSIS OF THE REL. PARTICLE

x' to x'' which never cross a given spacelike surface. (See Fig. 6). This is at first sight disconcerting. Every classical trajectory of the relativistic particle crosses every spacelike surface (unless it is tachyonic). And in the quantum theory, a solution to the Klein-Gordon equation cannot be zero on one side of a spacelike surface and non-zero on the other.

To investigate this issue, we consider the following coarse graining: paths from x' to x'' which either cross or do not cross the surface x0 = τ. That is, we are interested in the question, given a solution to the Klein-Gordon equation, what is the probability that the particle will be found on the spacelike surface x0 = τ, or will never be found on that surface? Clearly the answer to this question must be probability unity for crossing the surface, and probability zero for not crossing.

The sum over paths which do not cross x0 = τ is easily constructed using the path integral representations (2.1.6), (2.1.7). We take T to have an infinite range and we sum over all paths which never cross the surface. In Ref.[42] it was shown that this is in fact equivalent to a method of images construction for g(x'', T|x', 0), and we obtain, for the class operator for paths restricted to not cross the surface,

\[ C_{NC}(x'', x') = \left( \theta(x''^0 - \tau)\theta(x''^0 - \tau) + \theta(\tau - x''^0)\theta(\tau - x''^0) \right) \]

\[ \times \left( G^{(1)}(x'', x') - G^{(1)}(\tilde{x}'', x') \right) \]

(2.5.1)

where \( \tilde{x} \) denotes the reflection of the point x about x0 = τ, that is,

\[ \tilde{x}^\mu = (2\tau - x^0, x) \]  

(2.5.2)

\( C_{NC} \) vanishes on x''^0 = τ and x''^0 = τ. Both \( G^{(1)}(x'', x') \) and \( G^{(1)}(\tilde{x}'', x') \) are solutions to the KG equation, but the presence of the \( \theta \)-functions means that \( C_{NC} \) does not satisfy it,

\[ (\Box + m^2)C_{NC}(x'', x') = 2\delta(x''^0 - \tau) \epsilon(x''^0 - \tau) \partial_0 G^{(1)}(\tau, \tilde{x}''^0|0, x') \]

(2.5.3)

where \( \epsilon(x) \) is the signum function. This is the difficulty with the path integral-defined class operators mentioned in Section 1.3.1 and the introduction to this chapter. The sum over paths which always cross x0 = τ, which we denote \( C_C(x'', x') \), is constructed using the relation

\[ G^{(1)}(x'', x') = C_C(x'', x') + C_{NC}(x'', x') \]

(2.5.4)
from which one can see that $C_C(x'', x')$ will also not satisfy the constraint (although to actually compute the crossing class operator we will use a different method below).

Since the constraint is associated with reparametrization invariance, it might seem that failure to satisfy it is associated with a breaking of that invariance. However, the connection between constraints and invariance can be rather subtle for the case of reparametrizations. In particular, the path integral (2.1.6), (2.1.7) between fixed end-points over paths restricted to pass through certain spacetime regions is clearly reparametrization invariant. These issues are discussed more fully in Refs.[41, 50].

Note also that we have now encountered two potential difficulties which are not obviously related: first, the possibility of a physically unreasonable result, and second, the fact that the naturally defined class operator does not satisfy the constraint. We will now see that both of these problems are solved simultaneously by appropriate modification of the class operator.

Following the suggestion of Hartle and Marolf [51], we will deal with this issue by replacing $C_{NC}$ by another object $C'_{NC}$ which satisfies the most important boundary conditions defining $C_{NC}$ but which also satisfies the constraint everywhere. The boundary conditions satisfied by $C_{NC}$ are that, (a), it vanishes on $x^{0''} = \tau$, $x^{0'} = \tau$ and when $x''$ and $x'$ are on opposite sides of the surface. One might also be tempted to impose that, (b), $C'_{NC}$ coincides with (the non-zero) $C_{NC}$ when $x''$ and $x'$ are on the same side of the surface. It appears to be impossible for a function satisfying the constraint everywhere to satisfy all of these conditions. The essence of the non-crossing propagator appears to be contained in the conditions (a), so we drop conditions (b). The unique solution to the constraint equation satisfying conditions (a) is then quite simply

$$C'_{NC}(x'', x') = 0 \quad (2.5.5)$$

This is because for fixed $x'$, $C'_{NC}(x'', x')$ is zero for all values of $x''$ on the opposite side of the surface to $x'$. This means that both $C'_{NC}$ and its normal derivative are zero on all spacelike surfaces on the opposite side of the surface $x^0 = \tau$, and the solution to the Klein-Gordon equation with these conditions is simply $C'_{NC} = 0$. The only way of getting a non-zero result as $x''$ moves from the opposite side to the same side as $x'$ is to have a
discontinuity in the normal derivative; but this can only be achieved with a delta-function source, as in Eq. (2.5.1).

The conclusion (2.5.5) for the modified class operator for non-crossing paths implies that the modified class operator for paths that always cross is quite simply $G^{(1)}(x, y)$. It now follows that histories partitioned according to whether or not they cross $x^0 = \tau$ are exactly decoherent, the probability of not crossing is zero, and the probability of crossing is 1. We have therefore shown that by sufficiently careful treatment of the class operators and their boundary conditions, we obtain the expected and physically sensible result.

2.5.2 Crossing Propagators and the Path Decomposition Expansion

Having resolved the issue of how to modify class operators that do not satisfy the constraint, we may now turn to the issue of computing the class operators for crossing the spacelike surface $x^0 = \tau$ in a spatial region $\Delta$. These operators (before modification) will be constructed by a path integral of the form (2.1.6), (2.1.7) in which the paths cross the spacelike surface in the region $\Delta$. Because the paths go backwards and forwards in time, they will typically cross a given spacelike surface many times; so the notion of crossing needs to be specified more precisely. We will see however, that for the path integral representations of the Klein-Gordon propagators, first and last crossings are in fact the only useful notions of crossing.

A very useful result for our purposes is the path decomposition expansion, or PDX [3, 42]. For a propagator of the non-relativistic form (2.1.7), it implies that when $x''$ and $x'$ are on opposite sides of the surface of constant $x^0$, we have

$$g(x'', T|x', 0) = 2i \epsilon (\tau - x'^0) \int_0^T dt_c \int d^3x \ g(x'', T|x, t_c) \ \overrightarrow{\partial_0 g(x, t_c|x', 0)} \quad (2.5.6)$$

This formula is obtained by partitioning the paths in the sum over histories (2.1.7) according to the parameter time $t_c$ and position $x$ at which they cross the surface of constant $x^0$.
for the first time\(^2\) (See Fig. 7). If we partition according to the last crossing, we get
\[ g(x''\!, T|x', 0) = -2i \, \epsilon(x^{0''} - \tau) \int_0^T dt_c \int d^3 x \, g(x''\!, T|x, t_c) \partial_0g(x, t_c|x', 0) \] (2.5.7)

When \(x''\) and \(x'\) are on the same side of the surface, there is the possibility of paths between these points which do not cross the surface. The appropriate formulae then are
\[ g(x''\!, T|x', 0) = g_r(x''\!, T|x', 0) + 2i \, \epsilon(\tau - x^{0'}) \int_0^T dt_c \int d^3 x \, g(x''\!, T|x, t_c) \partial_0g(x, t_c|x', 0) \] (2.5.8)
for the first crossing and
\[ g(x''\!, T|x', 0) = g_r(x''\!, T|x', 0) - 2i \, \epsilon(x^{0''} - \tau) \int_0^T dt_c \int d^3 x \, g(x''\!, T|x, t_c) \partial_0g(x, t_c|x', 0) \] (2.5.9)
for the last crossing, where \(g_r\) denotes the restricted propagator given by a sum over paths which never cross the surface. The formulae (2.5.6)–(2.5.9) imply that the sum over paths which cross the surface is given by either (2.5.6) or (2.5.7), irrespective of whether \(x'\) and \(x''\) are on the same side or opposite sides of the surface. (But only in the latter case are these expressions then equal to the full propagator).

These results were used in Ref.[42] to derive the composition laws of relativistic propagators from the path integral. Here, we note that the propagators for first or last crossing the surface \(x^0 = \tau\) in the region \(\Delta\) are readily obtained by simply restricting the \(d^3 x\) integration to the region \(\Delta\).

### 2.5.3 First and Last Crossing Relativistic Propagators

Turning now to the relativistic propagators, the class operator for crossing the surface \(x^0 = \tau\) in the region \(\Delta\) is
\[ C_{\Delta}(x'', x') = \int_{-\infty}^{\infty} dT \, g_{\Delta}(x'', T|x', 0) \] (2.5.10)

\(^2\)The full version of the PDX actually involves the normal derivative of the restricted propagator \(g_r\), but in this simple case, \(g_r\) may be computed using the method of images and it follows that \(\partial_0g_r = 2\partial_0g\), which is what is used in Eq.(2.5.6). See Ref.[42] for more details.
We first take the case where \( g_\Delta(x'', T, x', 0) \) is the sum over paths from \( x' \) to \( x'' \) in fixed proper time \( T \) which cross the surface for the first time in \( \Delta \), that is,

\[
g^f_\Delta(x'', T | x', 0) = 2i \epsilon(\tau - x'^0) \int_0^T dt_c \int_\Delta d^3x \ g(x''(t), T | x, t_c) \overleftarrow{\partial_0}g(x, t_c | x', 0)
\]  

(2.5.11)

(See Fig. 8). This is valid for \( x'', x' \) on either the same or opposite sides of the spacelike surface. Inserting in Eq.(2.5.10), writing the integral as a sum of two parts corresponding to the positive and negative ranges of \( T \), and changing variables to \( v = T - t_c, u = t \) (see Ref.[42] for more details), this yields,

\[
C^f_\Delta(x'', x') = -2i \epsilon(\tau - x'^0) \int_\Delta d^3x \ \left[ G_F(x'', x) \overleftarrow{\partial_0}G_F(x, x') - G^*_F(x'', x) \partial_0 G^*_F(x, x') \right]
\]  

(2.5.12)

This is the formula for first crossing the region \( \Delta \) for all end-points. It is also conveniently written as

\[
C^f_\Delta(x'', x') = -\int_\Delta d^3x \ \left[ G^{(1)}(x'', x) \overleftarrow{\partial_0}G(x, x') + \epsilon(x'^0 - \tau)\epsilon(\tau - x'^0) G(x'', x) \overleftarrow{\partial_0}G^{(1)}(x, x') \right]
\]  

(2.5.13)

It is also of interest to consider the class operator defined by the last crossing, which is easily shown to be

\[
C_\Delta^l(x'', x') = 2i \epsilon(x'^0 - \tau) \int_\Delta d^3x \ \left[ G_F(x'', x) \overleftarrow{\partial_0}G_F(x, x') - G^*_F(x'', x) \partial_0 G^*_F(x, x') \right]
\]  

= \int_\Delta d^3x \ \left[ \epsilon(x'^0 - \tau)\epsilon(\tau - x'^0)G^{(1)}(x'', x) \overleftarrow{\partial_0}G(x, x') + G(x'', x) \partial_0 G^{(1)}(x, x') \right]
\]  

(2.5.14)

When the initial and final points are on opposite sides of the surface, we have

\[
\epsilon(x'^0 - \tau)\epsilon(\tau - x'^0) = 1
\]  

(2.5.15)

It is then convenient to average the first and last crossing class operators to obtain

\[
C_\Delta(x'', x') = \frac{1}{2} \left( C_\Delta^f(x'', x') + C_\Delta^l(x'', x') \right)
\]  

= \frac{1}{2} \int_\Delta d^3x \ \left[ G^{(1)}(x'', x) \overleftarrow{\partial_0}G(x, x') + G(x'', x) \overleftarrow{\partial_0}G^{(1)}(x, x') \right]
\]  

= i \int_\Delta d^3x \ \left( G^+(x'', x) \overleftarrow{\partial_0}G^+(x, x') - G^-(x'', x) \overleftarrow{\partial_0}G^-(x, x') \right)
\]  

(2.5.16)
It is then readily confirmed, using the properties Eq.(2.3.2) and (2.3.7), that this class operator become $G^{(1)}$ in the limit that $\Delta$ becomes $\mathbb{R}^3$, as expected.

As one of $x''$ or $x'$ is moved from the opposite to the same side of the surface, the class operator undergoes a discontinuity. This is reflected in the fact that it does not satisfy the constraint. The first crossing class operator, for example, satisfies the equation,

$$\left(\Box + m^2\right) C'_\Delta(x'', x') = 2 \epsilon(\tau - x'^0) \delta(x''^0 - \tau) \partial_0 G^{(1)}(\tau, x'' | x'^0, x')$$  \hspace{1cm} (2.5.17)

when $x''$ is in $\Delta$ and zero otherwise. Note that Eq.(2.5.3) and Eq.(2.5.17) are consistent, since $C_\Delta + C_{NC} = G^{(1)}$ when $\Delta = \mathbb{R}^3$, and $G^{(1)}$ satisfies the constraint.

As in Section 2.5.1, some doctoring of this basic class operator must therefore be carried out before we get the final expression for a modified class operator $C'_\Delta$ which satisfies the constraint. It is clear in this case how to proceed. From the above the obvious strategy is to take $C'_\Delta$ to be given by Eq.(2.5.16) for all values of the end-points $x''$, $x'$, whether they lie on the same side of the surface or opposite sides. This is clearly a solution to the constraint everywhere. It matches the path integral-defined object when the end-points are on opposite sides of the surface. Furthermore, when $\Delta = \mathbb{R}^3$, it is equal to $G^{(1)}$ and so this is consistent with the modified class operator for not crossing. We will return below to the question of a more general prescription for constructing modified class operators.

If we now look at the definition of the propagator for not entering $\Delta$, $C'_\Delta = G^{(1)} - C'_\Delta$, we find using (2.5.16) and $G^{(1)} = G^{(1)} \circ I G^{(1)}$

$$C'_\Delta(x'', x') = i \int d^3x \left( G^+(x'', x) \frac{\partial}{\partial_0} G^+(x, x') - G^-(x'', x) \frac{\partial}{\partial_0} G^-(x, x') \right)$$

$$- i \int_\Delta d^3x \left( G^+(x'', x) \frac{\partial}{\partial_0} G^+(x, x') - G^-(x'', x) \frac{\partial}{\partial_0} G^-(x, x') \right)$$

$$= i \int d^3x \left( G^+(x'', x) \frac{\partial}{\partial_0} G^+(x, x') - G^-(x'', x) \frac{\partial}{\partial_0} G^-(x, x') \right)$$

$$= C'_\Delta(x'', x')$$  \hspace{1cm} (2.5.18)

This equality between $C'_\Delta$ and $C'_\Delta$ is analogous to the fact that classically the particle has only the choice between $\Delta$ and $\bar{\Delta}$. It has to cross $x^0 = \tau$ somewhere. This physical argument also led us to set $C'_{NC} = 0$.

We therefore may now consider the decoherence functional for histories which cross the spacelike surface $x^0 = \tau$ either in the region $\Delta$ or in its complement $\bar{\Delta}$, for an initial
DECOHERENT HISTORIES ANALYSIS OF THE REL. PARTICLE

state $\psi = \psi_+ + \psi_-$. The off-diagonal terms of the decoherence functional are

$$D(\Delta, \bar{\Delta}) = \psi^* \circ I (C'_{\Delta})^\dagger \circ I C'_{\bar{\Delta}} \circ I \psi$$

(2.5.19)

We have

$$C'_\Delta \circ I \psi = i \int_{\Delta} d^3 x \left( G^+(x''', x) \overrightarrow{\partial_0} \psi_+(x) + G^-(x'''', x) \overrightarrow{\partial_0} \psi_-(x) \right)$$

(2.5.20)

so the decoherence functional is

$$D(\Delta, \bar{\Delta}) = \int_{\Delta} d^3 x \int_{\bar{\Delta}} d^3 y \left( \psi^*_+(y) \overrightarrow{\partial_0} G^+(y, x) \overrightarrow{\partial_0} \psi_+(x) + \psi^*_-(y) \overrightarrow{\partial_0} G^-(y, x) \overrightarrow{\partial_0} \psi_-(x) \right)$$

(2.5.21)

The key feature of this expression is that the decoherence functional is not exactly diagonal. It is, however, approximately diagonal in the sense that the two-point functions $G^\pm(y, x)$ decay for increasing spatial separations. In particular, we expect that approximate diagonality can be obtained if both regions $\Delta$ and $\bar{\Delta}$ are much larger than the Compton wavelength $m^{-1}$ (the decay length scale of $G^\pm(x, y)$).

Given decoherence, the probability for crossing $\Delta$ is then

$$\psi^* \circ I C'_{\Delta} \circ I \psi = i \int_{\Delta} d^3 x \left( \psi^*_+(x) \overrightarrow{\partial_0} \psi_+(x) - \psi^*_-(x) \overrightarrow{\partial_0} \psi_-(x) \right)$$

(2.5.22)

This is exactly the expected answer, coinciding with Eq.(2.4.23), although recall that the probabilities are only approximately defined because of approximate decoherence.

2.5.4 General Prescription for Constructing Modified Class Operators

We have so far constructed the modified class operators using some general arguments, but the question remains as to whether it is possible to find a more general formula for constructing them. Connected to this is the question of how the modified class operators are related to the original path operators, such as Eq.(2.5.10), which were defined using path integrals in a simple and obvious way.

