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Quantum Mechanics for Totally Constrained Dynamical Systems and Evolving Hilbert Spaces

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We analyze the quantization of dynamical systems that do not involve any background notion of space and time. We give a set of conditions for the introduction of an intrinsic time in quantum mechanics. We show that these conditions are a generalization of the usual procedure of deparametrization of relational theories with Hamiltonian constraint that allow one to include systems with an evolving Hilbert space. We apply our quantization procedure to the parametrized free particle and to some explicit examples of dynamical systems with an evolving Hilbert space. Finally, we conclude with some considerations concerning the quantum gravity case.

1. INTRODUCTION

The concept of time enters in the basic formalism of quantum mechanics in two ways: to mark the evolution of the system and to order a sequence of measurements. In terms of von Neumann's (1955) axiomatic formulation, time enters as an evolution-labeling parameter in axiom IV, through the evolution equation (Schrödinger equation) and implicitly in axiom II through the possible dependence of the operators corresponding to observables on time. On the other hand, time appears as a sequence-ordering label in axiom V, through the fact that the outcome of a measurement depends on previous measurements. Furthermore, this time parameter is assumed to be given in advance. The picture that we get is a unit vector in a Hilbert space (which depends on the system and is given once and forever, following axiom I) with a smooth time evolution generated by the Hamiltonian operator via the Schrödinger equation with discontinuous leaps corresponding to measurements.

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The Dirac (1964) quantization procedure for constrained systems does not introduce major changes in this picture, considering that it assumes the existence of a nonvanishing Hamiltonian in addition to the set of constraints, and a standard Schrödinger equation with that Hamiltonian. There exists, however, a wide class of models for which, at the end of the application of the usual rules of thumb of quantization, one is left only with a set of constraint equations (in addition, of course, to the commutation algebra of the fundamental dynamical variables), with neither a nonzero Hamiltonian nor a natural choice of a time parameter. This situation is characteristic, for instance, of reparametrization-invariant systems (Sundermeyer, 1982), sometimes called generally covariant systems. The example of greatest physical interest of this kind of theory is undoubtedly general relativity, where the problem is known as "the issue of time" (Kuchar, 1992a; Isham, 1992).

Our aim in this paper is twofold. First we propose the necessary changes in the standard formalism of quantum mechanics in order to deal with the above-mentioned kind of systems, which we will call "totally constrained systems." This involves putting forward a prescription to slice the representation space in which we will realize the commutation algebra of the dynamical variables into equal "time" spaces as well as defining this "time." Then we will explore the logical possibility of the slices being nonisomorphic. This could be considered, from the point of view of standard quantum mechanics, as a change in time or evolution of the Hilbert space describing the system.

The motivation to consider the possibility of "evolving Hilbert spaces" comes from the suggestion due to Unruh (1993) that quantum gravity should have this property. The main point of his argument is the following: Does the Big Bang theory for the origin of the universe mean that because there was less space early, there were also fewer physical attributes that the universe had? His answer is yes and it is based on the fact that there should be some limit at the Planck length to the number of different values that any field could take. If this observation is true, one should describe the universe with a finite-dimensional Hilbert space and a set of operators which both change in time.[3] This proposal seems to be very appealing both from a physical and philosophical point of view. In fact in a description of the universe in terms of fixed Hilbert space, the set of possible behaviors of the universe is fixed at all times from the very beginning. That means that the state that describes the present behavior of the universe with its enormous complexity was a vector of the Hilbert space since the Big Bang. In practice the observed evolution from the simple to the complex is nothing but the evolution between different possible behaviors. In quantum mechanics a system is identified

[3] A similar proposal was made by Jacobson (1991).

with its Hilbert space, the set of all its possible behaviors (states). Hence, in this picture, the universe is given once and for all.

Furthermore, if the Hilbert space is fixed, the initial conditions of the universe are not determined by its dynamical laws and the actual initial conditions remains completely unexplained. Hartle (1991) has stressed the reasons for searching for a theory for the initial conditions of the universe. Initial conditions are crucial to explain the large-scale homogeneity and isotropy of the universe, its approximate spatial flatness, the spectrum of density fluctuations, the homogeneity of the arrow of time, and the existence of a classical space-time.

Of course, usual quantum mechanical systems, such as particles, are described by a fixed set of attributes such as position and momentum and a fixed Hilbert space, but for these systems we have no reason to expect different behaviors for different times, and in principle any conceivable initial state may be prepared by measuring a suitable complete set of commuting observables.

In this work, as we said before, we are interested in the identification of an intrinsic time in totally constrained dynamical systems. We shall give a set of conditions for the definition of a physical time that generalize the usual deparametrization procedure. We shall see that the introduction of a physical time in these systems naturally leads to the possibility of evolving Hilbert spaces.

