Decoherent Histories Analysis of the Relativistic Particle

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ABSTRACT: The Klein-Gordon equation is a useful test arena for quantum cosmological models described by the Wheeler-DeWitt equation. We use the decoherent histories approach to quantum theory to obtain the probability that a free relativistic particle crosses a section of spacelike surface. 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. The notion of crossing a spacelike surface requires some attention, given that the paths in the path integral may cross such a surface many times, but we show that first and last crossings are in essence the only useful possibilities. 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). In the Klein-Gordon quantization, the decoherence is only approximate, due to the fact that the paths in the path integral may go backwards and forwards in time. We compare with the results obtained using operators which commute with the constraint (the “evolving constants” method).
1. INTRODUCTION

If the state of a quantum system obeys a wave equation of the form

\[ H \Psi = 0, \quad (1.1) \]

how do we extract probabilities from the wave function? Quantum cosmological models are described by precisely such a wave equation – the Wheeler-DeWitt equation – where \( H \) is the total Hamiltonian of the matter and gravitational fields [1,2]. A simpler but important example of an equation of this type is the Klein-Gordon equation

\[ \left( \Box + m^2 \right) \phi = 0 \quad (1.2) \]

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. These questions are closely related to the problem of time in quantum gravity [3,4,5]. Furthermore, it is likely that they will also be present in other approaches to quantum gravity, such as the loop variable approach [6].

A number of approaches to this problem have been considered. One is the decoherent histories approach, in which the wave function is associated with a set of histories to which probabilities may be assigned [7,8,9]. Another approach involves the use of operators which commute with \( H \) [10,11,12,13,14,15]. The purpose of this paper is to explore the application of these methods to some simple probability questions involving the relativistic particle in flat spacetime. We will concentrate on the decoherent histories approach,
extending and developing earlier work in this area [1,16]. At the present (rather early) stage of development of this field it is not possible to say whether it is equivalent to an operator approach, and an important part of this paper is to compare the approaches where possible. Indeed, there are many different and potentially inequivalent quantization methods applicable to simple parametrized systems [17,18].

We 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 parameterized 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, which will be considered elsewhere.

We begin by briefly reviewing the various aspects of the formalism relating to the wave equations (1.1), (1.2).

1(A). Inner Products

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

$$
\Psi^* \circ_{KG} \Phi = (\Psi, \Phi)_{KG} = i \int_{\Sigma} d^3x \, \Psi^* \overset{\rightarrow}{\partial_0} \Phi
$$

$$
= i \int_{\Sigma} d^3x \left( \Psi^* \overset{\rightarrow}{\partial_0} \Phi - \Psi^* \overset{\leftarrow}{\partial_0} \Phi \right)
$$

(1.3)

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, it is positive on the positive frequency sector and negative on the negative frequency sector.
An essential part of our approach here is to use the methods of refined algebraic quantization, in which we work with the so-called induced (or Rieffel) inner product \([16,19]\). This starts through the introduction of an auxiliary inner product

\[
(\Psi, \Phi)_A = \int d^4 x \, \Psi^*(x)\Phi(x)
\]  

(1.4)

We then consider eigenstates of the constraint

\[
H\Psi_{\lambda k} = \lambda \Psi_{\lambda k}
\]  

(1.5)

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

\[
(\Psi_{\lambda k}, \Psi_{\lambda' k'})_A = \delta(\lambda - \lambda')\delta(k - k')
\]  

(1.6)

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 solutions to the constraint. This procedure may also be understood by starting from the observation that solutions to the constraint (1.5) may be written in the form \(\delta(H - \lambda)|\chi\rangle\) for some fiducial state \(|\chi\rangle\). The induced inner product between such states is then effectively equivalent to replacing \([\delta(H - \lambda)]^2\) with \(\delta(H - \lambda)\), that is, taking \(\delta(H - \lambda)\) to be a projection operator (which it clearly is in the case of a discrete spectrum).

When a split into positive and negative frequency solutions is possible, \(\Psi = \Psi^+ + \Psi^-\), 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:

\[
\Psi^* \circ I \Phi = (\Psi, \Phi)_I = (\Psi^+, \Phi^+)_{KG} - (\Psi^-, \Phi^-)_{KG}
\]  

(1.7)

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
provides a good inner product even when the split into positive and negative frequencies is not possible. (See Refs. [16,19] for more details).

1(B). An Operator Approach

Given the constraint equation (1.1) and its inner product structure we would like to be able to assign probabilities to various dynamical variables of interest. It is generally believed that the interesting dynamical variables are those that commute with the constraint $H$ [10,11,12,13,14,15]. This is because the constraint is associated with reparametrization invariance (diffeomorphism invariance in the general case) and we are interested in variables that are invariant.