Consider first, therefore, the question of why the expressions (2.5.10) and (2.5.11) fail to satisfy the constraint. Using the fact that the propagators of the form $g(x, t|x', 0)$ satisfy the Schrödinger equation, it is easy to see that (2.5.10) fails to satisfy the constraint at
DECOHERENT HISTORIES ANALYSIS OF THE REL. PARTICLE

$x''$ because of the finite integration range for $t_c$. Recall that $t_c$ is the parameter time of first crossing and is not a physically observable quantity. Because it is unobservable, and because the total parameter time $T$ is integrated over an infinite range, it seems reasonable to explore the possibility that $t_c$ could also be integrated over an infinite range, in such a way that a solution to the constraint equation is obtained.

Proceeding along these lines, one can see that one way to obtain a solution to the constraint is to extend the integration range of $t_c$ to $-\infty < t_c < \infty$, but with a signum function $\epsilon(t_c)$ included. That is, we define the modified class operator

$$C_\Delta'(x'', x') = 2i \epsilon(\tau - x'') \int_{-\infty}^{\infty} dT \int_{-\infty}^{\infty} dt_c \epsilon(t_c) \int_\Delta d^3x \, g(x'', T|x, t_c) \overrightarrow{\partial_0}g(x, t_c|x', 0)$$

(2.5.23)

Now we note that

$$\int_{-\infty}^{\infty} dt_c \epsilon(t_c) \, g(x, t_c|x', 0) = iG_F(x, x') + iG_F^*(x, x')$$

(2.5.24)

where recall $x^0 = \tau$. Furthermore, we have that

$$\overrightarrow{\partial_0} \left( \epsilon(\tau - x'') \, G(x, x') \right) = \epsilon(\tau - x'') \, \overrightarrow{\partial_0}G(x, x')$$

(2.5.25)

since $G(x, x')$ vanishes when $\tau = x''$. The modified class operator is therefore

$$C_\Delta''(x'', x') = -2 \int_\Delta d^3x \, G^{(1)}(x'', x) \overrightarrow{\partial_0}G(x, x')$$

(2.5.26)

which, apart from the factor of 2, coincides with the first term in Eq.(2.5.13). It is easy to see that the second term in Eq.(2.5.13), but without the $\epsilon$ factors (and again up to a factor of 2) may be obtained by a slightly different modification of the integration range over parameter times, that is,

$$2i \epsilon(\tau - x'') \int_{-\infty}^{\infty} dT \epsilon(T - t_c) \int_{-\infty}^{\infty} dt_c \epsilon(t_c) \int_\Delta d^3x \, g(x'', T|x, t_c) \overrightarrow{\partial_0}g(x, t_c|x', 0)$$

(2.5.27)

$$= -2 \int_\Delta d^3x \, G(x'', x) \overrightarrow{\partial_0}G^{(1)}(x, x')$$

Hence averaging these two results gives the class operator Eq.(2.5.13), but crucially, without the $\epsilon$ factors that cause (2.5.13) to fail to satisfy the constraint. We may finally perform a further averaging with the last crossing versions of the above modified class operators to
obtained a modified class operator with the following properties: it satisfies the constraint everywhere, and, when \( x'' \) and \( x' \) are on opposite sides of the surface, coincides with the path-integral defined object (2.5.16).

In summary, we therefore now have two different methods of defining modified class operators which satisfy the constraint. One is to use the usual path integral construction to compute the class operators when \( x'' \) and \( x' \) are on opposite sides of the surface, and then declare that this is valid for all values of \( x'', x' \). The second is to use the path integral defined object but modify the integrations over the unphysical parameter time labels, as in Eqs.(2.5.23), (2.5.27). The two methods are equivalent for the simple model of this Chapter. The benefit of introducing the second method is that it shows that the modification procedure does not fundamentally modify the class of paths in configuration space summed over in the path integral, only the way their parametrizations are summed over. The modified class operators therefore still have equal claim to be a sum over paths which cross the surface.

These issues concerning modified class operators will be taken up in more detail in the next chapter.

### 2.5.5 A Multiple Crossings Decomposition?

The results of Section 2.5.2 show that it is a partition of paths according to their first and last crossing of a spacelike surface that leads to the expected Klein-Gordon probability expression Eq.(2.4.23). It is, however, of interest to explore other notions of surface crossings. This is partly by way of a digression, but it is also relevant to the recovery of the Newton-Wigner probability expression.

We begin by considering the first-crossing path decomposition expansion Eq.(2.5.6), with \( T \) integrated over a half-infinite range. We restrict to the case \( x''_0 > \tau > x'_0 \), and for simplicity restrict to the positive frequency sector. In this subsection we will take \( \Delta = \mathbb{R}^3 \). We thus obtain

\[
G^+(x'', x') = 2i \int d^3x \ G^+(x'', x) \overrightarrow{\partial_0}G^+(x, x')
\]  

(averaged with the last crossing PDX this gives the composition law in Eq.(2.3.2)). From
Section 2.3 we also have that

\[ 2i\partial_0 G^+(x'', x') = G_{NW}(x'', x') \]  

and Eq.(2.5.28) becomes

\[ G^+(x'', x') = \int d^3x \ G^+(x'', x)G_{NW}(x, x') \]  

In this expression the Newton-Wigner propagator therefore represents paths that start at \( x' \), move forwards and backwards in time but without crossing the final surface, except to end on it at point \( x \). (See Fig. 5). Similarly, one can see from the last crossing PDX Eq.(2.5.7), that a sum over paths which move backwards and forwards in time but without crossing the initial surface, except to start on it, is \(-2iG^+(x'', x')\partial_0\). (See Fig. 9). This is in fact again the Newton-Wigner propagator \( G_{NW}(x, x') \), as may be seen from Eq.(2.3.13), and we may write

\[ G^+(x'', x') = \int d^3x \ G_{NW}(x'', x)G^+(x, x') \]  

Using these two relations, we may carry out an iteration of Eq.(2.5.30) to yield

\[ G^+(x'', x') = \int d^3x_1 d^3x_2 \ G_{NW}(x'', x_2)G^+(x_2, x_1)G_{NW}(x_1, x') \]  

The two Newton-Wigner propagators represent restricted propagation to the first crossing and from the last crossing of the surface, and the propagator \( G^+(x_2, x_1) \) is unrestricted propagation between two points which both lie on the spacelike surface. (See Fig. 10).

It is now reasonable to ask whether this expression can be further decomposed according to the detailed number of surface crossings entailed in the path integral representation of \( G^+(x_2, x_1) \). Interestingly, this does not appear to be possible. For suppose we apply a first or last crossing expansion of the type Eq.(2.5.30) or Eq.(2.5.31) to the propagator \( G^+(x_2, x_1) \). It is then the case that all three points involved (initial point, final point, crossing point) all have the same value of \( x^0 \), hence the expression would contain the Newton-Wigner propagator \( G_{NW}(x, y) \) at \( x^0 = y^0 \). But this is simply the delta function \( \delta^{(3)}(x - y) \), leading to a trivial result. Hence a further decomposition according to the specific number of crossings appears to be impossible.

The explanation for this is that in a path integral representation of \( G^+(x_2, x_1) \), generic paths cross the surface an infinite number of times, and the set of paths crossing a finite
number of times is of measure zero. This result is due in essence to Hartle [46], who considered a lattice version of the Euclideanized sum over histories. He attempted to factor the usual propagator of non-relativistic quantum mechanics across an arbitrary surface in spacetime by partitioning according to the number of crossings each path makes. He showed that paths with a finite number of crossings generally have zero amplitude in the continuum limit, and deduced that such a factoring is not in fact possible. (This is not in contradiction with the path decomposition expansion, Eq.(2.5.6), which partitions the paths according to their first crossing).

On the face of it, therefore, it might seem like there are a number of different notions of surface crossing. The above results show, however, that first and last crossings are the only ones that can be defined in this case, hence are the only useful ones for defining the class operators of interest here.

### 2.6 The Newton-Wigner Case

Consider now the question of how to obtain the Newton-Wigner probability Eq.(2.4.14) from the decoherent histories approach. Since this is like non-relativistic quantum mechanics but with the Hamiltonian $h = \sqrt{-\nabla^2 + m^2}$, it is simpler than the previous case and we describe it only briefly.

The decoherence functional is given by Eq.(2.3.17) in which the inner product $\circ$ is the Schrödinger inner product, with the initial states normalized in this product. The main issue is the construction of the class operator representing crossing a spacelike surface $x^0 = \tau$ in a spatial region $\Delta$. We first give the result and then explain its origin. (For simplicity we concentrate on the positive frequency sector only). It is clear that the class operator is

$$C_\Delta(x'',x') = \int_\Delta d^3x \ G_{NW}(x'',x^{0''},x,\tau) \ G_{NW}(x,\tau,x',x^{0'})$$

Note that when $\Delta = \mathbb{R}^3$ this gives the standard composition property of the Newton-Wigner propagator

$$G_{NW}(x'',x') = \int d^3x \ G_{NW}(x'',x^{0''},x,\tau) \ G_{NW}(x,\tau,x',x^{0'})$$
Inserting in the decoherence functional (2.3.17), it is readily shown this gives exact decoherence, and the probabilities coincide with Eq.(2.4.14) (this is very similar to standard calculations in non-relativistic quantum mechanics). It is necessary also to use here the fact that the Newton-Wigner propagator is the overlap of two Newton-Wigner states,

\[ G_{NW}(x, x^0 | y, y^0) = \langle x, x^0 | y, y^0 \rangle_I \]  (2.6.3)

There are (at least) two path integral representations of the path integral for the Newton-Wigner propagator that lead to the class operator (2.6.1). The first is the one of the standard non-relativistic form:

\[ G(x'', \tau'', x', \tau') = \int Dx Dp \exp \left( i \int_{\tau'}^{\tau''} dx^0 \left[ p \cdot \frac{dx}{dx^0} - \sqrt{p^2 + m^2} \right] \right) \]  (2.6.4)

(The configuration space form of this path integral may also be considered, but the measure is then rather complicated [53]). In this representation, the paths move forwards in the time coordinate \( x^0 \). Summing over paths from \( x' \) to \( x'' \) which pass through \( \Delta \) on an intermediate spacelike surface then yields the class operator (2.6.1).

A second and perhaps more interesting path integral representation of \( G_{NW}(x'', x') \) is the one mentioned in the discussion of the path decomposition expansion of the previous section. This is to use a path integral representation of the form (2.1.6), (2.1.7), in which the paths summed over do not cross the final surface except to end on it at \( x'' \), depicted in Fig. 5. (See also Refs.[42, 46]). Equivalently, they can be restricted so that they start at the initial point \( x' \) but do not cross it thereafter (see Fig. 9). In fact, it is easy to show from these representations, using Eq.(2.6.2), that \( G_{NW}(x'', x') \) is obtained more generally by choosing any surface of constant \( x^0 \) lying between initial and final points, and then summing over paths which cross it once and only once, as depicted in Fig. 11. The first two representations then correspond to the limit in which the intermediate surface tends to the initial or final surface. From this third representation, we see that the class operator Eq.(2.6.1) is obtained by summing over paths which cross the intermediate spacelike surface once and only once, in the spatial region \( \Delta \).

Note that there is no conflict here with the statement in Section 2.5.5 that the set of paths crossing a surface only a finite number of times is of zero measure in the set
of all paths. Section 2.5.5 concerned path integral representations of the Klein-Gordon propagators, which involve a sum over all paths between two points, and the set of paths making single crossings of given surface are indeed insignificant. However, the path integral representation of the Newton-Wigner propagator considered is defined from the outset by a sum over the much smaller class of paths which cross an intermediate surface only once.

2.7 Summary and Discussion

As already mentioned, this thesis is part of a programme whose general aim is to supply a reasonable predictive framework for quantum cosmological models. In connection with that aim, the main achievement of this Chapter is the derivation of the probability formula Eq.(2.5.22) (or Eq.(2.4.23)) from the decoherent histories approach, and the demonstration that the associated histories are approximately decoherent.

Along the way we derived a number of other relevant results. We showed how to modify in a physically sensible way class operators which do not satisfy the constraints. We also showed that first and last crossings are essentially the only ways of defining surface crossings (in the Klein-Gordon quantization). In particular, partitions of paths according to multiple crossings are not possible. These results will be relevant to more complicated models in quantum cosmology.

The main result of Section 2.4 is the computation of an evolving constraints operator for the relativistic particle, proof that its eigenstates are the Newton-Wigner states, and that the operator is essentially the same as the Newton-Wigner operator. We discussed some novel path integral representations of the NW propagator in Section 2.6, involving single surface crossings and computed the decoherence functional (although noted that it is very similar to the case of non-relativistic quantum mechanics).

We do not expect that a Newton-Wigner quantization based on a Schrödinger equation such as Eq.(2.3.12) will be relevant to more complicated models in quantum cosmology, since it is only under very special circumstances that the constraint may be solved to produce a real, positive Hamiltonian $h$ to go in Eq.(2.3.12). The comparison with this case has, however, proved quite useful in the present Chapter. Furthermore, here, our
starting point for an operator quantization was the evolving constants method, based on
Eq.(2.1.4), which does not require the solution to the constraints, and this method will be
valid for more complicated models (and indeed has been used already in such a context
[80–82, 84]). We also note that we find agreement between the operator methods of Section
2.4 and the decoherent histories results of Sections 2.5 and 2.6.

We may now return to the discussion initiated at the end of Section 2.2, on the rela-
tionship between decoherence, surface crossings and the existence of self-adjoint operators.
We see further evidence for this. It is striking that the NW quantization, which involves
single surface crossings in the decoherent histories approach, yields exact decoherence of
histories, whereas the KG quantization, which has multiple surface crossings, exhibits
only approximate decoherence. It is reasonable to conclude from this that the approxi-
mate nature of the decoherence is related to the fact that the paths in KG quantization go
backwards and forwards in time and cross a surface many times. In fact, generally speak-
ing, one might expect such multiple crossings to destroy decoherence altogether, since the
paths may pass through both $\Delta$ and its complement $\bar{\Delta}$, but with single crossings they
may pass through only one or the other. The interesting question is therefore why even
approximate decoherence is obtained. For the free relativistic particle considered here, the
answer is that the dominant contribution to the path integral representation of the class
operators comes from the immediate neighbourhood of the classical path from $x'$ to $x''$,
and this crosses the surface only once. Paths with multiple crossings therefore presumably
belong to the quantum fluctuations about the classical path, and these may be neglected
at sufficiently coarse-grained scales. Note also that the anticipated connection with self-
adjoint operators holds up. The NW probability is associated with a self-adjoint operator,
whilst the KG probability is not.

The difference of the expressions for the Newton-Wigner and Klein-Gordon probabil-
ity (2.4.14), (2.4.23) of entering the region $\Delta$ also motivates the question which of these
expressions is the physically correct one. If one would do an experiment which probability
would one obtain? That these expressions are different, is not a surprise, since, as we
mentioned, we have used two different quantization schemes. Moreover the position oper-
ators we defined have different momentum space representations. They act differently on
the same momentum space solution to the Klein-Gordon equation.
But can we argue for one of these expressions form a physical point of view? Although we only have approximate decoherence in the Klein-Gordon expression, it still incorporates relativistic invariance. This invariance is lost for the Newton-Wigner case, and in that sense the Klein-Gordon case is more complete. More arguments could be found if one would examine detector models that emulate the different position “measurements”. Ultimately the answer would have to be given by an explicit experiment.
Chapter 3

Life in an Energy Eigenstate: 
Decoherent Histories Analysis of a 
Model Timeless Universe

3.1 Introduction

In this chapter we study in a more general context the quantization and interpretation of simple timeless models described by an equation of the Wheeler-DeWitt type

\[(\hat{H} - E)\Psi(x) = 0\] (3.1.1)

We still study the question: what is the probability that the system passes through a region \(\Delta\) of configuration space without reference to time? But in contrast to the previous chapter we won’t specify the region further. (For some calculations we have to assume that \(\Delta\) is an open subset). Also all the results presented are applicable to quantum cosmological models with an Hamiltonian of the form

\[H = \sum_{k,j=1}^{n} \left( g^{kj}(x)p_k p_j + V(x) \right)\] (3.1.2)

where \(g^{kj}(x)\) is an inverse metric of hyperbolic signature. Most quantum cosmological models are of this type.
We begin in Section 3.2 by analyzing our question in the classical case. We introduce a classical phase space distribution function \( w(p, x) \) that obeys \( \{ H, w \} = 0 \) and compute the probability that a trajectory in configuration space passes through a region \( \Delta \). Most of the key ideas for this chapter are in fact contained in this classical result. In particular, we discuss the reparametrization invariance of the system, and introduce observables corresponding to entire classical trajectories. We write the classical result in a number of different forms, including a form in terms of a flux across a hypersurface, closely related to the heuristic WKB interpretation of quantum cosmology. We also show how the induced inner product for the quantum case implies a useful normalization for the classical phase space distribution function.

We begin the quantum case in Section 3.3, with the construction of the decoherence functional for timeless models in the way we have set it out in Chapter 1. The main aspect is again the construction of the class operators, which in this case are propagators describing coarse-grained sets of histories passing through restricted regions of configurations space.

In Section 3.4, we discuss the semiclassical limit of the decoherence functional. A key step is the construction of class operators corresponding to restricted sets of histories entering the region \( \Delta \). The obvious candidates for these class operators are not in fact compatible with the constraint equation, and we therefore show how they may be appropriately modified. This turns out in fact to be the crucial step in the construction of the decoherence functional. We then show that, for the special initial states for which the histories are decoherent, the probabilities for the histories approximately coincide with the classical case, with the phase space distribution function \( w(p, x) \) replaced by the Wigner function \( W(p, x) \) of the quantum system.

In Section 3.5, we consider the special case in which the system is a collection of harmonic oscillators in a fixed energy eigenstate. For this system it is possible to introduce a special class of eigenstates of the Hamiltonian sometimes called “timeless coherent states”, which have the property that they are concentrated about an entire classical phase space trajectory. We discuss the decoherence and probabilities associated with these states and obtain the intuitively expected physical results for the probabilities of entering a region.
Since decoherence is only obtained for special initial states, we consider, in Section 3.6, the addition of an environment to produce decoherence for a wide variety of initial states. We repeat the calculation of decoherence and probabilities with intuitively expected results, in agreement with classical expectations.