Some systems that usually require the introduction of a nonpositive-definite inner product or a decomposition between positive- and negative-frequency states may now be quantized in terms of a positive-definite inner product with an evolving Hilbert space. In general, evolving Hilbert spaces seem to be naturally related to systems with boundaries or involving operators that satisfy a noncanonical algebra.

As noticed by Unruh, evolving Hilbert spaces are naturally related to systems with a finite number of degrees of freedom. In fact, in the infinite-dimensional case, it is always possible to describe the system in terms of a fixed Hilbert space, but we shall prove that in this case relational systems may behave as the continuum limit of systems with a finite-dimensional evolving vector space. In particular, the transition amplitudes will remain invariant while the system evolves into the future, but the system will not be invariant under time reversal, and the evolution will not be unitary. We shall call this kind of infinite-dimensional system an evolving system.

In Section 2 we introduce a description of the quantum mechanics of totally constrained dynamical systems and show that this description naturally generalizes the quantization procedure of deparametrizable systems. In Section 3 we apply this description to three examples: The parametrized classical free particle, a finite-dimensional constrained system with an evolving vector space of states, and an infinite-dimensional evolving system associated with the Klein–Gordon model.

Finally, in Section 4, we make some remarks concerning the application of this procedure to the quantum gravity case.

2. TIME AND QUANTIZATION OF TOTALLY CONSTRAINED DYNAMICAL SYSTEMS

We will assume that we have, in general, as the outcome of a standard Hamiltonian formulation of the theory under study a set of constraint equations

$$\phi_i(q_a) = 0 \qquad \text{with} \quad i = 1, \ldots, n + 1 \tag{1}$$

written in terms of the dynamical variables q_a, with $a = 1, \ldots, f$, of the theory as well as the commutation (or anticommutation) algebra of these variables

$$[q_a, q_b]_\pm = \alpha^c_{ab} q_c + \beta_{ab} \tag{2}$$

Notice that if

$$\alpha^c_{ab} = 0 \tag{3}$$

$$\beta_{ab} = i \tag{4}$$

then q_a and q_b are canonically conjugated variables. From the algebra of the q's follows the algebra of the constraints

$$[\phi_i, \phi_j]_\pm = f^k_{ij}(q_a)\phi_k \tag{5}$$

which we assume closed (or the constraints to be first class), but allowing the "structure constants" to depend on the q's. We will assume furthermore that one of the constraints is singled out (as in concrete examples) from a physical point of view or considerations from the classical theory as containing implicitly the information about the time evolution of the system, and we will call it the *Hamiltonian constraint* $\mathcal{H}$. We will call the remaining n constraints *kinematic constraints* $\mathcal{D}_i$.

In order to have a sensible quantum theory from the previous information we need to follow several steps.

The first ones, more or less straightforward, are:

1. To find a vector space $\mathscr{E}_R$, which we will call *representation space*, in which realize the algebra of the q's.

2. To construct the subspace $\mathscr{E}_K$, which we will call *kinematic space*, given by the solutions $|\psi_K\rangle$ of the whole set of kinematic constraints

$$\mathcal{D}_i|\psi_K\rangle = 0 \tag{6}$$

3. To construct the subspace $\mathscr{E}_F$, which we will call *physical space*, given by the solutions $|\psi_F\rangle$ of the whole set of constraints

$$\mathcal{D}_i | \psi_F \rangle = 0 \tag{7}$$

$$\mathcal{H} | \psi_F \rangle = 0 \tag{8}$$

At this point we will consider a function $T(q_a)$ of the dynamical variables and we will discuss which conditions should be satisfied by this function in order for it to be considered a time variable for the system.

I. The first condition that we will require is

$$[T, \mathcal{D}_i] = 0 \qquad \text{and} \qquad [T, \mathcal{H}] \neq 0 \tag{9}$$

The vanishing of the commutator between T and $\mathcal{D}_i$ implies that T is a well-defined operator in $\mathcal{E}_K$ ($T | \psi_K \rangle \in \mathcal{E}_K$), while the nonvanishing of the commutator between the Hamiltonian constraint and T, together with conditions III and IV, ensures that the Hamiltonian restricts the evolution in t of the wavefunctions. This condition is not independent of the other conditions. In fact, if the Hamiltonian commutes with T, condition IV obviously fails.

II. We will require that the eigenvectors of T span the kinematic space $\mathcal{E}_K$. In other words, there exist a basis $|x, t\rangle$ of $\mathcal{E}_K$ such that

$$T | x, t \rangle = t | x, t \rangle \tag{10}$$

where the x corresponds to additional labels necessary to characterize the vector unambiguously.