Because the wave equation 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

$$[A]_{B=\tau} = \int_{-\infty}^{\infty} ds \ A(s) \frac{dB(s)}{ds} \delta(B(s) - \tau) \quad (1.8)$$

where $A(s) = e^{iHs} A e^{-iHs}$, and similarly for $B(s)$ [14,15]. (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 $H$. The study of operators of this type is the basis of the operator approach (sometimes know as the “evolving constants” method). The spectrum of the operator Eq(1.8) is computed from
which one may compute a projection operator $P_\alpha$ say, onto a range of the spectrum. The
associated probability is then of the form $\text{Tr}(P_\alpha \rho)$.

1(C). Decoherent Histories

In this paper we are primarily concerned with the decoherent histories approach to
quantum theory, and this provides a second method of calculating probabilities of interest
On the face of it this method is quite different to the operator method outlined above, and
as stated in the Introduction, there is no particular reason to assume that the methods are
equivalent.

In the usual formulation in non-relativistic quantum mechanics [7,8,9], the central
object of interest is the decoherence functional,

$$D(\alpha, \alpha') = \frac{1}{N} \text{Tr} \left( \rho_f C_\alpha \rho C^\dagger_{\alpha'} \right)$$

(1.9)

where the histories are characterized by the class operators $C_\alpha$, which satisfy

$$\sum_\alpha C_\alpha = 1$$

(1.10)

In the simplest case, for non-relativistic systems, the class operators are given by time-
ordered sequences of projection operators

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

(1.11)

where $\alpha$ denotes the string of alternatives $\alpha_1, \alpha_2 \cdots \alpha_n$. The theory is, however, more
general than this and we will exploit this generality here [1,20]. We have included the possi-
bility 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 $N = (\text{Tr}(\rho_f \rho))^{-1}$.

Intuitively, the decoherence functional is a measure of the interference between pairs
of histories $\alpha, \alpha'$. When its real part is zero for all pairs of histories with $\alpha \neq \alpha'$, we say
that the histories are consistent and probabilities

\[ p(\alpha) = D(\alpha, \alpha) \]  

(1.12)

obeying the usual probability sum rules may be assigned to them. Typical physical mechanisms which produce this situation usually cause both the real and imaginary part of \( D(\alpha, \alpha') \) to vanish. This condition is usually called decoherence of histories, and is related to the existence of so-called generalized records [7,21]. Note also that when there is decoherence, using (1.10) the probabilities may be written

\[ p(\alpha) = \frac{1}{N} \text{Tr} \left( \rho_f C_\alpha \rho \right) \]  

(1.13)

In its application to the parametrized systems considered here, the initial and final states are attached to the class operators using the induced inner product scheme [16]. So for pure initial and final states, the decoherence functional is

\[ D(\alpha, \alpha') = \frac{1}{N} \left( \psi_f \circ C_\alpha \circ \psi \right) \left( \psi_f \circ C_{\alpha'} \circ \psi \right)^* \]  

(1.14)

where \( \circ \) here denotes the induced inner product. (We may of course sum over initial or final pure states to get mixed ones.) The key question for the models considered here is then the construction of class operators corresponding to questions of interest. This is the step analogous to the construction of operators above in Eq.(1.8), 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 paper is therefore to explore possible constructions and examine their properties.

One very natural approach to calculating the class operators for reparametrization-invariant systems is to use path integrals [16,1]. For the relativistic particle these have the form

\[ C_\alpha(x'', x') = \int dT \ g_\alpha(x'', T|x', 0) \]  

(1.15)
where
\[ g_\alpha(x'', T | x', 0) = \int_\alpha D x^\mu \exp \left( -i \int_0^T ds \left[ \frac{\eta_{\mu\nu} \dot{x}^\mu \dot{x}^\nu}{4} + m^2 \right] \right) \] (1.16)

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 constraint surface. 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 \( C_\alpha \) [16].

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 (1.8) and the class operators \( C_\alpha \)), but the operator method looks at a projection operator onto ranges of the spectrum of (1.8), whilst the decoherent histories approach works with the class operators \( C_\alpha \) and the decoherence functional (1.14). 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 histories Eq.(1.12) may be written in the form $\text{Tr}(R_\alpha \rho)$ where $R_\alpha$ is a projection operator (corresponding to the existence records mentioned earlier [7,21]).

1(D). Summary of this Paper

As stated, the main aim of this paper 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 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 3.

Our main results are described in Sections 4 and 5 where we apply the formalism outlined above to the relativistic particle. In Section 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 [22]. 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.(1.7)). 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 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). 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 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 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 expect NW probability expressions are easily recovered.

We summarize and conclude in Section 7.
This paper is related to a number of other works in the field. It exploits and extends the general formalism of the decoherent histories approach applied to quantum cosmology set out by Hartle [23], and more recently by Hartle and Marolf [16]. The application of this formalism appears to have been applied to particular models in only two other places. Whelan [24] considered probabilities on timelike surfaces for the relativistic particle (but not using the induced inner product structure, as here). Craig and Hartle [25] have applied the formalism to a Bianchi IX quantum cosmological model. There is also some connection with the work on probabilities for non-trivial spacetime coarse grainings in non-relativistic quantum mechanics [26]. A more general investigation of these ideas applied to quantum cosmological models is currently being pursued in Ref.[27].