The calculations of Sections 3.4 and 3.6 used initial states consisting of single WKB wave packets. In Section 3.7, we therefore extend to the case of superpositions of such wave packets. This turns out in fact to be straightforward, and very similar to earlier calculations performed with the reduced density matrix. We easily find that the interference terms between different WKB wave packets are very small. We summarize and conclude in Section 3.8.

### 3.2 The Classical Case

We are interested in the question, “What is the probability associated with a given region of configuration space when the system obeys an energy eigenstate equation?” We begin by analyzing the classical problem.

We will consider a classical system described by a $2n$-dimensional phase space, with coordinates and momenta $(x, p) = (x_k, p_k)$, and Hamiltonian

$$H = \sum_{k=1}^{n} \left( \frac{p_k^2}{2M} + V(x) \right)$$

(3.2.1)

More generally, as already mentioned, we are interested in a system for which the kinetic part of the Hamiltonian has the form $g^{kj}(x)p_k p_j$, where $g^{kj}(x)$ is an inverse metric of hyperbolic signature. Most minisuperspace models in quantum cosmology have a Hamiltonian of this form. However, the focus of this research is the timelessness of the system, and the form of the configuration space metric turns out to be unimportant. So for simplicity, we will concentrate on the form Eq.(3.2.1).

We assume that there is a classical phase space distribution function $w(p, x)$, which is normalized according to

$$\int d^n p \, d^n x \, w(p, x) = 1$$

(3.2.2)
and obeys the evolution equation

$$\frac{\partial w}{\partial t} = \sum_k \left( -\frac{p_k}{M} \frac{\partial w}{\partial x_k} + \frac{\partial V}{\partial x_k} \frac{\partial w}{\partial p_k} \right) = \{H, w\}$$

(3.2.3)

where \{ , \} denotes the Poisson bracket. The interesting case is that in which \(w\) is the classical analogue of an energy eigenstate, in which case \(\partial w/\partial t = 0\), so the evolution equation is simply

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

(3.2.4)

It follows that

$$w(p^{cl}(t), x^{cl}(t)) = w(p_0, x_0)$$

(3.2.5)

where \(p^{cl}(t), x^{cl}(t)\) are the classical solutions with initial data \(p_0 = p^{cl}(0), x_0 = x^{cl}(0)\). So \(w\) is constant along the classical orbits. (The normalization of \(w\) then becomes an issue if the classical orbits are infinite, but we will return to this at the end of this Section.)

Given a set of classical solutions \((p^{cl}(t), x^{cl}(t))\), and a phase space distribution function \(w\), we are interested in the probability that a classical solution will pass through a region \(\Delta\) of configuration space. For the following construction to work we have to assume that \(\Delta\) is open, other we would miss trajectories that only touch the region in one point. First of all we introduce the characteristic function of the region \(\Delta\),

$$f_\Delta(x) = \begin{cases} 
1, & \text{if } x \text{ in } \Delta; \\
0 & \text{otherwise}
\end{cases}$$

(3.2.6)

To see whether the classical trajectory \(x^{cl}(t)\) intersects this region, consider the phase space function

$$A(x, p_0, x_0) = \int_{-\infty}^{\infty} dt \, \delta^{(n)}(x - x^{cl}(t))$$

(3.2.7)

(In the case of periodic classical orbits, the range of \(t\) is taken to be equal to the period). This distribution is positive for points \(x\) on the classical trajectory labelled by \(p_0, x_0\) and zero otherwise. Hence intersection of the classical trajectory with the region \(\Delta\) means,

$$\int d^n x \, f_\Delta(x) \int_{-\infty}^{\infty} dt \, \delta^{(n)}(x - x^{cl}(t)) > 0$$

(3.2.8)

Or equivalently, that

$$\int_{-\infty}^{\infty} dt \, f_\Delta(x^{cl}(t)) > 0$$

(3.2.9)
This quantity is essentially the amount of parameter time the trajectory spends in the region $\Delta$. We may now write down the probability for a classical trajectory entering the region $\Delta$. It is,

$$p_\Delta = \int d^n p_0 d^n x_0 \ w(p_0, x_0) \ \theta \left( \int_{-\infty}^{\infty} dt \ f_\Delta(x^{cl}(t)) - \epsilon \right)$$  \hspace{1cm} (3.2.10)

In this construction, $\epsilon$ is a small positive number that is eventually sent to zero, and is included to avoid possible ambiguities in the $\theta$-function at zero argument. The $\theta$-function ensures that the phase space integral is over all initial data whose corresponding classical trajectories spend a time greater than $\epsilon$ in the region $\Delta$.

The classical solution $x^{cl}(t)$ depends on some fiducial initial coordinates and momenta, $x_0$ and $p_0$, say. In the case of a free particle, for example,

$$x^{cl}(t) = x_0 + p_0 t M$$  \hspace{1cm} (3.2.11)

The construction is independent of the choice of fiducial initial points. If we shift $x_0$, $p_0$ along the classical trajectories, the measure, phase space distribution function $w$ and the $\theta$-function are all invariant. Hence the integral over $x_0$, $p_0$ is effectively a sum over classical trajectories. The shift along the classical trajectories may also be thought of as a reparametrization, and the quantity (3.2.10) is in fact a reparametrization-invariant expression of the notion of a classical trajectory. This means that the probability (3.2.10) has the form of a phase space overlap of the “state” with a reparametrization-invariant classical observable.

It is useful also to write this result in a different form, which will be more relevant to the results we get in the quantum theory case. In the quantum theory, we generally deal with propagation between fixed points in configuration space, rather than with phase space point. Therefore, in the free particle case, consider the change of variables from $x_0, p_0$ to $x_0, x_f$, where

$$x_f = x_0 + \frac{p_0 \tau}{M}$$  \hspace{1cm} (3.2.12)

Hence $x_f$ is the position after evolution for starting from $x_0$ for parameter time $\tau$. The probability then becomes

$$p_\Delta = \left( \frac{M}{\tau} \right)^n \ \int d^n x_f d^n x_0 \ w(p_0, x_0) \ \theta \left( \int_{-\infty}^{\infty} dt \ f_\Delta(x^{cl}_f(t)) - \epsilon \right)$$  \hspace{1cm} (3.2.13)
where \( p_0 = M(x_f - x_0)/\tau \) and
\[
x_{0f}(t) = x_0 + \frac{(x_f - x_0)}{\tau} t
\]
(3.2.14)
The parameter \( \tau \) may in fact be scaled out of the whole expression, hence the probability is independent of it.

The result now has the form of an integral over “initial” and “final” points, analogous to similar results in quantum theory. The result is again essentially a sum over classical trajectories with the trajectories now labelled by any pair of points \( x_0, x_f \) along the trajectories, and is invariant under shifting \( x_0 \) or \( x_f \) along those trajectories. Naively, one might have thought that the restriction to paths that pass through \( \Delta \) is imposed by summing over all finite length classical paths which intersect \( \Delta \) as they go from the “initial” point \( x_0 \) to “final” point \( x_f \); that is, \( \Delta \) lies between the initial and final points. This is also what one might naively expect in the quantum theory version. However, one can see from the above construction that the correct answer is in fact to sum over all classical paths (which can be of infinite length) passing through \( x_0 \) and \( x_f \) that intersect \( \Delta \) at any point along the entire trajectory, even if \( \Delta \) does not lie between the two points (see Fig. 12). This feature is related to the reparametrization invariance of the system.

The above point turns out to be quite crucial to what follows in the rest of this chapter, so it is worth saying it in an alternative form. Loosely speaking, the statement is that only the entire classical path respects the reparametrization invariance associated with the constraint equation. A section of the classical path does not. This may be expressed more precisely in terms of the function \( A(x, p_0, x_0) \) introduced in Eq.(3.2.7). This function is concentrated on the entire classical trajectory, and is zero when \( x \) is not on the trajectory. It is easy to see that it has vanishing Poisson bracket with the Hamiltonian \( H = H(p_0, x_0) \), since we have
\[
\{H, A(x, p_0, x_0)\} = \int_{-\infty}^{\infty} dt \{ H, \delta^{(n)}(x - x^{cl}(t)) \}
\]
\[
= -\int_{-\infty}^{\infty} dt \frac{d}{dt} \delta^{(n)}(x - x^{cl}(t))
\]
(3.2.15)
\[
= 0
\]
This is the precise sense in which the entire trajectory is reparametrization invariant, and the phase space function \( A \) may be regarded as an observable – a quantity which Poisson
bracket with the constraint $H$ vanishes \[82, 100, 102\]. By way of comparison, consider a second phase space function similarly defined, but on only a finite section of trajectory,

$$B(x, p_0, x_0) = \int_0^\tau dt \, \delta^{(n)}(x - x^{cl}(t))$$  \hfill (3.2.16)

It is easily seen that

$$\{H, B(x, p_0, x_0)\} = -\delta(x - x^{cl}(\tau)) + \delta(x - x^{cl}(0))$$  \hfill (3.2.17)

Hence $B$ “almost” commutes with $H$, failing only at the end points, and it is in this sense that a finite section of trajectory does not fully respect reparametrization invariance.

A third version of the classical result is also useful. It is of interest to obtain an expression for the probability for intersecting an $(n - 1)$-dimensional surface $\Sigma$. Since the result (3.2.10) involves the parameter time spent in a finite volume region $\Delta$ it does not apply immediately. However, suppose that the set of trajectories contained in the probability distribution $w$ intersect the $(n - 1)$-dimensional surface $\Sigma$ only once. Then we may consider a finite volume region $\Delta$ obtained by thickening $\Sigma$ along the direction of the classical flow. If this thickening is by a small (positive) parameter time $\Delta t$, then the quantity appearing in the $\theta$-function in (3.2.10) is

$$\int dt \int_\Delta d^n x \, \delta^{(n)}(x - x^{cl}(t)) = \Delta t \int dt \int_\Sigma d^{n-1} x \, n \cdot \frac{dx^{cl}(t)}{dt} \, \delta^{(n)}(x - x^{cl}(t))$$  \hfill (3.2.18)

where $n$ is the normal to $\Sigma$, and we suppose that the normal is chosen so that $n \cdot \frac{dx^{cl}}{dt}$ is positive. The quantity $I[\Sigma, x^{cl}(t)]$, in a more general context, is the intersection number of the curve $x^{cl}(t)$ with the surface $\Sigma$, and takes the value 0 for no intersections, or $k \in \mathbb{N}$ otherwise (depending on the number of intersections). In this case we have assumed that the trajectories intersect at most once, hence $I = 0$ or 1. We then have

$$\theta(\Delta t I - \epsilon) = \theta(I - \epsilon') = I$$  \hfill (3.2.19)

(where $\epsilon = \Delta t \epsilon'$) and the probability for intersecting $\Sigma$ may be written

$$p_\Sigma = \int dt \int d^n p_0 d^n x_0 \, w(p_0, x_0) \int_\Sigma d^{n-1} x \, n \cdot \frac{dx^{cl}(t)}{dt} \, \delta^{(n)}(x - x^{cl}(t))$$  \hfill (3.2.20)
At each $t$, we may perform a change of variables from $p_0, x_0$ to new variables $p' = p^c(t)$, $x' = x^c(t)$, and using that $w$ is constant along the trajectories (Eq.(3.2.5)), we obtain the result

$$p_\Sigma = \frac{1}{M} \int dt \int_\Sigma d^n p' d^{n-1} x' \ n \cdot p' \ w(p', x')$$  \hspace{1cm} (3.2.21)

Finally, the integrand is now in fact independent of $t$, so the $t$ integral leads to an overall factor. (This might be infinite but is regularized as discussed below). We therefore drop the $t$ integral.

This result is relevant for the following reason. In the heuristic “WKB interpretation” of quantum cosmology, one considers WKB solutions to the Wheeler-DeWitt equation of the form

$$\Psi = C e^{iS}$$  \hspace{1cm} (3.2.22)

It is usually asserted that this corresponds to a set of classical trajectories with momentum $p = \nabla S$, and with a probability of intersecting a surface $\Sigma$ given in terms of the flux of the wave function across the surface [36, 55, 56]. As we shall show, from the decoherent histories analysis, the quantum theory gives a probability for crossing a surface $\Sigma$ proportional to Eq.(3.2.21) with $w$ replaced by the Wigner function of the quantum theory. The Wigner function of the WKB wave function is, approximately [33],

$$W(p, x) = |C(x)|^2 \delta(p - \nabla S)$$  \hspace{1cm} (3.2.23)

Inserting in Eq.(3.2.21), we therefore obtain, up to overall factors, the probability distribution,

$$p_\Sigma = \int_\Sigma d^{n-1} x \ n \cdot \nabla S \ |C(x)|^2$$  \hspace{1cm} (3.2.24)

We therefore have agreement with the usual heuristic analysis of (3.2.22) in quantum cosmology.

### 3.2.1 Normalization of the classical phase space distribution function

The induced inner product scheme of Section 1.2.2 suggests a normalization scheme for the classical phase space distribution function $w$, which, recall, is not normalizable in the case where the classical trajectories are infinite (since $w$ is constant along those trajectories).
The idea is to consider the normalization of the phase space Wigner function $W$ corresponding to a density operator $\rho$. $W$ is defined by

$$W(p, X) = \frac{1}{(2\pi)^n} \int d^n v \, e^{-ip \cdot v} \rho(X + \frac{1}{2}v, X - \frac{1}{2}v)$$

(3.2.25)

with inverse

$$\rho(x, y) = \int d^n p \, e^{ip \cdot (x-y)} W(p, \frac{x+y}{2})$$

(3.2.26)

(See Refs. [4, 59, 105] for properties of the Wigner function.)

We now consider the normalization of $\rho$ in the induced inner product. For an energy eigenstate $|\Psi_E\rangle$ we first of all construct an auxiliary operator $\tilde{\rho}_{EE'}$ for regularization,

$$\tilde{\rho}_{EE'} = |\Psi_E\rangle\langle\Psi_{E'}|$$

(3.2.27)

which is a density operator for $E = E'$ and is normalized by

$$\text{Tr} (\tilde{\rho}_{EE'}) = \delta(E - E')$$

(3.2.28)

hence the corresponding Wigner function is normalized according to

$$\int d^n p d^n x \, \tilde{W}_{EE'}(p, x) = \delta(E - E')$$

(3.2.29)

Now notice that the operator $\tilde{\rho}_{EE'}$ obeys the equation

$$[H, \tilde{\rho}_{EE'}] = (E - E')\tilde{\rho}_{EE'}$$

(3.2.30)

Taking the Wigner transform of this equation we obtain

$$\mathcal{L}\tilde{W}_{EE'} = i(E - E')\tilde{W}_{EE'}$$

(3.2.31)

where $\mathcal{L}$ is the phase space operator

$$\mathcal{L} = \sum_k \left(-\frac{p_k}{M} \frac{\partial}{\partial x_k} + \frac{\partial V}{\partial x_k} \frac{\partial}{\partial p_k}\right) + \mathcal{L}_q$$

(3.2.32)

It is a sum of the classical Liouville operator, plus a term $\mathcal{L}_q$ describing quantum modifications.

We may now see how to normalize the classical case. We take the classical distribution function to be described by Eq.(3.2.31) with the quantum term $\mathcal{L}_q$ set to zero. The Liouville operator may then be written as

$$\mathcal{L} = -\frac{d}{ds}$$

(3.2.33)
for some parameter $s$, and Eq.(3.2.31) may be solved, with the result,

$$w_{EE'} = e^{-is(E-E')}w_{EE} \tag{3.2.34}$$

since $Lw_{EE} = 0$. The exponential factor now effectively regularizes the phase space distribution function. $w_{EE}$ is constant along the classical trajectories, but $w_{EE'}$ is not, and, in the normalization (3.2.29), the part of the integral along the trajectories is an integral over $s$ which produces the $\delta$-function.

## 3.3 The Quantum Case

### 3.3.1 Construction of the Decoherence Functional.

Following our approach of Section 1.3, the decoherence functional has the form (like the probability (1.3.1))

$$D(\alpha, \alpha') = \text{Tr}_{\text{ind}} \left[ C_\alpha |\Psi\rangle \langle \Psi | C_{\alpha'}^\dagger \right], \tag{3.3.1}$$

where the subscript “ind” reminds us that we have to take the trace using the induced inner product. We will implement it by using different energies for the class operators and the wave functions (see below).

The essential part of the construction of the decoherence functional is to find the class operators, $C_\alpha$. These are to describe histories of fixed energy which do or do not pass through the region $\Delta$ without regard to time, denoted $\alpha = \Delta$ and $\alpha = \Delta'$ respectively. As mentioned in Chapter 1, we partly follow Refs.[50, 51].

We consider first the amplitude to go from $x_0$ at time $t = 0$ to $x_f$ at time $t = \tau$ passing through the region $\Delta$, or not, at any time in between. This is given by

$$g_\alpha(x_f, \tau|x_0, 0) = \int_\alpha D_x(t) \exp \left( \frac{i}{\hbar} S[x(t)] \right) \tag{3.3.2}$$

where the sum is over all paths $x(t)$ with $t$ in the range $[0, \tau]$ which pass through $\Delta$, or never pass through $\Delta$. It therefore satisfies,

$$\sum_\alpha g_\alpha = g_\Delta + g_{\Delta'} = g \tag{3.3.3}$$
where \( g = g(x_f, \tau | x_0, 0) \) is the unrestricted propagator. There are many ways of constructing this sort of object more explicitly (see Refs.\[3, 37, 42, 43\] for example), but here it is useful to exploit the construction used in the classical case. The amplitude to pass through \( \Delta \) is therefore given by

\[
g_{\Delta}(x_f, \tau | x_0, 0) = \int \mathcal{D}x(t) \exp \left( iS[x(t)] \right) \theta \left( \int_0^\tau dt \ f_\Delta(x(t)) - \epsilon \right)
\]

(3.3.4)

Here, the \( \theta \)-function ensures that only paths \( x(t) \) that spend a time in excess of \( \epsilon \) in \( \Delta \) contribute to the sum.