We shall consider the vector space $\mathcal{E}_{Kt}$ defined as the subspace of $\mathcal{E}_K$ spanned by $|x, t\rangle$ for a given t. One can define an analogous vector space $\mathcal{E}_{Ft}$ with the projection of the vectors of the physical space

$$| \psi_F \rangle = \sum_{xt} \psi_{Ft}(x, t) | x, t \rangle \tag{11}$$

for a given t

$$| \psi_F, t \rangle = \sum_{x} \psi_{Ft}(x, t) | x, t \rangle \tag{12}$$

$\mathcal{E}_{Ft}$ may be considered as the projection of $\mathcal{E}_F$ on $\mathcal{E}_{Kt}$. We will introduce evolving systems by considering the logical possibility that the components of a given $\psi_F(x, t)$ of vectors in the physical space $|\psi_F\rangle$ might vanish identically for $t < t_0$. Thus, one may classify these vectors by the value t_0. We shall say that $|\psi'^0_F\rangle$ is from level t_0 if and only if

$$\psi'^0_F(x, t) \equiv 0 \qquad \forall t < t_0$$

We will consider now the operators $O_i(q_a)$ in $\mathcal{E}_K$ that commute with all the constraints (including the Hamiltonian constraint). Following Kuchar, we shall call these operators perennials.

III. The next condition that we are going to require is that there exist a subset of $\mathscr{E}_{Kt}$, denoted $\mathscr{E}^{*}_{Kt}$, with a positive-definite inner product

$$\langle \psi_K | \phi_K \rangle_t = \sum_x \psi^{*}_K(x, t)\phi_K(x, t)\mu(x, t) \tag{13}$$

and that there is a set of perennials such that:

(a) They are self-adjoint with this inner product, provided their classical counterpart be real, and commute with T, $[T, O_i] = 0$.

It follows that this subset of operators does not mix vectors lying in different time sections, which implies that they are block diagonal in $\mathscr{E}_K$; in other words,

$$O_i \mathscr{E}_{Kt} \subseteq \mathscr{E}_{Kt} \tag{14}$$

and

$$O_i \mathscr{E}_{Ft} \subseteq \mathscr{E}_{Ft} \tag{15}$$

(b) Their eigenvectors in $\mathscr{E}_{Ft}$; labeled by $|\psi'^{\alpha}_{F_\alpha}, t\rangle$, satisfy

$$O_i |\psi'^{\alpha}_{F_{\alpha_i}}, t\rangle = \alpha_i |\psi'^{\alpha}_{F_{\alpha_i}}, t\rangle \tag{16}$$

for any t and α_i independent of t.

The eigenvectors corresponding to different eigenvalues are orthogonal.

(c) Their restriction to $\mathscr{E}_{Ft}$ is a complete set of commuting observables (CSCO).

We impose that the inner product in $\mathscr{E}^{*}_{Ft}$ (induced by the inner product in $\mathscr{E}^{*}_{Kt}$) is such that the eigenvectors of the perennial operators satisfy the orthonormality condition

$$\langle \psi'^{\alpha}_{F\alpha} | \psi'^{\beta}_{F_\beta} \rangle_t = \theta(t - t_\alpha)\theta(t - t_\beta)\delta_{\alpha\beta} \tag{17}$$

where $\theta(t - t_\alpha)$ is the Heaviside function.

Notice that a basis in $\mathscr{E}^{*}_{Ft}$ includes all the vectors $|\psi'^{\alpha}_{F_\alpha}\rangle$ of level less than or equal to t.

We are going to be interested in considering as physical observables, not only constants of the motion, but more general operators. We shall call an operator A an observable if and only if

$$[A, \mathscr{D}_i] = [A, T] = 0 \tag{18}$$

and therefore A is block diagonal in $\mathscr{E}_K$, A is self-adjoint with respect to the inner product, and the eigenvectors of A expand $\mathscr{E}_{Kt}$. Notice that while we have required that any perennial commuting with T is self-adjoint, here one may have classical real dynamical variables that are not associated with a self-adjoint operator and consequently they are not observables.

IV. The last property that we shall require for our time variable is that

$$\mathscr{E}^*_{Kt} \equiv \mathscr{E}^*_{Ft} \tag{19}$$

This condition essentially implies that the Hamiltonian constraint determines the evolution of the states, but it does not restrict their functional dependence at a given t.

In general, $A\,|\psi_F\rangle$ will not be an element of $\mathscr{E}_F$. However, condition IV allows us to determine a vector of the physical space that coincides in $\mathscr{E}_t$ with any eigenvector of A. Let

$$A\,|a_\mu, t\rangle = a_\mu(t)\,|a_\mu, t\rangle \tag{20}$$

Then the restriction of the physical state

$$|\psi_F(a_\mu, t_0)\rangle = \sum_{\substack{\alpha \\ t_\alpha \le t_0}} \langle \psi'^{\alpha}_{F_\alpha}\,|\,a_\mu, t_0\rangle_{t_0}\,|\psi'^{\alpha}_{F_\alpha}\rangle \tag{21}$$

to $\mathscr{E}_{Kt_0}$ is equal to $|a_\mu, t_0\rangle$, and then

$$\langle x, t\,|\,a_\mu, t\rangle = \sum_{\substack{\alpha \\ t_\alpha \le t}} \langle x, t\,|\,\psi'^{\alpha}_{F_\alpha}\rangle_t \langle \psi'^{\alpha}_{F_\alpha}\,|\,a_\mu, t\rangle_t \tag{22}$$