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

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

(2.1)

where $\dot{}$ denotes differentiation with respect to the parameter $s$. $N$ is a Lagrange multiplier enforcing the constraint

$$H = p_t + h = 0$$

(2.2)

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

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

(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 Section 1.

Following the general scheme, we normalize solutions to the constraint by first considering eigenstates of $H$, as in Eq.(1.5). They are normalized using the auxiliary inner product according to

$$(\Psi_{\lambda k}, \Psi_{\lambda' k'})_A = \int dt dx \, \Psi_{\lambda k}^*(x,t) \Psi_{\lambda' k'}(x,t) = \delta(\lambda - \lambda') \delta(k - k') \quad (2.4)$$

Since $H = \dot{p} + h$, the solutions to the eigenvalue equation may be written

$$\Psi_{\lambda k}(x,t) = \frac{1}{(2\pi)^{1/2}} e^{i\lambda t} \psi_k(x,t) \quad (2.5)$$

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

$$\frac{1}{2\pi} \int dt \int dx \, e^{-i\lambda t + i\lambda' t} \psi_k^*(x,t) \psi_{k'}(x,t) = \delta(\lambda - \lambda') \delta(k - k') \quad (2.6)$$

The integral contains within it the usual inner product

$$(\psi_k, \psi_{k'})_S = \int dx \, \psi_k^*(x,t) \psi_{k'}(x,t) \quad (2.7)$$

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.(2.6), pulling down a delta function $\delta(\lambda - \lambda')$, and it follows that

$$(\psi_k, \psi_{k'})_S = \delta(k - k') \quad (2.8)$$

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

$$p_\Delta = \int_\Delta dx \, |\psi(x,t_0)|^2 \quad (2.9)$$
To express this in the language of Section 1, 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

$$X = \int_{-\infty}^{\infty} ds \, \frac{dt(s)}{ds} \, x(s) \, \delta(t(s) - t_0) \quad (2.10)$$

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

$$x(s) = e^{iHs} xe^{-iHs}, \quad t(s) = e^{iHs} te^{-iHs} \quad (2.11)$$

Since $H = p_t + h$ this is

$$x(s) = e^{ihs} xe^{-ihs} = x + \frac{ps}{m} \quad (2.12)$$
$$t(s) = e^{ip_s} te^{-ip_s} = t + s \quad (2.13)$$

The integral over $s$ may be done in Eq.(2.10) with the result

$$X = x - \frac{p(t - t_0)}{m} \quad (2.14)$$

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

$$X u_{\lambda\bar{x}}(x,t) = \bar{x} u_{\lambda\bar{x}}(x,t) \quad (2.15)$$

with solutions

$$u_{\lambda\bar{x}}(x,t) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\lambda t} g(x,t|\bar{x},t_0) \quad (2.16)$$

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

$$(u_{\lambda\bar{x}}, u_{\lambda'\bar{x}'})_A = \delta(\lambda - \lambda') \, \delta(\bar{x} - \bar{x}') \quad (2.17)$$

The amplitude for an eigenstate of the constraint of the form

$$\Psi_{\lambda'}(x,t) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\lambda t} \psi(x,t) \quad (2.18)$$
to be in an eigenstate of $X$ is

$$
(u_{\lambda \bar{x}}, \Psi_{\lambda'})_A = \frac{1}{(2\pi)} \int dt dx \, e^{it(\lambda - \lambda')} g^*(x, t|\bar{x}, t_0) \psi(x, t)
$$

$$
= \delta(\lambda - \lambda') \psi(\bar{x}, t_0)
$$

(2.19)

The probability is then computed from the expression

$$
\int_{\Delta} d\bar{x} \, (\Psi_{\lambda''}, u_{\lambda \bar{x}})_A (u_{\lambda \bar{x}}, \Psi_{\lambda'})_A = \delta(\lambda'' - \lambda) \delta(\lambda - \lambda') \int_{\Delta} d\bar{x} \, |\psi(\bar{x}, t_0)|^2
$$

(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.(2.9).

The operator formalism with Eq.(1.8) 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

$$
T = t_0 + \frac{m(x - x_0)}{p}
$$

(2.21)

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 Ref.[28], for example). 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 [29].

Both of the above questions in non-relativistic quantum mechanics may also be analysed 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.(2.9) 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(C), exact decoherence of histories implies that records exist [7,21], 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 (2.14) from which the probabilities Eq.(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 [26]), 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.(2.21) 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 5 and 7.