As in Eq. (1.3.3), the class operator \( C_\alpha \) is a propagator at fixed energy \( E \) and is given by

\[
\langle x_f | C_\alpha | x_0 \rangle = \int_{-\infty}^{\infty} d\tau \frac{e^{-iE\tau}}{2\pi} \ g_\alpha(x_f, \tau | x_0, 0)
\]

(3.3.5)

When \( g_\alpha \) is replaced with an unrestricted propagator, we require that (3.3.5) is annihilated by \( H - E \), and this is why we choose an infinite range for \( \tau \), rather than a half-infinite one [34, 41, 106–108]. (As we shall see below, when \( g_\alpha \) is a restricted propagator, we encounter some difficulties here, although the correct range for \( \tau \) is still the infinite one). The total decoherence functional (regularized by using different energies) is therefore given by (like Eq. (1.3.5))

\[
D(\alpha, \alpha') = \frac{1}{(2\pi)^2} \int d^n x_f d^n x_0 d^n x'_f d^n x'_0 \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' e^{-iE\tau} e^{iE'\tau'}
\]

\[
\times g_\alpha(x_f, \tau | x_0, 0) \ g^{\ast}_{\alpha'}(x_f, \tau' | x'_0, 0) \ \Psi_{E_0}(x_0) \Psi^{\ast}_{E_0'}(x'_0)
\]

(3.3.6)

This may also be written,

\[
D(\alpha, \alpha') = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' e^{-iE\tau} e^{iE'\tau'}
\]

\[
\times \int_{\alpha} \mathcal{D}x(t) \int_{\alpha'} \mathcal{D}x'(t) \exp \left( iS_0^\ast[x(t)] - iS_0'[x'(t)] \right)
\]

\[
\times \Psi_{E_0}(x_0) \Psi^{\ast}_{E_0'}(x'_0)
\]

(3.3.7)

where note that the two actions in the path integral are over different ranges of time. It is straightforward to show that

\[
\sum_{\alpha, \alpha'} D(\alpha, \alpha') = \delta(E - E_0) \delta(E' - E'_0) \delta(E_0 - E'_0)
\]

(3.3.8)

In the induced inner product scheme we therefore replace the righthand side by 1, verifying that the construction is correctly normalized.
3.3.2 Modified Class Operators

The basic scheme described above runs into the same difficulty we encountered in the previous chapter. The class operators defined by (3.3.5) do not necessarily satisfy the constraint equation. We have, for example, for the class operator for paths that enter the region $\Delta$,

$$C_{\Delta}(x_f, x_0) = \int_{-\infty}^{\infty} d\tau e^{-iE\tau} \int D_x(t) \exp \left( iS[x(t)] \right) \theta \left( \int_{0}^{\tau} dt f_{\Delta}(x(t)) - \epsilon \right)$$  (3.3.9)

It may be shown that this satisfies the constraint everywhere except on the boundaries of the region $\Delta$. That is, there is a discontinuity as one of the end-points crosses the boundary of $\Delta$. This is an issue because a basic rule of the game of constructing the decoherence functional for these systems is that we only work with objects which satisfy the constraint equation (or operators which commute with it). Mathematically, this is to ensure that the underlying symmetry, reparametrization invariance, is fully respected (the induced inner product, note, is defined only between objects which satisfy the constraint). Physically, it is related to the fact that the universe is a closed system, and measurements of it (the class operators are generalizations of the notions of measurement) must not lead out of the physical state space.

Because of this difficulty, it is necessary to define a modified class operator $C'_{\Delta}$ which is as close as possible to the path integral one, but satisfies the constraint equation everywhere [51]. A way to do this is to first compute the class operator $C_{\Delta}$ when one of the end-points is inside $\Delta$. (This is the way we found the physically reasonable noncrossing operator (2.5.5) in the previous chapter). This defines a solution to the constraints for one end-point inside and the other outside. We then define $C'_{\Delta}$ to be the object which satisfies the constraint everywhere and matches this expression for one end-point inside and the other outside.

This issue concerning the replacement of the original class operators with modified ones is related to the fact that in the original class operator (3.3.9), the functions restricting the paths to enter the region $\Delta$ involve a time integral over a finite interval $[0, \tau]$, whereas the classical result (3.2.13) involves a similar restricting function but with a time integral over an infinite range. If a finite range is used in the classical result, it is no longer
reparametrization invariant, as we saw in Section 3.2. This is why we discussed the classical result at such length.

The construction of these modified class operators is crucial to the construction of the decoherence functional for reparametrization-invariant theories. It is probably fair to say that the method suggested above for constructing them has not at this stage been fully explored. We will show below that a physically plausible modified class operator is readily constructed in the semiclassical approximation, but a more thorough investigation of this issue for the full path integral is necessary. It should also be noted that reparametrization-invariance can be rather subtle. For example, the path-integral constructed class operators Eq.(3.3.9) certainly appear to be reparametrization-invariant at the level of Lagrangian symmetry transformations, yet do not quite satisfy the constraint. Here, we have used the expression “reparametrization-invariant” to mean satisfying the constraint everywhere (or having a vanishing Poisson bracket with the Hamiltonian everywhere, in the classical case). This issue is related to the connections between Lagrangian and Hamiltonian symmetries, and between the path integral and Dirac quantizations. (See also Refs.[41, 50] for further discussion).

3.4 The Semiclassical Approximation to the Decoherence Functional and Probabilities

We may now compute the decoherence functional. It is

\[ D(\alpha, \alpha') = \int d^n x_f d^n x_0 d^n y_0 \ C'_\alpha(x_f, x_0) C'^*_\alpha'(x_f, y_0) \ \Psi(x_0) \Psi^*(y_0) \quad (3.4.1) \]

(For convenience, here and in what follows we will in fact drop the notation involving different values of \( E \) to regularize the expressions, unless necessary). To see how the semiclassical approximation works out, we will in this Section assume decoherence (for example, by restricting to special initial states) and concentrate on the construction of the probabilities that the system passes through the region \( \Delta \). We will return to the question of decoherence for general initial states in Section 3.6.

We begin by computing the semiclassical approximation to the modified class operator \( C'_\Delta(x_f, x_0) \). In the absence of any restrictions on the paths, the path integral will be
dominated by the classical paths connecting the initial and final points. The classical
paths will be the solutions to the equations of motion

\[ M\ddot{x} + \nabla V(x) = 0 \quad (3.4.2) \]

which satisfy the boundary conditions

\[ x(0) = x_0, \quad x(\tau) = x_f \quad (3.4.3) \]

In addition, these paths must satisfy the constraint equation

\[ \frac{1}{2} M\dot{x}^2 + V(x) = E \quad (3.4.4) \]

This equation determines the time \( \tau \) in terms of \( x_0, x_f \) and \( E \), hence the final form of the
extremizing paths have no reference to time. It is also useful to introduce \( A(x_f, x_0) \), the
classical action from \( x_0 \) to \( x_f \). It obeys the time-independent Hamilton-Jacobi equation
with respect to each end point,

\[ \frac{1}{2M} (\nabla A)^2 + V(x) = E \quad (3.4.5) \]

The initial and final momenta are given by derivatives of the classical action,

\[ p_f = \nabla f A(x_f, x_0), \quad p_0 = -\nabla 0 A(x_f, x_0) \quad (3.4.6) \]

The semiclassical approximation to the unrestricted propagator \( \langle x_f | \delta(H - E) | x_0 \rangle \) is
given by a sum of terms each of the form

\[ G(x_f, x_0) = P(x_f, x_0) e^{iA(x_f, x_0)} \quad (3.4.7) \]

The quantity \( P \) is a prefactor, whose specific form is lengthy to calculate, but will not
in fact be required. (For the case of the time-dependent propagator, the prefactor would
be given in terms of the determinant of the matrix of second derivatives of \( A(x_f, x_0) \).
Here, because of the constraint equation (3.4.5), this matrix is in fact singular and the
expression for the prefactor is more complicated \([8, 9, 74, 104]\)).

The semiclassical form (3.4.7) satisfies the constraint equation \( \langle i.e., is annihilated by \( (H - E) \)) in the WKB approximation, as it should. If the classical trajectory from \( x_0 \)
to \( x_f \) is unique there will be just one term in the semiclassical approximation. If there
is more than one, there will be a sum of similar terms, one for each trajectory. For the moment we will assume that there is just one. We will also assume that the extremizing classical solution is real, and thus the action \( A(x_f, x_0) \) is real. We do not want to consider any Euclidean solutions.

With the restriction that the paths must pass through \( \Delta \), we expect that the class operator will be given again by (3.4.7) when the classical path passes through \( \Delta \), and will be zero when the classical path does not pass through \( \Delta \). It is then not difficult to see that the modified class operator for this case may therefore be written,

\[
C'_{\Delta}(x_f, x_0) = \theta \left( \int_{-\infty}^{\infty} dt \ f_{\Delta}(x_0'(t)) - \epsilon \right) P(x_f, x_0) e^{iA(x_f, x_0)} \tag{3.4.8}
\]

The \( \theta \)-function here is the same as in the (rewritten) classical case Eq.(3.2.13) in terms of “initial” and “final” points, where \( x_0'(t) \) denotes that classical path from \( x_0 \) to \( x_f \). (This is exactly as in the classical case depicted in Fig. 12). Note also that

\[
\nabla A \cdot \nabla \theta \left( \int_{-\infty}^{\infty} dt \ f_{\Delta}(x_0'(t)) - \epsilon \right) = 0 \tag{3.4.9}
\]

as may be shown by shifting the \( t \) integration. It follows that the modified class operator \( C'_{\Delta} \) is a WKB solution to the constraint equation, as required. We have therefore succeeded in computing, in the semiclassical approximation, a modified class operator satisfying the constraint equation everywhere, corresponding to the restriction to paths passing through the region \( \Delta \). This is a very simple result but turns out to be crucial to the rest of the derivation.

It is important that \( t \) is integrated over an infinite range in the quantity inside the \( \theta \)-function, otherwise the modified class operator would not in fact satisfy the constraint. Recall that the originally defined class operator Eq.(3.3.5) contained a similar \( \theta \)-function, with a finite range of time integration, which one might have been tempted to use in the semiclassical approximation, but this class operator does not in fact satisfy the constraint.

Hence we see that the difference between the modified and original class operators in the semiclassical approximation is the difference between using the entire classical trajectory or using finite segments of it in the \( \theta \)-functions. We also see that these modified class operators are the correct ones to use in order to be consistent with the discussion of the classical case and Eq.(3.2.13). There, we saw that it is appropriate to sum over classical
paths intersecting $\Delta$ even if $\Delta$ does not lie on the segment of classical trajectory between $x_0$ and $x_f$. This feature therefore appears to be necessary for the particular type of reparametrization invariance used here. Only the entire trajectory is reparametrization-invariant notion. A finite section of trajectory is not.

The off-diagonal terms of the decoherence functional are now given in the semiclassical approximation by

$$D(\Delta, \Delta) = \int d^n x f d^n x_0 d^n y_0 \theta \left( \int_{-\infty}^{\infty} dt f_{\Delta}(x_0^I(t)) - \epsilon \right)$$

$$\times \left( 1 - \theta \left( \int_{-\infty}^{\infty} dt f_{\Delta}(y_0^I(t)) - \epsilon \right) \right) \times P(x_f, x_0) P^*(x_f, y_0) \exp \{ iA(x_f, x_0) - iA(x_f, y_0) \} \rho(x_0, y_0) \tag{3.4.10}$$

It is now essentially a sum over pairs of classical paths, and the $\theta$-functions restrict the paths to either pass or not pass through the region $\Delta$. We see also from the invariance property of the $\theta$-functions, (3.4.9), that they are invariant under shifting the regions $\Delta_\alpha$ along their classical trajectories. This is the expression of the idea that the decoherence functional, in the semiclassical approximation, knows only about entire trajectories.

It is now convenient to introduce the variables

$$X_0 = \frac{1}{2}(x_0 + y_0), \quad v = x_0 - y_0 \tag{3.4.11}$$

and thus

$$x_0 = X_0 + \frac{1}{2}v, \quad y_0 = X_0 - \frac{1}{2}v \tag{3.4.12}$$

and we also rewrite the density operator in terms of the Wigner function $W(p_0, q_0)$ (Eq.(3.2.25)). We will discuss the detailed mechanism of decoherence in the next Section. For the moment, we will simply assume decoherence, which essentially means assuming that $v$ is concentrated around zero, and work out the form of the probabilities. Although we note that this assumption can be justified for initial states $\rho(x_0, y_0)$ which are approximately diagonal in position. We now set $v = 0$ in the prefactors $P$ and in the $\theta$-functions, and we obtain the probability

$$p_\Delta = \int d^n x f d^n x_0 d^n v d^n p_0 \theta \left( \int_{-\infty}^{\infty} dt f_{\Delta}(X_0^I(t)) - \epsilon \right) |P(x_f, X_0)|^2$$

$$\times \exp \left( iA(x_f, X_0 + \frac{1}{2}v) - iA(x_f, X_0 - \frac{1}{2}v) + i\mathbf{p}_0 \cdot \mathbf{v} \right) W(p_0, X_0) \tag{3.4.13}$$
Expanding the action terms to linear order in $v$ (decoherence again allows us to drop the higher order terms), the $v$ integral may be performed and we obtain

$$p_{\Delta} = \int d^n x_f d^n X_0 d^n p_0 \, \theta \left( \int_{-\infty}^{\infty} dt \, f_{\Delta}(X'_0(t)) - \epsilon \right)$$

$$\times |P(x_f, X_0)|^2 \delta^{(n)}(p_0 + \nabla_0 A(x_f, X_0)) \, W(p_0, X_0)$$

(3.4.14)

where $\nabla_0$ operates on the initial point $X_0$. Finally, the integration over $x_f$ may be performed. The delta-function constraint then means that the quantity $X'_0(t)$ (the classical path from $X_0$ to $x_f$) is replaced by $X^{cl}(t)$ (the classical path with initial data $X_0, p_0$).

Although we have not worked out the explicit form of the prefactor $P$, we deduce that it must in fact drop out when the $x_f$ integration is carried out, because the probability must equal 1 when the $\theta$-function is removed. (From this we deduce that $|P(x_f, X_0)|^2$ must be the Jacobian factor in the change of integration variables from $x_f$ to $\nabla_0 A(x_f, X_0)$). We therefore obtain the final result,

$$p_{\Delta} = \int d^n X_0 d^n p_0 \, \theta \left( \int_{-\infty}^{\infty} dt \, f_{\Delta}(X^{cl}(t)) - \epsilon \right) \, W(p_0, X_0)$$

(3.4.15)

As expected, this is the classical result Eq.(3.2.10) with the classical phase space distribution function replaced by the Wigner function.

### 3.5 Systems of Harmonic Oscillators

There is one simple system for which the discussion of decoherence and probabilities is particularly simple, and this is the case of a collection of harmonic oscillators. It also enjoys the property that its spectrum is discrete, hence the induced inner product scheme is not required for normalization.

In non-relativistic quantum mechanics, in the search for emergent quasi-classical histories, it is of interest to consider histories characterized by strings of phase space quasi-projectors $P_\Gamma$. These are positive hermitian operators concentrated on a region $\Gamma$ of phase space, but are not quite projectors since they only have $P^2_\Gamma \approx P_\Gamma$. Omnès [89–95] has proved an important theorem about these projectors, which is essentially that they are approximately preserved in form under unitary evolution and moreover approximately
follow classical evolution. That is,
\[ e^{-iHt} P_{\Gamma} e^{iHt} \approx P_{\Gamma_t} \tag{3.5.1} \]
where \( \Gamma_t \) is the classical evolution of the phase space cell \( \Gamma \). The approximation holds when the phase space cells are significantly larger than a quantum sized cell, and for times not so long that wave packet spreading becomes significant. In the special case of the harmonic oscillator, the approximation holds for all time. This result allows one to show that firstly, histories of phase space projectors are approximately decoherent for a wide variety of initial states, and secondly, that their probabilities are peaked about classical evolution. Differently put, on sufficiently coarse grained scales, quantum systems have an approximate determinism that ensures decoherence and approximate correspondence with classical physics.

It seems reasonable to suppose that the timeless models considered here might have analogous properties. We will demonstrate this for a system of harmonic oscillators in an energy eigenstate. The Hamiltonian for a set of \( N \) identical harmonic oscillators is
\[ H_0 = \frac{1}{2} \left( p^2 + x^2 \right) - \frac{1}{2} N \tag{3.5.2} \]
(the factor of \( \frac{1}{2} N \) is included to subtract the vacuum state energy and avoid certain phase factors). The standard coherent states (see Ref. [21], for example) are denoted \( |p, x\rangle \) and they have the important property that they are preserved in form under unitary evolution,
\[ e^{-iH_0 t} |p, x\rangle = |p_t, x_t\rangle \tag{3.5.3} \]
where \( p_t, x_t \) are the classical solutions matching \( p, x \) at \( t = 0 \), hence they are strongly peaked about the classical path. In Ref. [40], a set of states were introduced which are timeless analogues of the usual coherent states. They are
\[ |\phi_{p, x}\rangle = \delta(H_0 - E)|p, x\rangle \]
\[ = \int_0^{2\pi} dt \frac{1}{2\pi} e^{-i(H_0 - E)t} |p, x\rangle \tag{3.5.4} \]
\[ = \int_0^{2\pi} dt \frac{1}{2\pi} e^{iEt} |p_t, x_t\rangle \]
These states were referred to in Ref. [40] as “timeless coherent states”. (See also [71–73, 99]). They are exact eigenstates of the Hamiltonian,
\[ H_0 |\phi_{p, x}\rangle = E |\phi_{p, x}\rangle \tag{3.5.5} \]
Furthermore, since the coherent states $|p_t, x_t\rangle$ are concentrated at a phase space point for each $t$, integrating $t$ over a whole period produces a state which is concentrated along the entire classical trajectory. They are therefore the natural analogues of the usual coherent states. Their properties are similar in many ways to the usual coherent states and are described in more detail in Ref.[40].