Notice that from condition III it follows that $|\psi_F(a_\mu, t_0)\rangle$ exists and is unique; therefore we know how to compute the transition amplitudes between the eigenvectors of two observables A and B at different times,

$$\langle b_\nu, t'\,||\,a_\mu, t\rangle = \sum_{\substack{\alpha \\ t_\alpha \le t}} \langle b_\nu, t'\,|\,\psi'^{\alpha}_{F_\alpha}\rangle_{t'} \langle \psi'^{\alpha}_{F_\alpha}\,|\,a_\mu, t\rangle_t \tag{23}$$

where we have introduced the notation $\langle\,||\,\rangle$ to distinguish the transition amplitudes from ordinary inner products at t. In another form we have

$$\langle b_\nu, t'\,||\,a_\mu, t\rangle = \langle \psi_F(b_\nu, t')\,|\,\psi_F(a_\mu, t)\rangle_{t'} \tag{24}$$

These amplitudes contain all the basic information required to determine the evolution of the system. Notice that within this context neither all the perennials are observables nor all the observables are perennials.

The state $|\psi_F(a_\mu, t_0)\rangle$ has been prepared by the measurement of the observable A at time t_0. Notice that two states prepared at times t_0 and t_1 are such that $\langle \psi_F(a_\mu, t_0)\,|\,\phi_F(b_\nu, t_1)\rangle$ is time independent for all $t \ge t_0$ and $t \ge t_1$; *this is the "unitarity" condition for an evolving system.*

In the next section, we shall see that these conditions define a natural extension of the deparametrizable systems.

3. DEPARAMETRIZABLE MODELS

In this section we want to determine the set of necessary and sufficient conditions that a totally constrained dynamical system should obey in order to be deparametrizable. We are going to prove that the set of conditions given in the previous section contains as a particular case the deparametrizable systems. Consequently our formalism may be considered as an extension of the usual quantization procedure for deparametrizable systems. In a deparametrizable model there is a (noncanonical) transformation leading from the original set of dynamical variables q_a to a new set of variables T, p_T, and k_a, $a = 1, \ldots, f - 2$, satisfying the algebra

$$[k_a, k_b]_\pm = \alpha^c_{ab} k_c + \beta_{ab} \tag{25}$$

$$[T, p_T]_- = i \tag{26}$$

$$[k_a, T]_- = [k_a, p_T]_- = 0 \tag{27}$$

such that the Hamiltonian constraint takes the form

$$\mathcal{H} = p_T + H(k_a, T) \tag{28}$$

The other kinematic constraints have the form

$$\phi_j(k_a, T) = 0 \tag{29}$$

Here we shall restrict our analysis to the case where the only constraint is the Hamiltonian constraint. The generalization of the following considerations to the case in which there is a set of time-independent kinematic constraints $\phi_j(k_a) = 0$ is straightforward.

From the algebra it follows that we can write the representation space as a tensor product of two spaces $\mathscr{E}_R \equiv \mathscr{E}_T \otimes \mathscr{E}_Q$ in which one realizes on one hand T and p_T and on the other hand the k_a. We will choose the basis

$$|x, t\rangle = |x\rangle |t\rangle \tag{30}$$

where x corresponds to the set of labels required to specify the vector in $\mathscr{E}_Q$. An arbitrary vector in $\mathscr{E}_R$ will be

$$|\psi\rangle = \sum_{xt} \psi(x, t) |x\rangle |t\rangle \tag{31}$$

A positive-definite inner product is introduced in $\mathscr{E}_Q$,

$$\langle \psi | \phi \rangle = \sum_x \psi^*(x, t) \phi(x, t) \tag{32}$$

such that H is a Hermitian operator in $\mathscr{E}_Q$.

The action of the operators will be

$$T\psi(x, t) = t\psi(x, t) \tag{33}$$

$$p_T\psi(x, t) = -i \frac{\partial}{\partial t} \psi(x, t) \tag{34}$$

$$k_a\psi(x, t) = \sum_{x'} (k_a)_{xx'}\psi(x', t) \tag{35}$$

With these definitions the Hamiltonian constraint

$$\mathcal{H} | \psi_F\rangle = [p_T + H(k_a, T)]|\psi_F\rangle = 0 \tag{36}$$

becomes a Schrödinger equation

$$-i \frac{\partial}{\partial t} \psi_F(x, t) + \sum_{x'} (H(t))_{xx'}\psi(x', t) = 0 \tag{37}$$