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.[30] (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
\[
G^\pm(x, y) = \frac{1}{(2\pi)^3} \int \frac{d^3k}{2\omega_k} e^{-ik \cdot (x-y)}
\]  
where \( \omega_k = \sqrt{k^2 + m^2} \). They satisfy the composition laws
\[
G^\pm = \pm G^\pm \circ G^\pm, \quad G^\pm \circ G^\mp = 0
\]
where here and in the remainder of this section \( \circ \) denotes the Klein-Gordon inner product (unless explicitly denoted otherwise). The causal Green function is defined by
\[
iG(x, y) = G^+(x, y) - G^-(x, y)
\]
Its main property is that it propagates all solutions to the Klein-Gordon equation
\[
\phi = iG \circ \phi
\]
It also obeys the composition law
\[
G = iG \circ G
\]
The Hadamard function is defined by
\[
G^{(1)}(x, y) = G^+(x, y) + G^-(x, y)
\]
and obeys the composition laws,
\[
G^{(1)} = iG \circ G^{(1)} = iG^{(1)} \circ G, \quad G = -iG^{(1)} \circ G^{(1)}
\]
All of the above are solutions to the Klein-Gordon equation.

The Feynman Green function is
\[
iG_F(x, y) = \theta(x^0 - y^0)G^+(x, y) + \theta(y^0 - x^0)G^-(x, y)
\]
and satisfies
\[
(\Box + m^2) G_F(x, y) = -\delta^{(4)}(x - y)
\]
It obeys the composition laws
\[ G_F = iG_F \circ G_F \] (3.10)

Also of interest is the Newton-Wigner propagator
\[ G_{NW}(x, x^0, y, y^0) = \frac{1}{(2\pi)^3} \int d^3 k \ e^{-ik \cdot (x-y)} \] (3.11)
which is the propagator associated with the positive square root of the Klein-Gordon equation
\[ i \frac{\partial \phi}{\partial x^0} = h\phi \] (3.12)
where \( h = \sqrt{-\nabla^2 + m^2} \). It is also useful to define a negative frequency Newton-Wigner propagator, given by (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
\[ G_{NW}(x, y) = 2i \frac{\partial}{\partial x^0} G^+(x, y) = -2i \frac{\partial}{\partial y^0} G^+(x, y) \] (3.13)

Some of these Green functions can be obtained from a path integral of the form (1.15), (1.16). An unrestricted sum with \( T \) integrated over an infinite range yields the Hadamard function \( G^{(1)} \). (See Fig(3.1)). A half-infinite range, \( 0 \leq T < \infty \), yields \( iG_F \), where \( G_F \) is the Feynman Green function. (See, for example, Ref.[31]). The Newton-Wigner propagator can also be obtained from (1.15), (1.16) 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.(3.2)). More details of this construction are discussed in Sections 5 and 6. (See also Ref.[30]).

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.(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 (1.7). For suppose we have a solution $\phi = \phi^+ + \phi^-$. Then

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

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

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

$$= iG \circ_{KG} \phi$$ \hspace{1cm} (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.[30] that there is no path integral of the form (1.15), (1.16) 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.[16]). We take it to be of the form (1.14). We take a fixed pure initial state and sum over a complete set of final states. This gives

$$D(\alpha, \alpha') = \sum_{\psi_f} (\psi_f \circ I C_\alpha \circ I \psi)(\psi_f \circ I C_{\alpha'} \circ I \psi)^*$$ \hspace{1cm} (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

$$\sum_{\psi_f} \psi_f^*(x)\psi_f(y) = G^{(1)}(x, y)$$ \hspace{1cm} (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

$$D(\alpha, \alpha') = \psi^* \circ I C_\alpha^\dagger \circ I C_\alpha \circ I \psi$$  \hspace{1cm} (3.17)

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

$$p(\alpha) = D(\alpha, \alpha') = \sum_{\alpha'} D(\alpha, \alpha')$$

$$= \psi^* \circ I C_\alpha \circ I \psi$$  \hspace{1cm} (3.18)

In the KG quantization, the induced inner product becomes the modified KG inner product (1.7), 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.

\section*{4. AN OPERATOR APPROACH FOR THE KLEIN-GORDON EQUATION}

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

$$H = p_0^2 - \mathbf{p}^2 - m^2 = 0$$  \hspace{1cm} (4.1)

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

$$[x^\mu, p^\nu] = -i\eta^{\mu\nu}$$  \hspace{1cm} (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(B). Following Eq. (1.8), the operator expressing this question is

\[ X^k = \int_{-\infty}^{\infty} ds \left\{ \frac{dx^0(s)}{ds}, \delta(x^0(s) - \tau) \right\} x^k(s) \quad (4.3) \]

where \( \{ , \} \) denotes the anticommutator, and we have

\[ x^0(s) = x^0 + p^0 s \quad (4.4) \]
\[ x^i(s) = x^i + p^i s \quad (4.5) \]

The object of interest is therefore given by

\[ X^k = x^k - \frac{p^k}{2} \left\{ \frac{1}{p^0}, (x^0 - \tau) \right\} \quad (4.6) \]

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 [14]).