Each state is labelled by a fiducial phase space point $p, x$ which determines the classical trajectory the state is peaked about. Under evolution of the fiducial point $p, x$ to another point, $p_s, x_s$, say, along the same classical trajectory, the state changes by a phase,

$$|\phi_{px}\rangle \rightarrow |\phi_{p_sx_s}\rangle = e^{iE_s} |\phi_{px}\rangle$$ (3.5.6)

Two timeless coherent states of different energy are exactly orthogonal. If they have the same energy then they are approximately orthogonal if they correspond to sufficiently distinct classical solutions. They also obey a completeness relation,

$$\int dN_p dN_x (2\pi)^N |\phi_{px}\rangle \langle \phi_{px}| = \delta(H_0 - E)$$ (3.5.7)

[Note that the notation $\delta(H_0 - E)$ is a rather loose one. This object is really the projection operator onto the subspace of energy $E$, for which it is exactly true that $[\delta(H_0 - E)]^2 = \delta(H_0 - E)]$. Since $\delta(H_0 - E)|\psi\rangle = |\psi\rangle$ on any solution to the eigenvalue equation $(H_0 - E)|\psi\rangle = 0$, this is essentially a completeness relation on the set of solutions to the eigenvalue equation. We may therefore write any solution $|\psi\rangle$ as a superposition of timeless coherent states,

$$|\psi\rangle = \int dN_p dN_x (2\pi)^N |\phi_{px}\rangle \langle \phi_{px}|\psi\rangle$$ (3.5.8)

Given these preliminaries, we may now discuss the decoherence functional. We will consider coarse grainings in which the paths in configuration space either pass or do not pass through a series of regions denoted $\Delta = \Delta_1, \Delta_2 \cdots$. We will take $\Delta_1, \Delta_2 \cdots$ to lie along a classical path. Hence we need at least two such regions to fix a configuration space path.

The decoherence functional, in terms of the modified class operators, is, in the semi-classical approximation,

$$D(\Delta, \Delta) = \int d^np_{xf} d^np_{x0} d^ny_0 C_\Delta(\mathbf{x}_f, \mathbf{x}_0) C^{*\Delta}(\mathbf{x}_f, \mathbf{y}_0) \Psi^{*} (\mathbf{x}_0) \Psi (\mathbf{y}_0)$$ (3.5.9)
The modified class operator \( C'_\Delta(x_f, x_0) \) is given by Eq. (3.4.8), so is equal to the unrestricted semiclassical propagator \( G \) when \( x_f \) or \( x_0 \) lie on the classical path specified by \( \Delta \) and is zero otherwise. Also, \( C'_\Delta = \delta(H_0 - E) - C'_\Delta \).

We first consider the case in which the initial state is a timeless coherent state, \( |\phi_{px}\rangle \). It is then straightforward to see that

\[
C'_\Delta |\phi_{px}\rangle \approx |\phi_{px}\rangle
\]

when the trajectory labelled by the fiducial points \( p, x \) passes through the regions \( \Delta \), and

\[
C'_\Delta |\phi_{px}\rangle \approx 0
\]

otherwise. Also, since

\[
\delta(H_0 - E)|\phi_{px}\rangle = |\phi_{px}\rangle
\]

it follows that

\[
C'_\Delta |\phi_{px}\rangle \approx 0
\]

when the trajectory labelled by \( p, x \) passes through \( \Delta \). From these results it is easy to see that the decoherence functional is approximately diagonal. Furthermore, the probability for entering the regions \( \Delta \) is then approximately 1 or 0, depending on whether the classical trajectory of the timeless coherent state passes through \( \Delta \).

Now consider the case of a more general initial state. We expand it in timeless coherent states, as in Eq. (3.5.8). Using the above results, we therefore find

\[
C'_\Delta |\psi\rangle \approx \int_D \frac{d^N p \ d^N x}{(2\pi)^N} |\phi_{px}\rangle \langle \phi_{px}|\psi\rangle
\]

Here, \( D \) denotes the set of phase space points \( p, x \) whose classical trajectories pass through the regions \( \Delta \) in configuration space. Similarly,

\[
C'_\Delta |\psi\rangle \approx \int_{\bar{D}} \frac{d^N p \ d^N x}{(2\pi)^N} |\phi_{px}\rangle \langle \phi_{px}|\psi\rangle
\]

where \( \bar{D} \) denotes the set of phase space points whose classical trajectories do not pass through all regions \( \Delta \). Clearly we again have approximate decoherence, because of the approximate determinism. We may therefore assign a probability for passing through \( \Delta \),

\[
p_{\Delta} \approx \int_D \frac{d^N p \ d^N x}{(2\pi)^N} |\langle \phi_{px}|\psi\rangle|^2
\]
It is the integral over the phase space region $D$ of the phase space distribution function $|\langle \phi_{px} \mid \psi \rangle|^2$. Because $|\psi\rangle$ is an eigenstate of the Hamiltonian, it is easy to see using the definition (3.5.4) of the timeless coherent states that

$$\langle \phi_{px} \mid \psi \rangle = \langle px \mid \psi \rangle \quad (3.5.17)$$

and so the probability now is

$$p_\Delta \approx \int_D \frac{d^Np \, d^Nx}{(2\pi)^N} |\langle px \mid \psi \rangle|^2 \quad (3.5.18)$$

It is then a standard result that the integrand is in fact a smeared Wigner function

$$|\langle px \mid \psi \rangle|^2 = \int d^Np' d^Nx' \, e^{-\frac{1}{2}[(p-p')^2-(x-x')^2]} W(p',x') \quad (3.5.19)$$

This object is positive even if the original Wigner function $W$ of $|\psi\rangle$ is not [21]. Hence we obtain a result which is essentially identical to the classically anticipated result (3.2.10), with a smeared Wigner function as the phase space distribution function.

It is also of interest to note that the result for the probability may be written in the form

$$p_\Delta = \langle \psi \mid P_D \mid \psi \rangle \quad (3.5.20)$$

where $P_D$ is the approximate projection operator

$$P_D = \int_D \frac{d^Np \, d^Nx}{(2\pi)^N} |\phi_{px}\rangle \langle \phi_{px}| \quad (3.5.21)$$

Moreover, since the timeless coherent states $|\phi_{px}\rangle$ are exact eigenstates of $H_0$, we have that

$$[P_D, H_0] = 0 \quad (3.5.22)$$

Hence, we see that the result may be written in the standard quantum-mechanical form for a probability, in terms of an operator which commutes with the constraint.

The result here, of approximate decoherence and simple expressions for the probabilities, like the corresponding non-relativistic result is due to the approximate determinism contained in the quantum theory. It works only when we ask for the probabilities for approximately classical histories. To obtain probabilities for more complicated histories, and for systems which are not harmonic oscillators (where there is wave packet spreading), we need an environment to produce decoherence.
3.6 Decoherence Through an Environment

As stated above, the decoherence functional is typically not diagonal for most initial states, and a physical mechanism is required to produce decoherence. In this section we therefore consider the addition of an environment to produce decoherence of histories. The results of this Section therefore simply justify the assumed decoherence of Section 3.4, and little affect the final result of the probabilities, but it is important to see in detail how this works.

3.6.1 Semiclassical Approximation to the Decoherence Functional with Environment

For what we will do here, the specific form of the environment turns out not to be very important. But for definiteness, we take the environment to be a large collection of harmonic oscillators with coordinates denoted \( q_A \), where \( A \) runs over a large number of values, with a linear coupling to the system. For notational simplicity we will assume that for each system coordinate \( x \) in the \( n \)-dimensional configuration space there is a set of \( n \) oscillators with coordinate \( q \) for the environment. The case of of more oscillators is easily obtained from this. The total action of the system is

\[
S = S_0[x] + S_\varepsilon[x, q] \tag{3.6.1}
\]

and the corresponding Hamiltonian is

\[
H = H_0(x) + H_\varepsilon(x, q) \tag{3.6.2}
\]

We shall assume that the state of the whole system has the form

\[
\Psi(x, q) = \psi(x)\chi(x, q) \tag{3.6.3}
\]

This may be inserted into the Wheeler-DeWitt type equation \((H - E)\Psi = 0\) to obtain a perturbative solution about the solution with no environment. We will concentrate on the case in which the wave function is of oscillatory form, so the background solution is of WKB form

\[
\psi(x) = C(x)e^{iS(x)} \tag{3.6.4}
\]
where $S$ obeys the Hamilton-Jacobi equation

$$\frac{1}{2} (\nabla S)^2 + V(x) = E \quad (3.6.5)$$

and $C$ obeys the equation

$$\nabla^2 C + 2\nabla S \cdot \nabla C = 0 \quad (3.6.6)$$

The environment wave functions obey the Schrödinger equation

$$i \nabla S \cdot \nabla \chi = H_E \chi \quad (3.6.7)$$

We will consider the case of a superposition of WKB states in Section 3.7.

The decoherence functional now is

$$D(\alpha, \alpha') = \int_0^\infty d\tau \int_0^\infty d\tau' e^{-iE\tau} e^{iE'\tau'}$$

$$\times \int_\alpha^\text{D}x(t) \int_{\alpha'}^\text{D}y(t) \exp \left( iS_0^x[x(t)] - iS_0^y[y(t)] \right)$$

$$\times F[x(t), y(t), \tau, \tau'] \psi_{E_0}(x_0) \psi_{E_0}^*(y_0) \quad (3.6.8)$$

(suspending for the moment the necessity to use modified class operators). Here $S_0^x$ denotes the action over the fixed time range $[0, \tau]$ (and note that the time ranges are different on either side of the decoherence functional). The influence functional $F[x(t), y(t), \tau, \tau']$ is given by,

$$F[x(t), y(t), \tau, \tau'] = \int \text{D}q(t) \text{D}r(t) \exp \left( iS_0^x[x(t), q(t)] - iS_0^y[y(t), r(t)] \right)$$

$$\times \chi(x_0, q_0) \chi^*(y_0, r_0) \quad (3.6.9)$$

It is different in form in two ways to the usual influence functional. Firstly, the time ranges on either side are not the same, and secondly, the initial state $\chi$ depends on the system variables $x$, with a different dependence on either side of the influence functional. The functional integral is over all pairs of paths $q(t), r(t)$ which meet at the final point

$$q(\tau) = r(\tau') \quad (3.6.10)$$

and this point is summed over. The paths also match the initial values $q_0, r_0$, which are then folded into the initial state.

It is useful to go now to the semiclassical approximation for the system variables. We also now recall that we must use modified class operators for the system variables (this
does not affect the environment dynamics, at this level of approximation). The off-diagonal terms of the decoherence functional are now given by

\[
D(\Delta, \Delta^*) = \int d^n x d^n y_0 \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(x_0^f(t)) - \epsilon \right) \times \left( 1 - \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(y_0^f(t)) - \epsilon \right) \right) \\
\times P(x_f, x_0, y_0) P^*(x_f, y_0) \exp \left( iA(x_f, x_0) - iA(x_f, y_0) \right) \\
\times F(x_f, x_0, y_0) \psi(x_0) \psi^*(y_0)
\]

(3.6.11)

Here, \( F(x_f, x_0, y_0) \) is the influence functional with the semiclassical approximation for the system variables inserted. That is, for \( x(t) \) we insert the classical trajectory from \( x_0 \) to \( x_f \) in time \( \tau \), and the value of \( \tau \) is then determined (in terms of \( x_0 \) and \( x_f \)) by the constraint equation, and similarly for \( y(t) \). The decoherence functional is again essentially a sum over pairs of classical paths for the system variables, the path from \( x_0 \) to \( x_f \), and the path from \( y_0 \) to \( x_f \).

### 3.6.2 Calculation of the Influence Functional

We may now calculate the influence functional with the semiclassical approximation for system variables inserted. The influence functional may be written,

\[
F(x_f, x_0, y_0) = \int d^n q_f \phi(q_f, x_f, x_0) \phi^*(q_f, x_f, y_0)
\]

(3.6.12)

where

\[
\phi(q_f, x_f, x_0) = \int d^n q_0 g(q_f, x_f|q_0, x_0) \chi(q_0, x_0)
\]

(3.6.13)

Here, we have introduced the propagator for the environment variables along the system classical trajectory from \( x_0 \) to \( x_f \),

\[
g(q_f, x_f|q_0, x_0) = \int Dq(t) \exp \left( iS^E_x[x(t), q(t)] \right)
\]

(3.6.14)

The environment state \( \chi \) may be normalized according to

\[
\int d^n q \left| \chi(q, x) \right|^2 = 1
\]

(3.6.15)

for all \( x \). Since \( g \) propagates \( \chi \) unitarily along a fixed system trajectory, it follows that

\[
\int d^n q_f \left| \phi(q_f, x_f, x_0) \right|^2 = 1
\]

(3.6.16)
This means that the influence functional satisfies

$$|F(x_f, x_0, y_0)|^2 \leq 1$$  \hspace{1cm} (3.6.17)$$

with equality when \(x_0 = y_0\), indicating that the influence functional is peaked about \(x_0 = y_0\), which is the decoherence effect we need.

The influence functional is difficult to evaluate in general. It can be evaluated exactly when both \(g\) and \(\chi\) are Gaussian. It is also effectively Gaussian in form if we have a large number of oscillators in the environment, for then the many-oscillator influence functional is essentially the original one, (3.6.9), raised to a high power. This strongly enhances the peaking about \(x_0 = y_0\). A simple and reasonably general form for the influence functional may therefore be obtained by expanding about \(x_0 = y_0\), and assuming either a Gaussian form, or a large number of oscillators (or both).

We again use the coordinates \(X_0, v\) defined in Eq.(3.4.11). We have

$$\phi(q_f, x_f, x_0) = \phi(q_f, x_f, X_0) + \frac{1}{2} v^a \partial_a \phi(q_f, x_f, X_0) + \frac{1}{8} v^a v^b \partial_a \partial_b \phi(q_f, x_f, X_0) + \cdots$$  \hspace{1cm} (3.6.18)$$

where \(\partial_a = \partial/\partial X_0^a\). Inserting in the influence functional, and also introducing the notation \(\phi_0 = \phi(q_f, x_f, X_0)\), we get

$$F = 1 + \frac{i}{2} v^a \int d^n q_f \phi_0^* \partial_a \phi_0 - \phi_0 \partial_a \phi_0^*$$
$$+ \frac{1}{8} v^a v^b \int d^n q_f (\phi_0^* \partial_a \partial_b \phi_0 + \phi_0 \partial_a \partial_b \phi_0^* - 2 \partial_a \phi_0 \partial_b \phi_0^*)$$
$$+ \cdots$$  \hspace{1cm} (3.6.19)$$

By differentiating the normalization of \(\phi\), (3.6.16), we see that

$$\int d^n q_f \phi_0 \partial_a \phi_0^* = - \int d^n q_f \partial_a \phi_0 \phi_0^*$$  \hspace{1cm} (3.6.20)$$

and

$$\int d^n q_f (\phi_0 \partial_a \partial_b \phi_0^* + \phi_0^* \partial_a \partial_b \phi_0) = - \int d^n q_f (\partial_a \phi_0 \partial_b \phi_0^* + \partial_b \phi_0 \partial_a \phi_0^*)$$  \hspace{1cm} (3.6.21)$$

Using these relations, we may now write the influence functional as

$$F = 1 + iv^a \Gamma_a - \frac{1}{2} v^a v^b \Sigma_{ab} + \cdots$$
$$\approx \exp \left( iv^a \Gamma_a - \frac{1}{2} v^a v^b (\Sigma_{ab} - \Gamma_a \Gamma_b) \right) + \cdots$$  \hspace{1cm} (3.6.22)$$
The coefficients $\Gamma_a$ and $\Sigma_{ab}$ are given by

$$\Gamma_a(x_f, X_0) = \frac{i}{2} \int d^n q_f \left( \phi_0 \partial_a \phi_0^* - \phi_0^* \partial_a \phi_0 \right)$$

$$\Sigma_{ab}(x_f, X_0) = \int d^n q_f \partial_a \phi_0 \partial_b \phi_0^*$$  \hspace{1cm} (3.6.23)

The approximation of writing $F$ as a Gaussian becomes exact when $g$ and $\chi$ are Gaussian, and is also true approximately when there are a large number of oscillators in the environment. We have therefore obtained the influence functional, as required.

### 3.6.3 Reparametrization Invariance in the Influence Functional

The form of the influence functional indicates, as expected, that there is a suppression of interference for paths with $x_0 \neq y_0$. This is the usual decoherence effect. However, the situation in the reparametrization-invariant theory considered here is not so simple. We expect that the decoherence functional depends, in some sense, only on reparametrization-invariant quantities, and in the semiclassical approximation used here, this means it depends on entire classical paths (rather than individual points). Differently put, we do not expect (or need) the destruction of interference for points $x_0, y_0$ lying on the same classical path (connecting each to $x_f$), since these points are effectively equivalent. What we expect is that the influence functional will not be exponentially small when $x_f, x_0, y_0$ lie along a single classical path. We must therefore see how reparametrization invariance is expressed in the influence functional.