Such systems will have $f - 2$ constants of the motion (or perennials) $O_i(k_a, t)$ associated to the initial conditions of the system. They satisfy

$$\frac{i\,\partial O}{\partial t} - [H, O] = 0 \tag{38}$$

Now, a complete set of compatible perennials defines a nondegenerate basis on E_Q,

$$O_i(t_0) | \alpha_i\rangle = \alpha_i | \alpha_i\rangle \tag{39}$$

and

$$| \psi_F^{\alpha_i}, t\rangle = U(t, t_0) | \alpha_i\rangle | t_0\rangle \tag{40}$$

where U is the evolution operator in E_Q,

$$\frac{i\,\partial U}{\partial t} = HU \tag{41}$$

The vectors $| \psi_F^{\alpha_i}, t\rangle$ are eigenvectors of $O_i(t)$ with eigenvalues α_i and span the physical space. Thus, there is an isomorphism for any t_0 between the restriction $\mathscr{E}_F^* t_0$ and $\mathscr{E}_Q^*$ which is also isomorphic to $\mathscr{E}_F^* t_0$, spanned by $|x\rangle | t_0\rangle$. To conclude, in the case of a deparametrizable system, conditions I, II, and IV, hold while condition III is satisfied with the usual time-independent inner product and the eigenvectors of the complete set O_i obey the orthonormality conditions

$$\langle\psi_{F_{\alpha_i}} | \psi_{F_{\alpha_j}}\rangle_t = \langle\alpha_i | \alpha_j\rangle = \delta_{ij} \tag{42}$$

instead of (17). Thus, all the states are of the same level $t = t_I$, taken as the origin of time.

Let us now study the converse. Let $T(q)$ be a time variable satisfying conditions I–IV in the particular case that all the states are of level $t = t_l$ and let the inner product have the form (32). Let O_i be a complete set of observables with eigenvectors $|\psi_{F_\alpha}\rangle$ that form a complete basis on $\mathscr{E}^*_{F_t} = \mathscr{E}^*_{K_t}$ and therefore satisfy the closure relation

$$\sum_\alpha |\psi_{F_\alpha}, t\rangle\langle\psi_{F_\alpha}, t| = I_t \tag{43}$$

where I_t is the identity operator in $\mathscr{E}^*_{K_t}$. Given an arbitrary state $|\phi\rangle \in \mathscr{E}^*_{K_{t0}}$, there is a vector of the physical space $|\phi_F\rangle$

$$|\phi_F\rangle = \sum_\alpha |\psi_{F_\alpha}\rangle\langle\psi_{F_\alpha}|\phi\rangle_{t0} \tag{44}$$

such that $|\phi_F, t_0\rangle = |\phi\rangle$. That implies

$$\begin{aligned}\phi_F(x, t) &= \sum_\alpha \sum_{x'} \psi_{F_\alpha}(x, t)\psi^*_{F_\alpha}(x', t_0)\phi(x', t_0)\\ &= \sum_{x'} D(x, t; x', t_0)\phi(x', t_0)\end{aligned} \tag{45}$$

Making use of the orthonormality conditions (17) for vectors of level t_l, one can show that this relation is invertible. Thus one can write

$$\begin{aligned}i\frac{\partial\phi}{\partial t}(x, t) &= \sum_{x',x''} i\frac{\partial D}{\partial t}(x, t; x'', t_0)D(x'', t_0; x', t)\phi(x', t)\\ &= \sum_{x'} H_{xx'}\phi(x', t)\end{aligned} \tag{46}$$

It is immediate to show from (45), making use of (43) and (17), that the inner product is conserved, $\langle\psi|\phi\rangle_t = \langle\psi|\phi\rangle_{t0}$, and therefore the Hamiltonian H is Hermitic. Thus we recover the Schrödinger equation for a deparametrizable system. One can easily prove by making use of (46) and the definition of the perennial operators that they also satisfy the evolution equation (38). Consequently the set of conditions given in the previous section is a generalization of the usual quantization procedure for deparametrizable systems. In the next section we will show several examples of evolving systems.

4. APPLICATIONS

We now apply the set of conditions that we have just established to several systems that require an intrinsic definition of time. The first and simpler example is the parametrized free particle in 1 + 1 dimensions. As a second example we consider a discrete constrained system with an evolving Hilbert space. As a third example we consider a continuous system that behaves as the continuum limit of the previous model. We introduce a unitary isomorphism that will allow us to describe this system in a fixed Hilbert space. We prove that the system still has perennials with new eigenvalues and eigenvectors at each level t satisfying the generalized orthonormality condition (17).