We choose a momentum representation, in which

\[ x^k \rightarrow -i \frac{\partial}{\partial p_k}, \quad x^0 \rightarrow -i \frac{\partial}{\partial p^0} \quad (4.7) \]

and \( X^k \) is

\[ X^k = \left( -i \frac{\partial}{\partial p_k} + i \frac{p^k}{p^0} \frac{\partial}{\partial p^0} - i \frac{p^k}{2(p^0)^2 p^0} + \frac{p^k \tau}{p^0} \right) \quad (4.8) \]

(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 Eq. (1.4). The eigenstates of \( X^k \) are the functions

\[ f(p) = \frac{1}{(2\pi)^{3/2}(2p^0)^{1/2}} e^{ip^0(\tau - i\mathbf{p} \cdot \mathbf{x})} g(p \cdot p) \quad (4.9) \]
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 $\langle p|p'\rangle = \delta^{(4)}(p - p')$), the eigenstates of $X^i$ may be written

$$|x, \tau\rangle = \frac{1}{(2\pi)^{3/2}} \int d^4p (2p^0)^{1/2} e^{i\vec{p}\cdot\vec{x}} \delta(p^2 - m^2) |p\rangle$$

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

$$= |x, \tau+\rangle + i|x, \tau-\rangle$$

(4.10)

(The factor of $i$ in the negative frequency term, not present in other definitions of these states [32,30], 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 according to

$$\langle p^\pm|p'^\pm\rangle = 2\omega_p \delta(p - p')$$

and also $\langle p^\pm|p'^+\rangle = 0$. The states $|x, \tau\rangle$ are the Newton-Wigner states [22]. They are orthogonal at equal times, and satisfy the completeness relation

$$1 = \int d^3x |x, \tau+\rangle\langle x, \tau+| + \int d^3x |x, \tau-\rangle\langle x, \tau-|$$

(4.12)

The probability of entering a region $\Delta$ at time $\tau$ is given by

$$P_\Delta = \int_\Delta d^3x |\langle x, \tau+|\psi\rangle|^2 + \int_\Delta d^3x |\langle x, \tau-|\psi\rangle|^2$$

(4.13)

where the states $\psi^\pm(x, \tau) = \langle x, \tau \pm |\psi\rangle$ obey the Klein-Gordon equation and its positive/negative square root, and are normalized in a Schrödinger inner product.

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

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

(4.14)
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 [22], which is, on the surface \( x^0 = 0 \), in the momentum representation

\[
X_{NW}^k = -i \frac{\partial}{\partial p_k} - \frac{p^k}{2\omega_p^2} \tag{4.15}
\]

This is in fact the same as the operator

\[
\int d^3x \, |x, \tau+\rangle \, x^k \langle x, \tau+| \tag{4.16}
\]

with \( \tau = 0 \), in terms of the Newton-Wigner states above. Eq.(4.15) is not the same as (4.6), since the constraint holds in Eq.(4.15), but has not yet been imposed in Eq.(4.6). Eq.(4.15) is, however, the same as Eq.(4.14), with \( \tau = 0 \), once one recognizes that the inner product structure (4.11) requires the replacement

\[
x^k \to -(2\omega_p)^{1/2} i \frac{\partial}{\partial p_k} \frac{1}{(2\omega_p)^{1/2}} = -i \frac{\partial}{\partial p_k} - \frac{p^k}{2\omega_p^2} \tag{4.17}
\]

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

\[
|x\rangle = \frac{1}{(2\pi)^{3/2}} \int_{p_0=\omega_p} d^3p \, e^{ip \cdot x} \, |p+\rangle + \frac{1}{(2\pi)^{3/2}} \int_{p_0=-\omega_p} d^3p \, e^{ip \cdot x} \, |p-\rangle \tag{4.18}
\]

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

\[
\langle x|y \rangle = G^{(1)}(x, y) \tag{4.19}
\]

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

\[
1 = i \int d^3x \left( |x+\rangle \hat{T}_0 \langle x + | - |x-\rangle \hat{T}_0 \langle x - | \right) \tag{4.20}
\]
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

$$p_\Delta = i \int_{\Delta} d^3x \left( \phi^*_+ \frac{\partial}{\partial x^0} \phi_+ - \phi^*_- \frac{\partial}{\partial x^0} \phi_- \right)$$

(4.21)

The states $\phi_\pm(x) = \langle x | \pm | \phi \rangle$ 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 $\Delta = IR^3$ this expression becomes the norm of $\phi$ in the induced inner product, as required.

5. DECOHERENT HISTORIES ANALYSIS

IN THE KLEIN-GORDON QUANTIZATION

We now come to the main point of this paper 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.(4.21), and we consider the NW quantization and Eq.(4.13) in Section 6.