We first note that

$$\phi_0 = \int d^n q_0 \ g(q_f, x_f | q_0, X_0) \ \chi(q_0, X_0)$$  \hspace{1cm} (3.6.24)

and let us see how this quantity varies with $X_0$. If this were the usual non-relativistic quantum mechanics, with propagation from initial time $t_0$ to final time $t_f$, then $\phi_0$ would in fact be independent of $t_0$. We expect a similar property here, that is, that $\phi_0$ is constant (as a function of $X_0$) along a certain vector field. The initial state $\chi(q_0, X_0)$ obeys the Schrödinger equation

$$i \nabla_0 S(X_0) \cdot \nabla_0 \chi = H_x(q_0, x_f, X_0) \chi$$  \hspace{1cm} (3.6.25)
The propagator \( g \) on the other hand, obeys Schrödinger equations with respect to both the final and initial points,

\[
i\nabla_f A(x_f, X_0) \cdot \nabla_f g = H_x(q_f, x_f, X_0)g \tag{3.6.26}
\]

\[
i\nabla_0 A(x_f, X_0) \cdot \nabla_0 g = H_x(q_0, x_f, X_0)g \tag{3.6.27}
\]

(Note that the expected minus sign in the Schrödinger equation with respect to the initial point is already contained through the fact that \( \nabla_0 A \) is minus the initial momentum, as in Eq.(3.4.6)). Now the point is here that \( g \) and \( \chi \) obey different Schrödinger equations, so at this stage, \( \phi_0 \) does not obviously have any constant directions in \( X_0 \) – neither \( \nabla_0 S \cdot \nabla_0 \phi_0 \) nor \( \nabla_0 A \cdot \nabla_0 \phi_0 \) are zero.

However, as we saw in the Section 3.4 (without environment), the path integral enforces the condition \( p = -\nabla_0 A \). We anticipate that this condition is approximately enforced with the environment in place. Furthermore, the initial Wigner function for a WKB state is of the approximate form,

\[
W(p, X_0) = |C(X_0)|^2 \delta(p - \nabla_0 S(X_0)) \tag{3.6.28}
\]

It follows that the sum over paths is dominated by configurations for which

\[
\nabla_0 A(x_f, X_0) \approx -\nabla_0 S \tag{3.6.29}
\]

This means that the trajectories of \( S \) are the same as the classical trajectories from \( X_0 \) to \( x_f \). From this it is then easy to show that

\[
\nabla_0 S(X_0) \cdot \nabla \phi_0 \approx 0 \tag{3.6.30}
\]

(essentially for the same reason that the analogous non-relativistic version is independent of the initial time \( t_0 \)). In the influence functional, two neighbouring points \( x_0, y_0 \) on the same classical trajectory have \( \mathbf{v} = x_0 - y_0 \) proportional to \( \nabla_0 S \). It follows that

\[
v^a \Gamma_a = 0, \quad v^a \Sigma_{ab} = 0 \tag{3.6.31}
\]

which means that the influence functional does not suppress interference between points on the same trajectories, only between points on different trajectories. That is, when the condition \( p = -\nabla_0 A \) is true, we get the expected result that the influence functional is a function only of entire trajectories, and not of the individual points along those trajectories.
3.6.4 Decoherence and the Evaluation of the $v$ Integral

The off-diagonal terms of the decoherence functional may now be written

$$D(\Delta, \Delta) = \int d^n x_f d^n X_0 d^n v d^n p \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(x_f(t)) - \epsilon \right) \times \left( 1 - \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(y_0(t)) - \epsilon \right) \right) \times P(x_f, X_0 + \frac{1}{2}v)P^*(x_f, X_0 - \frac{1}{2}v)$$

$$\times \exp \left( i \left( \nabla_0 A(x_f, X_0) + p \right) \cdot v + O(v^3) \right) W(p, X_0) \times \exp \left( iv^a \Gamma_a - \frac{1}{2} v^a v^b \sigma_{ab} \right)$$

(3.6.32)

where

$$\sigma_{ab} = \Sigma_{ab} - \Gamma_a \Gamma_b$$

(3.6.33)

and we have again introduced the Wigner function $W(p, X_0)$ and the variables $X_0$, $v$ in the exponential part. The decoherence functional is a sum over pairs of classical paths, one set of paths intersecting $x_0, x_f$ and passing through $\Delta$ at any stage along the path, the other set of paths intersecting $y_0, x_f$ and never passing through $\Delta$ at any stage along the path (see Fig. 12). It is easily seen that for this particular coarse graining, in which we are interested in paths that either pass or do not pass through the region $\Delta$, we do not in fact encounter the situation discussed in Section 3.6.3, in which $x_0, y_0, x_f$ lie along the same classical trajectory. That is, the coarse graining is such that $v$ is never proportional to $\nabla_0 A$, and the potentially singular situation (3.6.31) does not arise. The influence functional therefore does its job of suppressing the contribution from non-zero values of $v$ to a decoherence width determined by the inverse of the non-zero eigenvalues of $\sigma_{ab}$. If the size of the coarse graining region $\Delta$ is greater than this width then the off-diagonal terms of the decoherence functional are approximately zero.

We therefore have approximate decoherence and we may examine the probability for
passing through $\Delta$, which is

$$p(\Delta) = \int d^n x_f d^n X_0 d^n v d^n p \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(X_0^f(t)) - \epsilon \right) \times P(x_f, X_0 + \frac{1}{2} v) P^*(x_f, X_0 - \frac{1}{2} v) \times \exp \left( i (\nabla_0 A(x_f, X_0) + p) \cdot v + O(v^3) \right) W(p, X_0) \times \exp \left( iv^a \Gamma_a - \frac{1}{2} v^a v^b \sigma_{ab} \right)$$ (3.6.34)

where $v$ has been set to zero in the $\theta$-function. We are now summing over pairs of classical paths which both pass through the region $\Delta$, so now we do have the possibility of $x_0, y_0, x_f$ lying along the same path, and hence the matrix $\sigma_{ab}$ is potentially singular, by (3.6.31). This means that some care is necessary in the $v$ integral.

If we formally carry out the integral over $v$, we get,

$$p_\Delta = \int d^n x_f d^n X_0 d^n v d^n p \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(X_0^f(t)) - \epsilon \right) \times |P(x_f, X_0)|^2 W(p, X_0) \times \exp \left( -\frac{1}{2} (\nabla_0 A(x_f, X_0) + p + \Gamma)^a \sigma^{-1}_{ab} (\nabla_0 A(x_f, X_0) + p + \Gamma)^b \right)$$ (3.6.35)

Changing integration variables from $x_f$ to $p_0 = -\nabla_0 A(x_f, X_0)$ This is conveniently written

$$p_\Delta = \int d^n p_0 d^n X_0 \theta \left( \int_{-\infty}^{\infty} dt f_\Delta(X_0^d(t)) - \epsilon \right) \tilde{W}(p_0, X_0)$$ (3.6.36)

where we have defined the smeared Wigner function

$$\tilde{W}(p_0, X_0) = \int d^n p \exp \left( -\frac{1}{2} (p_0 - p - \Gamma)^a \sigma^{-1}_{ab} (p_0 - p - \Gamma)^b \right) W(p, X_0)$$ (3.6.37)

Again the prefactors $P$ drop out in the change of integration variables, as in Section 3.4. This smearing of the Wigner function represents environmentally induced fluctuations about the classical evolution, and the small additional term $\Gamma$ in the exponent represents the back reaction of the environment on the classical equations of motion.

As stated, the results (3.6.31) suggest that the matrix $\sigma_{ab}$ is singular, but it is easy to see the significance of this. When the matrix is non-singular, the $v$ integral produces a Gaussian peak about $p_0 = p + \Gamma$, which represents fluctuations about classical evolution. If the matrix is singular in a certain direction, it is easy to see from (3.6.34) that the $v$
integral in this direction will produce a $\delta$-function, instead of a Gaussian. It will still be peaked about the same configuration, but there are no fluctuations in that direction.

The result for the probabilities therefore approximately coincides with the classical result Eq.(3.2.10). We have concentrated on the case in which $\Delta$ is a single region of configuration space, but the result straightforwardly generalizes to the case in which $\Delta$ consists of a series of regions $\Delta_1, \Delta_2, \cdots$. The above result then shows that the probability is peaked when the series of regions lies along a classical path (plus the environmental effects of a small back reaction and small fluctuations).

### 3.7 Superposition States

The calculations of Sections 3.4 and 3.6 concerned only single WKB states of the form (3.6.4). It is therefore important to reconsider the decoherence calculation of Section 3.6 for the more general case of a superposition of semiclassical WKB states,

$$\Psi = \Psi_1 + \Psi_2 = C_1 e^{iS_1} \chi_1 + C_2 e^{iS_2} \chi_2$$  \hfill (3.7.1)

This turns out in fact to be quite straightforward, mainly because similar calculations (involving the reduced density matrix, not the decoherence functional) have already been done.

Inserting Eq.(3.7.1) in the decoherence functional, we obtain, a result of the form

$$D = D_{11} + D_{12} + D_{21} + D_{22}$$  \hfill (3.7.2)

where, in an obvious notation, $D_{11}$ is the decoherence functional with initial density matrix $|\Psi_1\rangle\langle\Psi_1|$, $D_{12}$ is the decoherence functional with the operator $|\Psi_1\rangle\langle\Psi_2|$ in the initial state slot, and so on. Clearly the analysis of $D_{11}$ and $D_{22}$ is identical to the case considered already – we get decoherence, and probabilities given in terms of the Wigner functions of $\Psi_1$ and $\Psi_2$. Hence these two terms correspond to a statistical mixture of the two initial states.

The interesting terms are $D_{12}$ and $D_{21}$ (= $D^{*}_{12}$), which correspond to interferences
between different WKB branches. From Section 3.6, we see that
\[
D_{12}(\alpha, \alpha') = \int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} d\tau' e^{-iE\tau} e^{iE'\tau'}
\times \int_{\alpha} D(x(t)) \int_{\alpha'} D(y(t)) \exp \left( iS_0^r[x(t)] - iS_0^{r'}[y(t)] \right) \times F_{12}[x(t), y(t), \tau, \tau'] C_1(x_0) e^{iS_1(x_0)} C_2^*(y_0) e^{-iS_2(y_0)}
\]
(3.7.3)
where
\[
F_{12}[x(t), y(t), \tau, \tau'] = \int Dq(t) Dr(t) \exp \left( iS^r_0[x(t), q(t)] - iS^r_0[y(t), r(t)] \right) \times \chi_1(x_0, q_0) \chi_2^*(y_0, r_0)
\]
(3.7.4)
(As in Section 3.6.1 we should then replace the class operators with their modified version and go to the semiclassical limit). Now it is easy to see that the influence functional is the overlap of the two initial states, but with each unitarily evolved along two different trajectories. That is, in the semiclassical approximation for the system,
\[
F_{12} = \langle \chi_2(y_0) | U^\dagger(x_f, y_0) U(x_f, x_0) | \chi_1(x_0) \rangle
\]
(3.7.5)
where \(U(x_f, x_0)\) denotes the unitary evolution of the environment states along the classical trajectory of the system from \(x_0\) to \(x_f\).

Clearly \(|F_{12}|^2 \leq 1\), and because \(F_{12}\) is an overlap between a pair of states it will typically be such that \(F_{12}\) is strictly less than 1. In this case, when raised to a high power, as happens when we take a large number of oscillators in the environment, we will get a very strong suppression of terms with \(x_0 \neq y_0\). In particular, even when \(x_0 = y_0\), we get
\[
F_{12} = \langle \chi_2(x_0) | \chi_1(x_0) \rangle
\]
which will be less than 1, quite simply because \(\chi_1\) and \(\chi_2\) are different states. We therefore find that \(D_{12}\) and \(D_{21}\) are much smaller than the diagonal terms \(D_{11}, D_{22}\). This destruction of interference between WKB states therefore comes about for essentially the same reason that the corresponding off-diagonal terms of the density matrix are very small, as discussed previously [35, 65, 68, 96].

It should be noted, that in Eq.(3.7.5), it could in fact happen that \(F_{12} = 1\), as a result of a careful choice of \(\chi_1 \neq \chi_2\) together with a suitable choice of \(x_0 \neq y_0\), in particular, if
\[
U(x_f, x_0) | \chi_1(x_0) \rangle = U(x_f, y_0) | \chi_2(y_0) \rangle
\]
(3.7.7)
The point here, however, is that this becomes very unlikely with a large environment. With a large collection of oscillators in the environment, the environment states are a tensor product over $A$ of states $|\chi^A_1(x_0)\rangle$, for example, and then

$$F_{12} = \prod_A \langle \chi^A_2(y_0)|U_d(x_f,y_0)U(x_f,x_0)|\chi^A_1(x_0)\rangle$$

(3.7.8)

As the size of the environment goes to infinity, the possibility of Eq.(3.7.8) being exactly 1 becomes negligible.

It is also of interest to look at the special case in which the wave function Eq.(3.7.1) is real (as is the case in the no-boundary wave function of Hartle and Hawking), so that $\Psi_2 = \Psi_1^*$, and $\chi_2 = \chi_1^*$. When $x_0 = y_0$, we then have that

$$|F_{12}|^2 = \left|\int dq_0 \chi^2_1(x_0,q_0)\right|^2$$

(3.7.9)

Since $\chi_1$ is generally complex (it obeys the complex Schrödinger equation (3.6.7)), the right-hand side of Eq.(3.7.9) will again be less than 1, so the argument still goes through [68]. The argument fails if $\chi_1$ is real. But then it would have to be an eigenstate of the environment Hamiltonian for all values of $x_0$, and this would not lead to decoherence, so we may disregard this case.

### 3.8 Summary and Discussion

In this chapter we have studied the quantization and interpretation of simple timeless models described by an equation of the type (3.1.1). In particular, we studied the question, what is the probability that the system passes through a region $\Delta$ of configuration space without reference to time?

We obtained the classical answer to this problem, in three different forms, in terms of a classical phase space distribution function $w(p,x)$, satisfying $\{H,w\} = 0$, the analogue of (3.1.1). This function needs some care in normalization since it is constant along the (possibly infinite) classical orbits. A very useful step in the classical case was the introduction of the phase space quantity Eq.(3.2.7), which is $\delta$-function peaked on the classical path and also has vanishing Poisson bracket with the Hamiltonian, so is an observable. This quantity assists in understanding some aspects of the quantum theory.
We constructed the decoherence functional, following the general scheme of Refs. [50, 51], using the induced inner product. Although the general scheme has been presented previously, a key part of our contribution to this area is the explicit identification (in the semiclassical approximation) of the class operator Eq. (3.4.8) satisfying the constraint everywhere describing histories restricted to pass through a region $\Delta$ of configuration space. The main point was that one has to consider entire trajectories.

Having made this identification, a major part of our work was to show that the decoherent histories approach then reduces, approximately, to the corresponding classical result, but with the classical phase space distribution function $w(p, x)$ replaced by the Wigner function $W(p, x)$ of the quantum theory. We also explored the decoherence and probabilities for a system of harmonic oscillators using the timeless coherent states, in terms of which the analysis is particularly transparent and fully agrees with intuitive expectations.

In brief, therefore, we have shown that heuristic classically inspired notions of interpretation for simple timeless models may in fact be derived from the decoherent histories analysis of such models. This result is by no means unexpected, but the key aspects of the derivation are the elucidation of the role of the constraint and the related reparametrization invariance in the construction of both the classical and quantum results. Furthermore, the complete absence of a time parameter is not an obstruction to quantization.

There are a number of issues which the present work chapters generates. We will mention them briefly in the final chapter of this thesis. But first we will study the master equation for quantum cosmological models. The master equation is a standard tool to study the physical process of decoherence for quantum mechanical systems with an environment and the results of this chapter should also be reflected in a master equation for the system-environment model considered in Section 3.6.
Chapter 4

The Master Equation in Quantum Cosmology

4.1 Introduction

A lot of effort has been made to understand how classical properties or a quasi-classical domain appear in a model for the universe that is governed by a Wheeler-DeWitt equation

\[ \hat{H} \Psi = 0, \]  

(4.1.1)

The split of the universe into a system and its environment has proven to be very useful for this enterprise. As we know from normal quantum systems (for a review see [26]), the coupling of an environment to a system leads to the suppression of quantum interferences in the reduced density matrix of the system. This is also called decoherence (and one can then easily find a family of approximately decoherent histories in the decoherent histories approach).

Several papers have investigated the reduced density matrix [35, 65, 86, 96] for quantum cosmological models, regarding certain degrees of freedom – perturbations for example – as the environment. This has been successful in showing that there is suppression of interferences, for example in the scale factor of the universe. On the other hand, it was shown that the Wigner function of the reduced density matrix indicates correlations
between coordinates and momenta that approximately obey the classical equations of motion [33, 98].

The influence functional [20] describes the effect of the environment on the system and one can read from it the variables whose interference is suppressed (the so called pointer basis). These variables also appear in the master equation, the effective equation for the dynamics of the reduced density matrix.

For quantum cosmological models the influence functional method has been used to study decoherence [67, 97], but the master equation has only been considered once for a particular model [66]. In this Chapter we want to give a derivation of a master equation for a general quantum cosmological model containing a system and an environment.

In the previous Chapter of this thesis we have seen that the influence functional in the decoherence functional, at least in a semiclassical approximation, respects the reparametrization invariance of the total system. Another goal of this Chapter is to understand if and how the reparametrization invariance leading to (4.1.1) is reflected in the master equation.

The Chapter is organized as follows. In Section 4.2 we discuss the master equation for the standard model: quantum Brownian motion. We particularly emphasize the effects of the different terms in the master equation. For that we also look at the equation of the corresponding Wigner function.