4.1. The Parametrized Particle

The parametrized particle obviously is a deparametrizable system and therefore there is a time variable satisfying conditions I–IV. However, it is interesting to discuss how these conditions determine the time variable. The dynamics of the parametrized particle is contained in the Hamiltonian constraint

$$\mathcal{H} = P_1 + \frac{P_2^2}{2m} = 0 \tag{47}$$

which is quadratic in the momentum P_2. Let us make the natural choice $t = x_1$. At the quantum level the kinematic space $\mathcal{E}_K$ is given in the basis $|x_1, x_2\rangle$ by functions $\psi(x_1, x_2)$, while the physical space is restricted by the Hamiltonian constraint

$$\mathcal{H}\psi_F(x_1, x_2) = -i\frac{\partial\psi_F}{\partial x_1} - \frac{1}{2m}\frac{\partial^2\psi_F}{\partial x_2^2} = 0 \tag{48}$$

The physical states may be written in terms of the Fourier transform as

$$\psi_F(x_1, x_2) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dp_2\, e^{i(p_2x_2-\omega(p_2)x_1)}f(p_2) \tag{49}$$

where

$$\omega(p_2) = \frac{1}{2m}p_2^2 \tag{50}$$

We introduce the inner product of two physical states ψ_1 and ψ_2 in $\mathcal{E}_{Ft}$,

$$\langle\psi_1|\psi_2\rangle_t = \int_{t=x_1} dx_2\, \psi_1^*(x_1, x_2)\psi_2(x_2, x_2) \tag{51}$$

In this particular case, the vector spaces $\mathcal{E}_{Ft}$ for different t are isomorphic. The perennial operators that commute with the time operator X_1 are

$$P_2 \qquad \text{and} \qquad X_2 - \frac{P_2}{m}X_1 \tag{52}$$

and a complete set of commuting perennials is formed by P_2, which obviously is self-adjoint with the inner product (31) and satisfy condition II. Their eigenvectors

$$\psi_{Fp_2}(x_1, x_2) = e^{i(p_2 x_2 - \omega(p_2) x_1)} \tag{53}$$

form an "improper" orthonormal basis of the physical state space, in accord with condition III. Finally, it is immediate to check that any square-integrable function $\psi(x_1^0, x_2)$ belonging to $\mathscr{E}^*_{Kx_1^0}$, the functional space of fixed $x_1 = x_1^0$, may be expanded in terms of the $\psi_{Fp_2}(x_1^0, x_2)$ that form a complete basis of the kinematic space at x_1^0. Thus the complete set of conditions is satisfied and the usual formalism of quantum mechanics is recovered with x_1 as the intrinsic time of the system. Before concluding this example, let us briefly mention what happens if we take as a "time variable" the coordinate x_2. Conditions I and II still hold, but one can easily check that III and IV cannot be simultaneously satisfied.

4.2. A Relational System with a Finite Dimensional Evolving Hilbert Space

In this example we show a system where the set of conditions for an intrinsic time holds provided its Hilbert space evolves in time. This kind of model shows how evolving Hilbert spaces arise within this approach.

We consider a system formed by the tensor product of two subsystems with angular momentum j, integer,

$$\mathscr{E}_K = \{ |j, m_1\rangle \otimes |j, m_2\rangle \equiv |m_1, m_2\rangle, m_1 \geq m_2 \} \tag{54}$$

The system is constrained by a Hamiltonian constraint

$$\mathscr{H} = J_0 - J_1 \tag{55}$$

where

$$J_0 |m_1, m_2\rangle = 2(j + m_2 + 1)|m_1, m_2 + 1\rangle \tag{56}$$

$$J_1 |m_1, m_2\rangle = 2(j + m_2)|m_1, m_2\rangle \tag{57}$$

We introduce a discrete time operator in $\mathscr{E}_K$ such that

$$T|m_1, m_2\rangle = (2j - m_1 + m_2)|m_1, m_2\rangle = t|m_1, m_2\rangle \tag{58}$$

One can easily see that $0 \leq t \leq j$. Any state of the basis $|m_1, m_2\rangle$ in $\mathscr{E}_K$ may be labeled by the value of t and the total third component of the angular momentum M.

We have

$$
\begin{array}{llll}
t = 0 & |j, -j\rangle & \Rightarrow |t = 0, M = 0\rangle & \dim \mathscr{E}_{K0} = 1 \\
t = 1 & \begin{cases} |j - 1, -j\rangle \\ |j, -j + 1\rangle \end{cases} & \Rightarrow |t = 1, M = \pm 1\rangle & \dim \mathscr{E}_{K1} = 2 \\
t = 2 & \begin{cases} |j - 2, -j\rangle \\ |j - 1, -j + 1\rangle \\ |j, -j + 2\rangle \end{cases} & \Rightarrow \begin{array}{l} |t = 2, M = \pm 2\rangle \\ |t = 2, M = 0\rangle \end{array} & \dim \mathscr{E}_{K2} = 3
\end{array} \tag{59}
$$

with

$$\dim \mathscr{E}_{Kt} = t + 1$$

and $M + t \geq 0$. The physical state space is defined by functions $\psi_F(t, M)\theta(M + t)$ such that

$$(M + t)[\psi_F(t, M) - \psi_F(t - 1, M - 1)] = 0 \tag{60}$$

The operator J_{1z}, explicitly given by

$$J_{1z}\psi(t, M) = \tfrac{1}{2}(2j - t + M)\psi(t, M) \tag{61}$$

is a perennial and commutes with T. The eigenvectors of J_{1z} define a basis in the physical state space

$$\psi_{Fm_1}^{j-m_1}(t, M) = \delta_{M,2m_1-2j+t}\theta(t - j + m_1) \tag{62}$$

These wave functions vanish for $t < j - m_1$ and therefore they have level $j - m_1$.