The decoherence functional is given by Eq.(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). However, in order to tackle a subtlety first noted in Section 1 concerning the definition of the class operators, we first need to consider a simpler question.
5(A). 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 $x'$ to $x''$ which never cross a given spacelike surface. (See Fig.(5.1)). 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 $x^0 = \tau$. 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 $x^0 = \tau$, 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 $x^0 = \tau$ is easily constructed using the path integral representations(1.15), (1.16). We take $T$ to have an infinite range and we sum over all paths which never cross the surface. In Ref.[30] 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,

$$
C_r(x'', x') = \left( \theta(x'^0 - \tau)\theta(x'^0 - \tau) + \theta(\tau - x'^0)\theta(\tau - x'^0) \right) \\
\times \left( G^{(1)}(x'', x') - G^{(1)}(\tilde{x}'', \tilde{x}') \right) 
$$

(5.1)

where $\tilde{x}$ denotes the reflection of the point $x$ about $x^0 = \tau$, that is,

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

(5.2)
$C_r$ vanishes on $x^0' = \tau$ and $x^0'' = \tau$. 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 $C_r$ does not satisfy it,

$$\left(\Box + m^2\right)C_r(x'', x') = 2\delta(x^{0''} - \tau) \epsilon(x^{0'} - \tau) \partial_0 G^{(1)}(\tau, x''|x^{0'}, x')$$  \hspace{1cm} (5.3)$$

where $\epsilon(x)$ is the signum function. This is the difficulty with the path integral-defined class operators mentioned in Section 1. The sum over paths which always cross $x^0 = \tau$, which we denote $C_c(x'', x')$, is constructed using the relation

$$G^{(1)}(x'', x') = C_c(x'', x') + C_r(x'', x')$$  \hspace{1cm} (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 (1.15), (1.16) 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.[1,33].

Note also that we have now encountered two potential difficulties which are not obviously related: firstly, the possibility of a physically unreasonable result, and secondly, 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 [16], we will deal with this issue by replacing $C_r$ by another object $C'_r$ which satisfies the most important boundary conditions defining $C_r$ but which also satisfies the constraint everywhere. The boundary conditions satisfied by $C_r$ 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), \( C_r' \) coincides with (the non-zero) \( C_r \) 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

\[
C_r'(x'', x') = 0
\] (5.5)

This is because for fixed \( y \), \( C_r'(x'', x') \) is zero for all values of \( x'' \) on the opposite side of the surface to \( x' \). This means that both \( C_r' \) 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 \( C_r' = 0 \). The only way of getting a non-zero results 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.(5.1).

The conclusion (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.

5(B). 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 (1.15), (1.16) 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 [34,30]. For a propagator of the non-relativistic form (1.16), it implies that when \( x'' \) and \( x' \) are on opposite sides of the surface of constant \( x^0 \), we have

\[
g(x'', T|x', 0) = 2i \epsilon(\tau - x^0') \int_0^T dt_c \int d^3x \ g(x'', T|x, t_c) \overset{\rightarrow}{\partial_0} g(x, t_c|x', 0)
\]

This formula is obtained by partitioning the paths in the sum over histories (1.16) according to the parameter time \( t_c \) and position \( x \) at which they cross the surface of constant \( x^0 \) for the first time\(^\dagger\). (See Fig.(5.2)). If we partition according to the last crossing, we get

\[
g(x'', T|x', 0) = -2i \epsilon(x''^0 - \tau) \int_0^T dt_c \int d^3x \ g(x'', T|x, t_c) \overset{\leftarrow}{\partial_0} g(x, t_c|x', 0)
\]

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

\[
g(x'', T|x', 0) = g_r(x'', T|x', 0)
\]

\[+ 2i \epsilon(\tau - x^0') \int_0^T dt_c \int d^3x \ g(x'', T|x, t_c) \overset{\rightarrow}{\partial_0} g(x, t_c|x', 0)
\]

(for the first crossing and

\[
g(x'', T|x', 0) = g_r(x'', T|x', 0)
\]

\[\quad - 2i \epsilon(x''^0 - \tau) \int_0^T dt_c \int d^3x \ g(x'', T|x, t_c) \overset{\leftarrow}{\partial_0} g(x, t_c|x', 0)
\]

\(^\dagger\) 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 \( \partial_0 g_r = 2\partial_0 g \), which is what is used in Eq.(5.6). See Ref.[30] for more details.
for the last crossing, where \( g_r \) denotes the restricted propagator given by a sum over paths which never cross the surface. The formulae (5.6)–(5.9) imply that the sum over paths which cross the surface is given by either (5.6) or (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.[30] 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 \( d^3x \) integration to the region \( \Delta \).