In Section 4.3 we derive the master equation. We recapitulate the situation in the context of quantum cosmology. In particular in Section 4.3.1 we investigate the semiclassical solution to the Wheeler-DeWitt equation for a model containing a system and an environment and discuss the predictions made by examining the reduced density matrix and the Wigner function for the system.

In Section 4.3.2 we calculate the commutator of the system Hamiltonian with the reduced density matrix to obtain the master equation. In Section 4.3.3 we examine the effect of the different terms in the master equation. In the discussion of which terms are relevant to generate the expected behaviour of the Wigner function and the reduced density matrix, we observe a crucial difference to the behaviour of the quantum Brownian
CHAPTER 4. THE MASTER EQUATION IN QUANTUM COSMOLOGY

motion master equation.

In Section 4.3.4 we compare our result with the quantum cosmological master equation derived in [66], examine if reparametrization invariance is respected, and in Section 4.4 we conclude.

4.2 The Master Equation for Quantum Brownian Motion

The dynamics of a quantum mechanical system is governed by the Schrödinger equation. Using it one gets the evolution equation for the density matrix \( \rho \) of the system,

\[
\frac{i}{\hbar} \frac{\partial \rho}{\partial t} = \{ \hat{H}, \rho \}
\]

(4.2.1)

If one can make the split of the system into a subsystem and its environment, all information about the subsystem is contained in the reduced density matrix \( \rho_{\text{red}} \) given by the trace over the environment,

\[
\rho_{\text{red}} = \text{Tr}_{\text{env}}(\rho)
\]

(4.2.2)

The master equation is an effective equation for the time evolution of this reduced density matrix. It depends on the initial state of the environment and the form of the coupling, but it can be given a quite general form and has for example been used highly successfully in quantum optics. A standard example is the quantum Brownian motion model. It consists of a particle with a potential \( V(x) \) linearly coupled to a bath of harmonic oscillators. For simplicity, we set \( V \) to be a harmonic oscillator potential with frequency \( \Omega \). The Hamiltonian for the total system is

\[
H(p_x, x, p_n, q_n) = \frac{p_x^2}{2M} + \frac{1}{2} M \Omega^2 x^2 + \sum_l c_l x q_l + \sum_l \left( \frac{p_l^2}{2m_l} + \frac{m_l \omega_l^2}{2} q_l^2 \right)
\]

(4.2.3)

A very general form of the master equation for this model (assuming only that the system and environment are initially uncorrelated) was found by Hu, Paz and Zhang using path
integral methods and the influence functional [60]. Their master equation is:

$$i \frac{\partial \rho_{\text{red}}(x, y, t)}{\partial t} = \left[ -\frac{1}{2M} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) + \frac{M \Omega_R^2}{2} (x^2 - y^2) \right] \rho_{\text{red}}(x, y, t)$$

$$+ \left[ -i \gamma(t)(x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) - i \gamma(t) h(t)(x - y)^2 \right] \rho_{\text{red}}(x, y, t)$$

$$+ \gamma(t) f(t)(x - y) \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right) \rho_{\text{red}}(x, y, t)$$

(4.2.4)

$\gamma(t)$, $h(t)$ and $f(t)$ are time-dependent coefficients depending on the initial state. (The well known equation of Caldeira and Leggett [14] for the case of a thermal environment in a high temperature limit (the so called Fokker-Planck limit) is a special case of this equation. For this case $\gamma$ and $h$ are constant and $f$ vanishes.)

The first square bracket is the commutator of the system Hamiltonian with the reduced density matrix where $\Omega_R$ is a renormalized frequency due to the back reaction of the environment. The second square bracket is due to the effects of the environment on the system. The term $(b)$ leads to a suppression of the non-diagonal terms of the density matrix. This is called decoherence. Term $(c)$ also contributes to this effect. The role of term $(a)$ becomes clear when one looks at the corresponding equation for the Wigner function $W$ of $\rho_{\text{red}}$:

$$W(X, p, t) = \int \frac{dv}{2\pi} e^{-ivp} \rho_{\text{red}}(X + v/2, X - v/2, t)$$

(4.2.5)

The dynamical equation for the Wigner function is of Fokker-Planck form,

$$\frac{\partial}{\partial t} W(X, p, t) = \left[ -\frac{p}{M} \frac{\partial}{\partial X} + M \Omega_R^2 X \frac{\partial}{\partial p} \right] W(X, p, t)$$

$$+ \left[ 2\gamma(t) \frac{\partial}{\partial p} p + \gamma(t) h(t) \frac{\partial^2}{\partial p^2} - \gamma(t) f(t) \frac{\partial^2}{\partial X \partial p} \right] W(X, p, t)$$

(4.2.6)

and one recognizes term $(a)$ as a friction or dissipation term.

Eq. (4.2.4) has the following physical consequences. The suppression of the non-diagonal terms of the reduced density matrix $\rho_{\text{red}}$ destroys interferences between different positions. This decoherence is not complete, since it is counteracted by wave packet spreading and the friction term. The dissipation term also leads to a departure from the
equations of motion describing the classical case. A very detailed overview about the whole topic of decoherence is given in [26].

In anticipation of the quantum cosmological results we obtain we want to emphasize that the main term responsible for decoherence in the case of quantum Brownian motion is the term proportional to \((x - y)^2\).

### 4.3 The Master Equation for a Quantum Cosmological Model

As a general model we take a mechanical system with a potential \(U(x)\) and couple an environment (given by the coordinates \(q = (q_1, \cdots, q_m)\)) via its coordinate \(x = (x_1, \cdots, x_n)\). The total Hamiltonian is\(^1\)

\[
H(x, q) = H_{\text{sys}}(x) + H_{\text{env}}(x, q) = \frac{1}{2M}p_ip_i + U(x) + H_{\text{env}}(x, q) \tag{4.3.1}
\]

where \(p_i\) is the conjugate momentum to \(x_i\) and \(H_{\text{env}}\) includes the coupling of the system to the environment which we do not specify further. The Wheeler-DeWitt equation will correspond to a stationary Schrödinger equation

\[
(\hat{H} - E)\psi = 0 \tag{4.3.2}
\]

A general quantum cosmological model will have a kinetic term of the form \(g_{ab}(x)p^ap^b\), but for simplicity we stick to the form (4.3.1).

The equation for the density matrix corresponding to (4.2.1) is also a stationary equation

\[
0 = [\rho, \hat{H}] \tag{4.3.3}
\]

Hence the master equation for the reduced density matrix \(\rho_{\text{red}}\) will be timeless as well and we expect it to be of the form

\[
0 = [\rho_{\text{red}}, \hat{H}_{\text{sys}}] + \ldots \text{ extra terms } \ldots \tag{4.3.4}
\]

\(^1\)Two identical indices are summed over.
This form inspires us to derive the master equation by calculating the commutator \([\rho_{\text{red}}, \hat{H}_{\text{sys}}]\). So first we have to discuss a typical reduced density matrix for quantum cosmological models.

### 4.3.1 The Semiclassical Reduced Density Matrix and the Corresponding Wigner Function

If one does a semiclassical analysis \([69, 70]\) one finds the following type of solution to the Wheeler-DeWitt type equation (4.3.2)

\[
\psi(x, q) = C(x)e^{iS(x)}\chi(x, q) \tag{4.3.5}
\]

where \(S\) obeys the Hamilton-Jacobi equation for the system,

\[
\frac{1}{2M} \frac{\partial S}{\partial x_a} \frac{\partial S}{\partial x_a} + U(x) = E \tag{4.3.6}
\]

A useful relation is obtained by differentiating this equation with respect to \(x_b\)

\[
\frac{1}{M} \frac{\partial^2 S}{\partial x_b \partial x_a} \frac{\partial S}{\partial x_a} + \frac{\partial U}{\partial x_b} = 0 \tag{4.3.7}
\]

\(C\) obeys

\[
2 \frac{\partial S}{\partial x_a} \frac{\partial C}{\partial x_a} + C \frac{\partial^2 S}{\partial x_a \partial x_a} = 0 \tag{4.3.8}
\]

which leads to

\[
\frac{\partial}{\partial x_a} \left( |C|^2 \frac{\partial S}{\partial x_a} \right) = 0 \tag{4.3.9}
\]

\(\chi\) obeys a Schrödinger-type equation

\[
\frac{i}{M} \nabla_x S \cdot \nabla_x \chi = \hat{H}_{\text{env}}(x, q)\chi \tag{4.3.10}
\]

The reduced density matrix for the system is then given by the trace over the environment

\[
\rho_{\text{red}}(x, y) = C(x)C^*(y)e^{iS(x) - iS(y)} \int d^mq \chi^*(y, q)\chi(x, q) \tag{4.3.11}
\]

We introduce new variables

\[
X = \frac{x + y}{2}, \quad v = x - y \tag{4.3.12}
\]
As said above, the effect of the environment is the suppression of the non-diagonal terms of the density matrix. These correspond to a large $v$. So we can expand around $v = 0$. $\rho_{\text{red}}$ then takes the form

$$\rho_{\text{red}}(X, v) = (|C(X)|^2 + O(v))e^{iv_a \nabla_a S(X) + O(v^3)}F(X, v) \tag{4.3.13}$$

$F$ is the expansion of $\int dq \chi^*(y, q)\chi(x, q)$, the trace over the environmental part of the wave function. It is less than or equal to 1 and equal to 1 for $x = y$ (i.e. $v = 0$), since $\chi$ is normalized. Therefore this expansion is similar to the expansion of the influence functional in Section 3.6.2 in the previous chapter. $F$ thus can be written as in the form of Eq. (3.6.22),

$$F(X, v) = e^{iv_a \Gamma_a - \frac{1}{2}v_a v_b \sigma_{ab}} + O(v^3) \tag{4.3.14}$$

where

$$\Gamma_a = \frac{i}{2} \int d^m q (\chi(X)\partial_a \chi^*(X) - \chi^*(X)\partial_a \chi(X)) \tag{4.3.15a}$$

$$\sigma_{ab} = \frac{1}{2} \left( \int d^m q \partial_a \chi(X)\partial_b \chi^*(X) - \int d^m q \partial_b \chi(X)\partial_a \chi^*(X) \right) - \Gamma_a \Gamma_b \tag{4.3.15b}$$

The Gaussian form of $F$ is exact in the case of Gaussian environmental states $\chi$ and certainly a good approximation for a large number of environmental degrees of freedom.

The Fourier transform with respect to $v$ gives us the Wigner function of $\rho_{\text{red}}$

$$W_{\text{red}}(X, p) = \sqrt{\frac{\det(\sigma^{-1})}{(2\pi)^n}} |C(X)|^2 \times \exp \left[ -\frac{1}{2} (p - \nabla S(X) - \Gamma) a \sigma^{-1}_{ab} (p - \nabla S(X) - \Gamma) b \right] \tag{4.3.16}$$

This function is peaked around trajectories obeying semiclassical equations of motion (see [33]) which shows the semiclassical property of the derived solution. The peak in $p$ obeys an total energy equation with semiclassical corrections [33, 69],

$$\frac{p^2}{2M} + \langle \hat{H}_\text{env} \rangle + U(X) + O(M^{-1}) = E \tag{4.3.17}$$

### 4.3.2 The Derivation of the Master Equation for $\rho_{\text{red}}$

To get the master equation we calculate the commutator of $\hat{H}_\text{sys}$ with the expanded $\rho_{\text{red}}$ of the previous Section up to order $v^2$. Since the master equation will be of the form (4.3.4),
this commutator will give the extra terms:

\[
[H_{\text{sys}}, \rho_{\text{red}}](X, v) = \left( -\frac{1}{M} \frac{\partial^2}{\partial X_a \partial v_a} + v_a \frac{\partial U}{\partial X_a} \right) |C(X)|^2 e^{i v_b \nabla_b S(X)} e^{i v_b \Gamma_b(X)} - \frac{i}{2} v_b v_c \sigma_{bc}(X)
\]

\[
= e^{i v_b \Gamma_b(X)} - \frac{1}{2} i v_b v_c \sigma_{bc}(X) \left( \frac{1}{M} \frac{\partial^2}{\partial X_a \partial v_a} + v_a \frac{\partial U}{\partial X_a} \right) |C(X)|^2 e^{i v_b \nabla_b S(X)} \frac{\partial}{\partial v_a} e^{i v_b \Gamma_b(X)} - \frac{i}{2} v_b v_c \sigma_{bc}(X)
\]

\[
- \frac{1}{M} \frac{\partial}{\partial X_a} \left( |C(X)|^2 e^{i v_b \nabla_b S(X)} \frac{\partial}{\partial v_a} e^{i v_b \Gamma_b(X)} - \frac{i}{2} v_b v_c \sigma_{bc}(X) \right)
\]

\[
- \frac{|C(X)|^2}{M} \frac{\partial}{\partial v_a} e^{i v_b \nabla_b S(X)} \frac{\partial}{\partial X_a} e^{i v_b \Gamma_b(X)} - \frac{i}{2} v_b v_c \sigma_{bc}(X)
\]

\[
= - \frac{i}{M} \frac{\partial}{\partial X_a} (\Gamma_a \rho_{\text{red}}) + v_b \nabla_b S(X) \frac{\partial \Gamma_b}{\partial X_a} \rho_{\text{red}}
\]

\[
+ \frac{1}{M} v_b \frac{\partial}{\partial X_a} (\sigma_{ab \text{red}}) + \frac{i}{2M} \nabla_a S(X) \frac{\partial \sigma_{bc}}{\partial X_a} v_b v_c \rho_{\text{red}}
\]

\[\text{(4.3.18)}\]

The term labelled with (a) vanishes due to the Eqs. (4.3.7) and (4.3.9) for \(S\) and \(C\).

Transforming back to the variables \(x\) and \(y\), we get as the master equation for \(\rho_{\text{red}}(x, y)\)

\[0 = \left[ -\frac{1}{2M} \left( \frac{\partial^2}{\partial x_a \partial x_a} - \frac{\partial^2}{\partial y_a \partial y_a} \right) + U(x) - U(y) \right] \rho_{\text{red}}
\]

\[+ \frac{i}{M} (\frac{\partial}{\partial x_a} + \frac{\partial}{\partial y_a}) (\Gamma_a \rho_{\text{red}}) - (x_b - y_b) \left( \frac{\partial S}{\partial x_a} + \frac{\partial S}{\partial y_a} \right) \left( \frac{\partial \Gamma_b}{\partial x_a} + \frac{\partial \Gamma_b}{\partial y_a} \right) \rho_{\text{red}}
\]

\[- \frac{1}{M} (x_b - y_b) \left( \frac{\partial \sigma_{ab}}{\partial x_a} + \frac{\partial \sigma_{ab}}{\partial y_a} \right) \rho_{\text{red}} - \frac{1}{M} (x_b - y_b) \sigma_{ab} \left( \frac{\partial}{\partial x_a} + \frac{\partial}{\partial y_a} \right) \rho_{\text{red}}
\]

\[- \frac{i}{2M} \frac{\partial S}{\partial x_a} + \frac{\partial S}{\partial y_a} \left( \frac{\partial \sigma_{bc}}{\partial x_a} + \frac{\partial \sigma_{bc}}{\partial y_a} \right) (x_b - y_b) (x_c - y_c) \rho_{\text{red}}
\]

\[\text{(4.3.19)}\]

The partial derivatives of \(S\), \(\Gamma\) and \(\sigma\) have to be taken at the point \(x^+ y^+ / 2\), so that \(\frac{\partial S}{\partial x_a} = \frac{\partial}{\partial x_a} S(\frac{x^+ y^+}{2})\) etc.

### 4.3.3 Discussion of the Derived Master Equation

To discuss this master equation, we write it in a compact form:

\[0 = [\hat{H}_{\text{sys}}, \rho_{\text{red}}] + \hat{O}_R \rho_{\text{red}}
\]

\[- \frac{1}{M} \sigma_{ab} (x_b - y_b) \left( \frac{\partial}{\partial x_a} + \frac{\partial}{\partial y_a} \right) \rho_{\text{red}} - \frac{i}{2M} \Upsilon_{bc} (x_b - y_b) (x_c - y_c) \rho_{\text{red}}
\]

\[\text{(4.3.20)}\]
\( \hat{O}_R \) includes the terms that can be regarded as corrections to the system evolution through the backreaction of the environment. They are

\[
\frac{i}{M} \Gamma_a \left( \frac{\partial}{\partial x_a} + \frac{\partial}{\partial y_a} \right) + \frac{i}{M} \left( \frac{\partial \Gamma_a}{\partial x_a} + \frac{\partial \Gamma_a}{\partial y_a} \right)
- (x_b - y_b) \left( \frac{\partial S}{\partial x_a} + \frac{\partial S}{\partial y_a} \right) \left( \frac{\partial \Gamma_b}{\partial x_a} + \frac{\partial \Gamma_b}{\partial y_a} \right) - \frac{1}{M} (x_b - y_b) \left( \frac{\partial \sigma_{ab}}{\partial x_a} + \frac{\partial \sigma_{ab}}{\partial y_a} \right)
\]

(4.3.21)

and mainly can be seen as corrections to the potential \( U \). Only the first term is special: It has the form of the coupling to a magnetic potential. This is not surprising since \( \Gamma \) gives a shift in the momenta analogously to a magnetic potential.

The term involving \( \Upsilon_{bc} \) (which is equal to \( \left( \frac{\partial S}{\partial x_a} + \frac{\partial S}{\partial y_a} \right) \left( \frac{\partial \Upsilon_{bc}}{\partial x_a} + \frac{\partial \Upsilon_{bc}}{\partial y_a} \right) \)) should be the main term for decoherence (following the case of quantum Brownian motion). A term corresponding to the term \((x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right)\) in the quantum Brownian motion master equation (4.2.4) is also present, but a friction term is missing in Eq. (4.3.20).