The inner product

$$\langle\psi|\phi\rangle_t = \sum_{M=-t}^{t} \psi^*(t, M)\phi(t, M) \tag{63}$$

ensures the Hermiticity of J_{1z}, and the inner product between the elements of the physical basis satisfies the orthonormality condition

$$\langle\psi_{Fm_1}^{j-m_1}|\psi_{Fm_1'}^{j-m_1'}\rangle_t = \delta_{m_1m_1'}\theta(t - j + m_1) \tag{64}$$

Thus conditions I–III are satisfied, and the last condition also holds; in fact, any function of M at a given t may be obtained by superposition of elements of the physical basis $\psi_{Fm_1}^{j-m_1}(t, M)$ at this t.

Now, it is very easy to compute a transition amplitude between two eigenstates of any observable. For instance, if we consider the operator J_{2z} given by

$$J_{2z}\psi(t, M) = \tfrac{1}{2}(M - 2j + t)\psi(t, M) \tag{65}$$

then it is self-adjoint and commutes with T. Now at time $t = 1$, $|t = 1, M = 1\rangle$ is an eigenvector

$$J_{2z}|1,1\rangle = (1-j)|1,1\rangle \tag{66}$$

If we label its eigenvectors at time t by $|m_2, t\rangle$, the transition amplitude between this state and $|m_2 = -j + 1, t\rangle$ is given by

$$\langle m_2 = -j + 1, t = 1 \| m_2, t\rangle = \delta_{m_2,-j+t} \tag{67}$$

4.3. An Evolving System with an Infinite-Dimensional Hilbert Space

Evolving systems in continuum space with a continuous intrinsic time may be simply introduced. The following example is the continuous extension of the model that we have just considered in Section 3.3:

$$\mathscr{E}_K = \{ |a, b\rangle, a, b \in R, a \geq b, -1 \leq a, b \leq 1 \} \tag{68}$$

with Hamiltonian constraint

$$\mathscr{H} = 4(a-1)(b+1)\frac{\partial}{\partial b}\psi(a, b) = 0 \tag{69}$$

Then if one chooses as a time variable $t = 2 - a + b$, and $x = a + b$, the Hamiltonian constraint takes the form

$$\mathscr{H}\psi(x, t) = (x^2 - t^2)\left[\frac{\partial}{\partial t}\psi(x, t) + \frac{\partial}{\partial x}\psi(x, t)\right] = 0 \tag{70}$$

A complete set of perennials satisfying condition III is given by

$$A\psi(x, t) = a\psi(x, t) \tag{71}$$

with eigenvectors belonging to the physical space given by

$$\psi_{Fa}^{1-a}(x, t) = \delta(x - t + 2 - 2a)\theta(t - 1 + a) \tag{72}$$

The inner product is given by

$$\langle\psi|\phi\rangle_t = \int_{-t}^{+t} dx\, \psi^*(x, t)\phi(x, t) \tag{73}$$

and the eigenfunctions satisfy the orthogonality condition

$$\langle\psi_{Fa}^{1-a}|\phi_{Fa'}^{1-a'}\rangle_t = \tfrac{1}{2}\delta(a - a')\theta(t - 1 + a)\theta(t - 1 + a') \tag{74}$$

Thus, conditions I–IV obviously hold in this system, which describes waves propagating in a region bounded by the future light cone. Now we have a description in terms of an inner product with a time-dependent measure. In the continuous case it is always possible to introduce a unitary isomorphism between the Hilbert spaces at two different times. Let us consider this transformation in the present case.