**5(C). 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

\[
C_{\Delta}(x'', x') = \int_{-\infty}^{\infty} dT \, g_{\Delta}(x'', T|x', 0)
\]  

(5.10)

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,

\[
g_{\Delta}(x'', T|x', 0) = 2i \epsilon(\tau - x^0') \int_0^T dt_c \int_{\Delta} d^3x \, g(x'', T|x, t_c) \frac{\partial}{\partial t_c} G_{F}(x, t_c|x', 0)
\]  

(5.11)

(See Fig.(5.3)). This is valid for \( x'', x' \) on either the same or opposite sides of the spacelike surface. Inserting in Eq.(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.[30] for more details), this yields,

\[
C_{\Delta}^f(x'', x') = -2i \epsilon(\tau - x^0') \int_{\Delta} d^3x \left[ G_{F}(x'', x) \frac{\partial}{\partial t_c} G_{F}(x, x') - G_{F}^*(x'', x) \frac{\partial}{\partial t_c} G_{F}^*(x, x') \right]
\]  

(5.12)
This is the formula for first crossing the region $\Delta$ for all end-points. It is also conveniently written,

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

(5.13)

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

$$C_\ell^\Delta(x'',x') = 2i \epsilon(x'' - \tau) \int_\Delta d^3x \left[ G_F(x'',x) \partial_0 G_F(x,x') - G^*_F(x'',x) \partial_0 G^*_F(x,x') \right]$$

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

(5.14)

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

$$\epsilon(x'' - \tau) \epsilon(\tau - x') = 1$$

(5.15)

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

$$C^\Delta(x'',x') = \frac{1}{2} \left( C_f^\Delta(x'',x') + C_\ell^\Delta(x'',x') \right)$$

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

$$= i \int_\Delta d^3x \left( G^+(x'',x) \partial_0 G^+(x,x') - G^-(x'',x) \partial_0 G^-(x,x') \right)$$

(5.16)

It is then readily confirmed, using the properties Eq.(3.2) and (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,
when \( x'' \) is in \( \Delta \) and zero otherwise. Note that Eq.(5.3) and Eq.(5.17) are consistent, since
\[ C_\Delta + C_r = G^{(1)} \] when \( \Delta = IR^3 \), and \( G^{(1)} \) satisfies the constraint. As in Section 5(A), 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, however, clear in this case how to proceed. From the above that the obvious candidate is to take \( C'_\Delta \) to be given by Eq.(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 \( \Delta = IR^3 \), it is equal to \( G^{(1)} \), so 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.

We 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 state \( \psi = \psi_+ + \psi_− \). The off-diagonal terms of the decoherence functional are

\[
D(\Delta, \bar{\Delta}) = \psi^* \circ I \left( C'_\Delta \right)^\dagger \circ I C'_\Delta \circ I \psi
\]  

(5.18)

We have

\[
C'_\Delta \circ I \psi = i \int_{\Delta} d^3x \left( G^+(x'', x) \hat{\partial}_0 \psi_+(x) + G^-(x'', x) \hat{\partial}_0 \psi_-(x) \right)
\]  

(5.19)

so the decoherence functional is

\[
D(\Delta, \bar{\Delta}) = \int_{\Delta} d^3x \int_{\Delta} d^3y \left( \psi^+_+(y) \hat{\partial}_0 G^+(y, x) \hat{\partial}_0 \psi_+(x) + \psi^+_-(y) \hat{\partial}_0 G^-(y, x) \hat{\partial}_0 \psi_-(x) \right)
\]  

(5.20)

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

$$\psi^* \circ I C'_\Delta \circ I \psi = i \int_\Delta d^3x \left( \psi^*_+ (x) \frac{\partial}{\partial 0} \psi_+(x) - \psi^*_- (x) \frac{\partial}{\partial 0} \psi_-(x) \right)$$

(5.21)

This is exactly the expected answer, coinciding with Eq.(4.21), although recall that the probabilities are only approximately defined because of approximate decoherence.

5(D). A 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.(5.10), which were defined using path integrals in a simple and obvious way.

Consider first, therefore, the question of why the expressions (5.10) and (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 (5.10) fails to satisfy the constraint at $x''$ 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

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

(5.22)
Now we note that
\[
\int_{-\infty}^{\infty} dt_c \, \epsilon(t_c) \, g(x, t| x', 0) = iG_F(x, x') + iG_F^*(x, x') = i\epsilon(\tau - x'^0) \, G(x, x')
\]
(5.23)

(where recall $x^0 = \tau$). Furthermore, we have that
\[
\partial_0 \left( \epsilon(\tau - x'^0) \, G(x, x') \right) = \epsilon(\tau - x'^0) \, \partial_0 G(x, x')
\]
(5.24)
since $G(x, x')$ vanishes when $\tau = x'^0$. The modified class operator is therefore
\[
C'_\Delta(x'', x') = -2 \int_\Delta d^3 x \, G^{(1)}(x'', x) \, \partial_0 G(x, x')
\]
(5.25)

which, apart from the factor of 2, coincides with the first term in Eq.(5.13). It is easy to see that the second term in Eq.(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,
\[
2i \, \epsilon(\tau - x'^0) \int_{-\infty}^{\infty} dT \, \epsilon(T - t_c) \int_{-\infty}^{\infty} dt_c \int_\Delta d^3 x \, g(x'', T| x, t_c) \, \partial_0 g(x, t_c| x', 0) = -2 \int_\Delta d^3 x \, G(x'', x) \, \partial_0 G^{(1)}(x, x')
\]
(5.26)

Hence averaging these two results gives the class operator Eq.(5.13), but crucially, without the $\epsilon$ factors that cause (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 (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.(5.22), (5.26). The two methods are equivalent for the simple model of this paper. 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.