What is a bit surprising is the following. The parameter \( \sigma_{ab} \) is a measure of decoherence since it determines the width of the peak in the reduced density matrix. In the quantum cosmological master equation however, the derivative of \( \sigma \) controls the term quadratic in \((x_a - y_a)\). As mentioned above, this quadratic term is normally associated with decoherence.

One can resolve this by examining how the semiclassical properties of the Wigner function (4.3.16) (the peak around \( \nabla S + \Gamma \)) are reflected in the master equation (4.3.20). To achieve this we solve the master equation (4.3.20) with a Gaussian ansatz. We can neglect the terms involving \( \Gamma \), since this is just a correction to the position of the peak of the Wigner function. Using the variables \( X \) and \( v \) from (4.3.12) again, we take as an ansatz

\[
\rho_A = \exp \left( -\frac{1}{2} v_a v_b A_{ab}(X) + iv_a B_a(X) + P(X) \right)
\]

(4.3.22)

The Wigner function to this density matrix is of the form

\[
W_A(X, p) = \sqrt{\det(A^{-1})} e^{P(X)} \exp \left( -\frac{1}{2} (p_a - B_a) A_{ab}^{-1} (p_b - B_b) \right)
\]

(4.3.23)

so the important coefficient for the form of the peak is \( A_{ab} \) and for the position it is \( B_a \). \( P \) will give us the prefactor.
We insert the ansatz in the master equation

$$0 = \left[ \frac{1}{M} \frac{\partial^2}{\partial X_a \partial v_b} + v_a \frac{\partial U}{\partial X_a} - \frac{1}{M} v_b \frac{\partial \sigma_{ab}}{\partial X_a} \right] \rho_A$$

(4.3.24)

Calculating the derivatives and ordering in powers of $v$, we find the following conditions for the coefficients $A$, $B$ and $P$.

$$\mathcal{O}(v^0) : \quad 0 = \frac{\partial B_a}{\partial X_a} + B_a \frac{\partial P}{\partial X_a}$$

(4.3.25)

$$\mathcal{O}(v^1) : \quad 0 = B_b \frac{\partial B_a}{\partial X_b} + M \frac{\partial U}{\partial X_a} + \frac{\partial P}{\partial X_b} (A_{ab} - \sigma_{ab}) + \frac{\partial A_{ab}}{\partial X_b} - \frac{\partial \sigma_{ab}}{\partial X_b}$$

(4.3.26)

$$\mathcal{O}(v^2) : \quad 0 = \frac{\partial B_a}{\partial X_c} (A_{bc} - \sigma_{bc}) + \frac{1}{2} \left( B_c \frac{\partial A_{ab}}{\partial X_c} - \frac{\partial S}{\partial X_c} \frac{\partial \sigma_{ab}}{\partial X_c} \right)$$

(4.3.27)

From (4.3.26) and (4.3.27) we deduce that $A_{ab} = \sigma_{ab}$. With this it follows from (4.3.27) that $B_a = \nabla_a S$. The remaining bit of Eq. (4.3.26) is then the differentiated Hamilton-Jacobi equation (4.3.7). And (4.3.25) then shows that $e^P$ obeys the same equation as $|C|^2$, i.e. Eq. (4.3.9). So far we have shown that our master equation leads to our semiclassical reduced density matrix (4.3.13).

The crucial step to examining the effects of the master equation now is to investigate which terms in (4.3.24) are responsible for the stated form of the coefficients $A$ and $B$. It turns out that term $(b)$ in connection with term $(a)$ gives $A_{ab} = \sigma_{ab}$, and that term $(c)$ and term $(a)$ lead to $B_a = \nabla_a S$. So in contrast to the quantum Brownian motion master equation (4.2.4) the term responsible for decoherence (the suppression of interference between different points $x$ and $y$) is the term of the form $(x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right)$. The term of the form $(x - y)^2$ that is normally considered to be responsible for decoherence is in quantum cosmology instead responsible for the position of the peak of the Wigner function, i.e. the semiclassical trajectories.

This surprising difference between quantum cosmology and quantum Brownian motion was already suggested by the calculations done by Kiefer in [66] and briefly mentioned in the discussion of Eq. (5.35) in [26]. In the next Section we will reexamine this calculation.
4.3.4 Relation to Other Work

In [66] a master equation was derived for a concrete model (a closed Friedman universe with small perturbations). The scale factor of the universe was regarded as the system variable \( x \) and the perturbations formed the traced over environment. In an approximation with \( x \approx y \) the master equation took the form (using our notations)

\[
\rho_{\text{red}} + \frac{2N^3}{3}(x-y)\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)\rho_{\text{red}} = 0 \tag{4.3.28}
\]

where \( N \) is a cut-off in the number of perturbation modes.

Comparing with our general form (4.3.20) there is no correction term \( \hat{O}_R \) and no term proportional to \((x - y)^2\). This has to do with the fact that phase factors were ignored in the reduced density matrix for this model. These phase factors are necessary to have a peak in the Wigner function around a momentum \( p_0 \) not equal to 0. As we had seen, the term proportional to \((x - y)^2\) produces this peak and therefore is missing here. The term proportional to \((x - y)\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\) is present and we have seen that this is the term responsible for decoherence in quantum gravity. This was already suggested in [26].

The original motivation for us to study the master equation in quantum cosmology were the results of the previous chapter. There, using decoherent histories, it was shown that decoherence should be suppressed for points lying on the same semiclassical trajectory of the system. This was due to the reparametrization invariance of the system. In the case of the master equation, this suppression of decoherence should be reflected in the fact that \( \sigma_{ab} \) becomes small when projected onto such a trajectory.

We calculate the projection of \( \sigma \) onto the trajectory (using the definition of \( \sigma \) in Eq. (4.3.15b) and the Eq. (4.3.10) for \( \chi \)):

\[
-\frac{1}{M^2}\partial_aS\partial_bS \sigma_{ab} = \int dq H_{\text{env}}\chi^*H_{\text{env}}\chi - (\int dq \chi^*H_{\text{env}}\chi)^2 = \langle H_{\text{env}}^2 \rangle - \langle H_{\text{env}} \rangle^2 \tag{4.3.29}
\]

For the semiclassical approximation it is often assumed that \( \chi \) behaves approximately adiabatically along the trajectories (analogous to the Born-Oppenheimer approximation in molecular physics). This means it will be approximately in an energy eigenstate of the environment Hamiltonian and in that case the calculated projection will approximately vanish.
CHAPTER 4. THE MASTER EQUATION IN QUANTUM COSMOLOGY

However our calculations with decoherent histories did not need this adiabatic approximation to respect reparametrization invariance. This has to do with the fact that the influence functional of the previous Chapter takes into account the whole evolution of $\chi$ along the trajectory whereas $F$ in this Chapter is only determined by $\chi$ at one point on the trajectory. In this sense the decoherent histories approach gives a more complete view of the timeless character of the model.

4.4 Conclusions and Discussion

For a general quantum cosmological model we have derived a master equation for a semiclassical reduced density matrix. It is of the form

$$0 = [\hat{H}_{\text{sys}}, \rho_{\text{red}}] + \hat{O}_R \rho_{\text{red}} - \frac{1}{M} \sigma_{ab} (x_b - y_b) \left( \frac{\partial}{\partial x_a} + \frac{\partial}{\partial y_a} \right) \rho_{\text{red}} - \frac{i}{2M} \Upsilon_{bc} (x_b - y_b)(x_c - y_c) \rho_{\text{red}}$$

and captures the heuristic behaviour which we expect from an analysis of the corresponding reduced semiclassical Wigner function.

We have confirmed and extended the suggestion made by Kiefer that the term responsible for decoherence in quantum cosmology is the one proportional to $(x - y) \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right)$. The term involving $(x - y)^2$ (normally associated with decoherence) is responsible for the position of the peak of the semiclassical reduced Wigner function.

We found some evidence that reparametrization invariance is also respected by the master equation, yet this is not as conclusive as in the decoherent histories approach.

The master equation we derive depends on the specific form of the semiclassical reduced density matrix. For a more general view and a fuller understanding, it would be nice to have a direct derivation from the equation $[\hat{H}, \rho] = 0$ analogous to the derivation of the master equation for quantum mechanical models. However the timelessness of $[\hat{H}, \rho] = 0$ seems to be quite an obstacle since it prevents the use of the methods applied in quantum mechanics.
Chapter 5

Summary and Outlook

In this thesis we attempted to find mathematical objects corresponding to physical properties for quantum cosmological models that obey a Wheeler-DeWitt equation. The question we concentrated on was finding the expression for the quantum probability of entering a region $\Delta$ in configuration space without any reference to time. The question was posed in this manner to reflect the timeless character of the Wheeler-DeWitt equation. The timelessness is a general feature of systems that are invariant under reparametrization of their time parameter.

This kind of question is not simply answered for quantum systems, since there the standard observables are related to a definite instant in time. There are several approaches to posing this kind of question for a quantum system. We mainly used the methods of the the decoherent histories approach to quantum theory. But we also compared with an operator approach (the “evolving constants” approach).

Another important ingredient was the use of the induced inner product scheme to guarantee that we always have a Hilbert space of physical states for the reparametrization invariant models we use.

In Chapter 1, after an introduction and a short review of reparametrization invariant systems, the induced inner product and the decoherence histories approach, we set up a decoherence functional for reparametrization invariant systems. We introduced class operators defined by restricted path integrals that should correspond to the question of
entering or not entering a region $\Delta$ in configuration space.

In Chapter 2 we applied the formalism to the relativistic particle that obeys the Klein-Gordon equation. We selected our region $\Delta$ to be a section of a spacelike hypersurface $x^0 = \tau$, since for this type of region we could also use the operator approach. In this approach we derived the standard Newton-Wigner and Klein-Gordon probabilities (being positive due to the induced inner product) for crossing the region $\Delta$. Using the decoherent histories approach we encountered a problem already recognized by Hartle and Marolf [51]. The class operators we defined by using restricted path integrals and rewrote with the help of the path decomposition expansion did not obey the constraint. But following the procedure suggested by Hartle and Marolf we were able to find the physically reasonable class operators. We found the same probability expressions as the ones in the operator approach. For the case of Klein-Gordon quantization we only found approximate decoherence. This seems to be related to the fact that in the operator approach, the operator in the Klein-Gordon scheme was not self-adjoint. We also managed to find a more mathematical way to find the correct class operators by changing the time parameter integrals of the path decomposition expansion such that reparametrization invariance was respected.

In Chapter 3 we then considered a more general quantum cosmological model and a general (open) region $\Delta$. We analyzed the classical case, constructed a phase space function as a classical observable and confirmed the standard heuristic interpretation of a WKB wavefunction in quantum cosmology.

For the quantum case, we used a semiclassical approximation to the class operators. The important step again was to find the correct operators. Here the main idea was to capture the behaviour of the entire trajectory. If there is decoherence, the decoherence functional then reduces to the classical result with the Wigner function as the classical phase space distribution function.

We also saw that approximate decoherence of the histories could be produced with the help of an environment. An interesting point was that the influence functional respected the reparametrization invariance of the model. In Chapter 4 we derived a master equation for the reduced density matrix of a quantum cosmological model in a semiclassical approximation. We extended a previous result and found a master equation that reproduced the
CHAPTER 5. SUMMARY AND OUTLOOK

semiclassical behaviour. We investigated how far reparametrization invariance is reflected in the master equation. This was only true for an adiabatic behaviour of the environment along the system trajectories. In this sense the decoherent histories approach gives a more complete view.

In this thesis we have seen that it is possible to use the decoherent histories approach for reparametrization invariant models like those used in quantum cosmology, and that it is possible to make probability statements about physical properties. But of course there are still open and new questions.

First of all, the main difficulty in computing the decoherence functional for our chosen coarse graining was the calculation of modified class operators that obey the constraint. Even before modification, the restricted propagators

\[ g_\alpha(x_f, \tau | x_0, 0) = \int_\alpha Dx(t) \exp \left( \frac{i}{\hbar} S[x(t)] \right) \]  

which we used to define the class operators are difficult to calculate (typically they can only be obtained exactly in the very simple situations where the method of images may be used). The suggested scheme for constructing the modified operators has not yet been explored fully. We have constructed physically plausible modified class operators in the semiclassical approximation, obtaining full agreement with the classical results and we found some exact modified class operators for simple coarse grainings of the relativistic particle. But it is not yet clear how general those results are. Hence a more detailed investigation of these modified class operators is called for. (We note in passing that, from the simple examples in which the modified class operators have been calculated, their calculation does in fact appear to be considerably easier than the original ones, Eq.(5.1.1)).

Second, we have assumed in Chapter 3 that both the initial states and the propagators are in the oscillatory regime. This means in the propagator that we assume the dominant contribution comes from real configurations (rather than Euclidean or complex ones). Many interesting models in quantum cosmology have a Euclidean region, corresponding, for example, to “tunnelling from nothing”. It is not immediately clear how the semiclassical calculations of Chapter 3 have to be modified to include this case, the main difficulty being...
understanding what the class operators are. This case is therefore probably related to the question of a more general formula for the modified class operators.

Third, it is generally understood that decoherence of histories is related to the existence of “records”[22–24, 39]. This means that it is possible to find a projection operator $R_\alpha$ which is perfectly correlated with the class operators $C_\alpha$ in terms of which the probabilities may be written,

$$p(\alpha) = \text{Tr} \left( C_\alpha \rho C_\alpha^\dagger \right) = \text{Tr} \left( R_\alpha \rho \right)$$

(5.1.2)

In the case of a non-relativistic model where decoherence is produced by an environment, it is possible to explicitly identify the environmental variables which store the information about the system [39]. It would be very desirable to do this in the timeless case considered here. It seems likely that the variables are very similar to the case of Ref.[39], but the interesting question is the role of reparametrization invariance in this situation, and whether the records are closely related to observables in the operator approach.

Last but not least, as already mentioned, it would be nice to have a derivation of the master equation for the reduced density matrix from the equation for the total density matrix

$$[H, \rho] = 0$$

(5.1.3)

in the case of reparametrization invariant models.
Figure 1: A possible region $\Delta$ defining an orbit for a system with a central potential
Figure 2: The construction of restricted propagators in the calculations of Yamada and Tagaki. The dotted path contributes to the restricted propagator $g_{\Sigma}(x_f, t_f|x_0, t_0)$ which represents the history of entering the space time region $\Sigma$. The solid path does not.
Figure 3: The construction of our restricted propagators. The dotted path contributes to the class operator $C_\Delta(x, y)$ which represents the history of entering the configuration space region $\Delta$. The solid path does not.
Figure 4: The propagators $G^{(1)}(x'', x')$ and $G_F(x'', x')$ are obtained by a path integral of the form (2.1.6), (2.1.7), involving a sum over all paths from $x'$ to $x''$ (hence the paths may move both backwards and forwards in the time coordinate $x^0$). An infinite range for $T$ gives $G^{(1)}(x'', x')$ and a half-infinite positive range gives $iG_F(x'', x')$.

Figure 5: The Newton-Wigner propagator $G_{NW}(x'', x')$ may be obtained by a path integral of the form (2.1.6), (2.1.7), in which the paths may move backwards and forwards in time, with the restriction that they do not cross the final surface, except to end on it at the final point $x''$. 

Figure 6: The class operator $C_{NC}(x''; x')$ for not crossing the spacelike surface $x^0 = \tau$ is given by a sum over paths from $x'$ to $x''$ which never cross the surface. It is equivalent to a method of images construction.

Figure 7: The path decomposition expansion (PDX) for the surface $x^0 = \tau$. A sum over paths from points $x'$ to $x''$ on opposite sides of a surface may be partitioned according to the position $x$ and the parameter time at which it makes its first crossing of the surface.
Figure 8: The class operator $C_\Delta(x'', x')$ for a first crossing of the surface $x^0 = \tau$ in the spatial region $\Delta$ is obtained by summing over paths which cross the surface for the first time in the region $\Delta$.

Figure 9: A second representation of the Newton-Wigner propagator $G_{NW}(x'', x')$ may be obtained by a path integral of the form (2.1.6), (2.1.7), in which the paths may move backwards and forwards in time, with the restriction that they do not cross the initial surface, except to start on it at the initial point $x'$. 
Figure 10: The path integral representation of Eq. (2.5.32). The paths go from the initial point \( x' \) to their first crossing of the surface at \( x_1 \), and this is represented by \( G_{NW}(x_1, x') \). The propagation from \( x_1 \) to \( x_2 \) is unrestricted and is represented by \( G^+(x_2, x_1) \). The paths make their last crossing at \( x_2 \) moving to their final point \( x'' \), and this is represented by \( G_{NW}(x'', x_2) \).
Figure 11: A more general path integral representation of the Newton-Wigner propagator $G_{NW}(x'', x')$. In the path integral expressions (2.1.6), (2.1.7), the paths move backwards and forwards in time with the restriction that they may cross a prescribed intermediate surface once and only once. The representation is independent of the choice of intermediate surface. The two previous representations (portrayed in Fig. 5 and Fig. 9) in the limit that the intermediate surface tends to the final or initial surface.
Figure 12: The rewritten classical probability Eq. (3.2.13) in terms of a sum over initial and final points $x_0$ and $x_f$. The probability for not entering $\Delta$ is a sum over paths as in case (a). The probability for entering $\Delta$ includes a sum over classical paths in which $\Delta$ lies between the initial and final points, as in case (b). But, to agree with the phase space form of the result Eq. (3.2.10), it must also include a sum over initial and final points for which $\Delta$ does not lie between them, as in case (c). This figure also applies to the semiclassical propagator Eq. (3.4.8) in the quantum case.
Bibliography


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