Let

$$\psi'(x, t) = \sqrt{t}\psi(xt, t) \tag{75}$$

Then

$$\langle\psi'(t)|\phi'(t)\rangle = \int_{-1}^{1} dx\, \psi'^*(x, t)\phi'(x, t)$$
$$= \int_{-t}^{t} du\, \psi^*(u, t)\phi(u, t) = \langle\psi|\phi\rangle_t \tag{76}$$

where $u = xt$. Thus the unitary transformation is given by

$$U_t^\dagger(u, x) = \sqrt{t}\delta(u - xt) = U_t(x, u) \tag{77}$$

and the eigenvalue equation for the perennial operator takes the form

$$A'\psi_a'(x, t) = \left[\frac{xt - t}{2} + 1\right]\psi_a'(x, t) = a\psi_a'(x, t) \tag{78}$$

while the Hamiltonian constraint now becomes

$$\mathcal{H}'\psi'(x, t) = (x^2t^2 - t^2)\left[\frac{(1 - x)}{t}\frac{\partial}{\partial x} + \frac{\partial}{\partial t} - \frac{1}{2t}\right]\psi'(x, t) = 0 \tag{79}$$

A complete set of eigenvectors of the perennial operator belonging to the physical space is

$$\psi_{Fa}'^{1-a}(x, t) = \sqrt{t}\delta[(x - 1)t + 2 - 2a] \tag{80}$$

Notice that these solutions still have level $1 - a$ and satisfy the orthogonality condition

$$\langle\psi_{Fa}^{1-a}(t)|\phi_{Fa'}^{1-a'}(t)\rangle = \tfrac{1}{2}\delta(a - a')\theta(t - 1 + a)\theta(t - 1 + a') \tag{81}$$

Thus, we see that the fundamental properties of the evolving relational systems—the appearance of new eigenvalues and eigenstates at each level and the conservation of the inner product among states of level t_0 for any $t \geq t_0$—are still present in this description in terms of a fixed Hilbert space. In general, evolving Hilbert spaces seem to be naturally related to systems with boundaries. For instance, the system we have just analyzed may be simply generalized to a Klein–Gordon system $\mathcal{H} = P_t^2 - P_x^2$ in a bounded region $R = (x, t)$: $t^2 - x^2 \geq 0$. This system may be treated as a deparametrizable system by introducing a time variable $\tau = (t^2 - x^2)^{1/2}$ leading to a usual Klein–Gordon equation with a nonpositive-definite inner product. However, an equivalent Hamiltonian in the bounded region $\mathcal{H}' = (x + t)(P_t^2 - P_x^2)$

may be quantized with a positive-definite inner product in an evolving Hilbert space.

5. CONCLUSIONS AND FINAL REMARKS

We have introduced a notion of intrinsic time in relational systems that allows us to recover the fundamental features of time in quantum mechanics. In the case of any standard quantum mechanical system in parametrized form our method reproduces the usual formalism of quantum mechanics.

However, the method allows us to include relational dynamical systems and leads naturally to quantum mechanical systems with an evolving Hilbert space. In that sense we are implementing the intuition that one can define fixed-time Hilbert spaces that contain subsets of all possible states of the system. These systems are not invariant under time translations or time reversal and have a defined arrow of time. The initial state of the system, as well as the evolution of the Hilbert space, are determined by the Hamiltonian constraint and therefore dictated by the dynamics. The number of accessible states increases in time.

Let us conclude with some final comments about the quantum gravity case. Even though very little is known about the physical state space of quantum gravity, a pure gravity system could behave as an evolving system of this type. In fact, it is natural to take as the configuration space of quantum general relativity the loop space (Rovelli and Smolin, 1990), because in this representation the domain of the wave functions seems to be simply related to the microscopic structure of space-time. In the loop representation, the kinematic space $\mathscr{E}_K$ is given by the knot-dependent functions (Rovelli and Smolin, 1990) $\psi[K]$ that satisfy the diffeomorphism constraint. As a candidate for the intrinsic time t, we would like to take a variable such that the simplest configuration corresponds to its initial value. A good candidate seems to be the minimum number of crossings of a knot; this knot invariant quantity may be used to characterize the complexity of each knot. The kinematic space of quantum gravity will be characterized by wave functions $\psi(t, \kappa)$, where κ are the remaining knot invariants necessary to describe a knot with a minimum number of crossings equal to t. If we do not include knots with more than triple self-intersections, the number of independent knot invariants with a fixed t is finite and increases with t. Of course, if we want to take as a time variable some knot invariant such that the number of independent knots and the dimension of the kinematic space increase with t, there is not a unique choice. For instance, one could define as time the degree of a universal polynomial associated with the link. However, it is not known how to classify any knot in terms of knot polynomials in such a way that inequivalent knots always correspond to different polynomials.

In general relativity no perennial is known, but a candidate for observable, in the sense used in this paper, is given by the volume of the universe. The eigenstates of the volume operator are knot states having a definite number of crossings and intersections and its eigenvalues are essentially proportional to the Planck volume times the number of intersections. This operator does commute with the diffeomorphism constraint and with our "time" and does not commute with the Hamiltonian constraint. These are the conditions required for our observables. The naive picture of the Big Bang that we get is a unique zero-volume state that evolves with certain probabilities to different states of finite volume. Within this description the recollapse of the universe will be associated with a decreasing volume, while the complexity of the knot space is still growing. Unfortunately, it does not seem to be easy to check a proposal of this type on a simple cosmological model. In fact, in that case the knot structure related to the diffeomorphism invariance is not present.

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