Theses issues concerning modified class operators will be taken up in more detail in Ref.[27].

5(E). A Multiple Crossings Decomposition?

The results of Section 5(C) 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.(4.21). 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.(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 $\Delta = IR^3$. We thus obtain

$$G^+(x'', x') = 2i \int d^3x \ G^+(x'', x) \partial_0 G^+(x, x')$$ (5.27)

(averaged with the last crossing PDX this gives the composition law in Eq.(3.2)). From Section 3 we also have that

$$2i \partial_0 G^+(x'', x') = G_{NW}(x'', x')$$ (5.28)
and Eq.(5.27) becomes

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

(5.29)

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.(3.2)). Similarly, one can see from the last crossing PDX Eq.(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.(5.4)). This is in fact again the Newton-Wigner propagator \( G_{NW}(x, x') \), as may be seen from Eq.(3.13), and we may write

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

(5.30)

Using these two relations, we may carry out an iteration of Eq.(5.29) to yield

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

(5.31)

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.(5.5)).

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.(5.29) or Eq.(5.30) to the propagator \( G^+(x_2, x_1) \). The point is 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 [23], 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 at variance with the path decomposition expansion, Eq.(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.

6. THE NEWTON-WIGNER CASE

Consider now the question of how to obtain the Newton-Wigner probability Eq.(4.13) 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.(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

\[ C_\Delta(x'', x') = \int_\Delta d^3x \ G_{NW}(x'', x, \tau) \ G_{NW}(x, \tau, x') \]  (6.1)

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

\[ G_{NW}(x'', x') = \int d^3x \ G_{NW}(x'', x, \tau) G_{NW}(x, \tau, x') \]  (6.2)

Inserting in the decoherence functional (3.17), it is readily shown this gives exact decoherence, and the probabilities coincide with Eq.(4.13) (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,

\[ G_{NW}(x, x^0|y, y^0) = \langle x, x^0|y, y^0 \rangle \]  (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 (6.1). The first is the one of the standard non-relativistic form:

\[ G(x'', \tau'', x', \tau') = \int \mathcal{D}x \mathcal{D}p \exp \left( i \int_{\tau'}^{\tau''} dx^0 \left[ p \cdot \frac{dx}{dx^0} - \sqrt{p^2 + m^2} \right] \right) \]  (6.4)

(The configuration space form of this path integral may also be considered, but the measure is then rather complicated [32]). 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 (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 (1.15), (1.16), in which the paths summed over do not cross the final surface except to end on it at \( x'' \), depicted in
Fig.(3.2). (See also Refs.[23,30]). Equivalently, they can be restricted so that they start at the initial point \( x' \) but do not cross it thereafter (see Fig.(5.4)). In fact, it is easy to show from these representations, using Eq.(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.(5.6). 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.(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 5(D) 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 5(D) 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.

7. SUMMARY AND DISCUSSION

This paper is a first step in 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 paper is the derivation of the probability formula Eq.(5.21) (or Eq.(4.21)) 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 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 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.(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.(3.12). The comparison with this case has, however, proved quite useful in the present paper. Furthermore, here, our starting point for an operator quantization was the evolving constants method, based on Eq.(1.8), 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 [14,15]). We also note that we find agreement between the operator methods of Section 4 and the decoherent histories results of Sections 5 and 6.

We may now return to the discussion initiated at the end of Section 2, on the relationship 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 approximate 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 speaking, 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.

These issues concerning multiple crossings become more complicated in non-trivial quantum cosmological models where typically even the classical paths have multiple surface crossings. This will be pursued elsewhere [27].

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Figure 3.1 The propagators $G^{(1)}(x'', x')$ and $G_F(x'', x')$ are obtained by a path integral of the form (1.15), (1.16), 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 3.2 The Newton-Wigner propagator $G_{NW}(x'', x')$ may be obtained by a path integral of the form (1.15), (1.16), 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 5.1 The class operator $C_{r}(x'', x')$ 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 5.2 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 5.3 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 5.4 A second representation of the Newton-Wigner propagator $G_{\text{NW}}(x'', x')$ may be obtained by a path integral of the form (1.15), (1.16), 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 5.5 The path integral representation of Eq.(5.31). 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 $G^+(x_1, x_2)$. 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 5.6 A more general path integral representation of the Newton-Wigner propagator $G_{NW}(x'', x')$. In the path integral expressions (1.15), (1.16), 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.(3.2) and Fig.(5.4)) in the limit that the intermediate surface tends to the final or initial surface.