A Discrete Time Presentation of Quantum Dynamics

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Abstract

Inspired by the discrete evolution implied by the recent work on loop quantum cosmology, we obtain a discrete time description of usual quantum mechanics viewing it as a constrained system. This description, obtained without any approximation or explicit discretization, mimics features of the discrete time evolution of loop quantum cosmology. We discuss the continuum limit, physical inner product and matrix elements of physical observables to bring out various issues regarding viability of a discrete evolution. We also point out how a continuous time could emerge without appealing to any continuum limit.

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I. INTRODUCTION

The recent work of Bojowald on Loop Quantum Cosmology (LQC) obtains the Wheeler-DeWitt equation (Hamiltonian constraint) as a difference equation [1]. The eigenvalues of the volume operator are discrete in quantum geometry and are taken as playing the role of a ‘discrete time’ in the context of isotropic LQC [2]. The order of the difference equation is typically high (16 for isotropic, Bianchi-I) and the number of independent (and non-degenerate) solutions is reduced by one due to the coefficient of the highest (lowest) order term vanishing for discrete time equal to zero [3]. This feature is crucial for the ‘singularity avoidance’ mechanism [4]. Furthermore, a continuum limit is defined wherein the Immirzi parameter plays a crucial role. This limit is used to distinguish the so called ‘pre-classical’ solutions and it is shown that the singularity avoidance mechanism also leads to a unique (up to normalization) pre-classical solution of the Wheeler-DeWitt equation [5, 6]. These are very interesting indications that the procedures of loop quantum gravity as applied to cosmological mini-superspaces, do lead to physically reasonable solutions. Although certain choices of definitions of constraint operators with certain factor orderings can be made with reasonable justification, the procedure is not devoid of ambiguities [3, 7]. While there are many issues to be resolved, we focus on one feature, namely ‘discrete evolution’, which seems to be robust.

For instance, mathematically, solutions of the Wheeler-DeWitt equation can be presented as a sequence of states (isotropic LQC). The sequence label is highly suggestive of a discrete ‘time’. This dynamical interpretation is something additionally attempted and its viability needs to be established. In a quantum theory, an evolution interpretation must be established at least at the level of expectation values, the states being not directly observable. Furthermore it is not enough to generate a family, continuous or discrete, of expectation values. It should be possible to detect the changes paying due attention to the uncertainties. By contrast, a continuum limit does not appear to be essential for a dynamical interpretation even though emergence of a continuous time description in a semi-classical limit is of course desirable. Presently, in the context of LQC, these issues are discussed somewhat schematically. One of the motivations for the present work is to have simple, well known examples which nonetheless mimic steps taken in LQC.
It is well known that the usual quantum mechanical systems (or classical for that matter) can also be viewed as a constrained system leading to a frozen-time description. The Dirac procedure nonetheless allows one to interpret the physical state condition as an evolution equation - the usual Schrödinger equation. By using the ‘Fock’ representation instead of the Schrodinger representation for the extra time degree of freedom, one can get a discrete ‘evolution’ equation which mimics all the features seen in the LQC work. The order of the difference equation is two but there is a reduction of number of non-trivial independent solutions; there is a parameter analogous to the Immirzi parameter which can play a similar role in exploring pre-classicality and a continuum limit.

To explore evolution at the level of expectation values of course needs definitions of physical inner products, observables and their matrix elements. The advantage in the quantum mechanical case however is that we know physical inner products and physical matrix elements so that we can push further the interpretation of the difference equation as “really” an evolution equation. Furthermore since the Schrodinger and the ‘Fock’ representations are equivalent, we can relate the continuous and the discrete evolutions by a transform. It turns out that the dynamical interpretation is not as straightforward as indicated by the LQC works.

‘Discrete Time’ has appeared in the literature several times in various forms and with various motivations. The present work is very different from these earlier works. In particular, we are not seeking a discrete time formulation, ab initio, for any particular reason. We observe that in a frozen time formulation of dynamics, a ‘time’ appears as a basis label which has an arbitrariness about it. The dynamics is then obtained as a family of states labeled by the ‘time’. One has natural choices of continuous and discrete labels. The choice of the continuous label leads to the usual quantum dynamics and we explore the discrete choice in detail, in particular with regards to observability of evolution.

In section II we detail the case of usual quantum mechanics cast in a frozen time form, both with continuous and discrete time and exhibit its analogy with LQC. We discuss the continuum limit and show the relation between the continuous and the discrete time
descriptions. In section III we discuss natural candidates for physical quantities needed to push the evolution interpretation further and the difficulties encountered. In the last section we discuss the issue of interpretation in some generality and point out a possible role of the parameter $\beta$ appearing in the discrete description. We conclude by making a series of remarks.

II. NON-RELATIVISTIC QUANTUM MECHANICS

A. Frozen Time Description: Continuum Case

Let $\Gamma_0$ denote a classical phase space and let $\mathcal{H}_0$ denote the Hilbert space of the corresponding quantum system. Let $\tau, \pi_\tau$ denote two extra phase space variables corresponding to the usual continuous time and its ‘conjugate momentum’. Let $\Gamma_{kin} := R^2 \times \Gamma_0$ denote an extended phase space and let $\mathcal{H}_{kin} := L_2(R, d\tau) \otimes \mathcal{H}_0$ the corresponding kinematical Hilbert space. At the classical level we impose the single constraint $\phi := \pi_\tau + H(\omega) \approx 0$. Here, $\omega$ denote the usual phase space coordinates and $H(\omega)$ denotes a time independent Hamiltonian on $\Gamma_0$. Quantum mechanically, the operator version of the constraint is imposed on to select the ‘physical states’. Explicitly, the physical states are those on which the operator $\pi_\tau + H$ vanishes. The constraint operator is of course is not identically zero. For definiteness one may think of $\Gamma_0 = R^{2N}, \mathcal{H}_0 = L^2(q^i, d^nq)$ and $H(\omega) = \frac{p^2}{2m} + V(q^i)$ though this is not necessary. There is no external time any more.

At the classical level, the Dirac observables, $A(\tau, \pi_\tau, \omega)$ are defined by $\{A, \phi\}_{PB} \approx 0$. Some simple examples of Dirac observables are: functions of only $\pi_\tau$ and functions independent of $\tau, \pi_\tau$ which Poisson commute with the Hamiltonian (in particular the Hamiltonian itself). This is a rather limited class of observables. One could however choose a $\tau$ dependent family of functions of $\omega$ satisfying the differential equation $\frac{\partial A}{\partial \tau} + \{A(\tau, \omega), H(\omega)\}_{PB} = 0$ with the initial condition $A(0, \omega) = A_0(\omega)$. Such solutions of the differential equation are trivially Dirac observables. In particular, the usual solutions of Hamilton’s equation are also Dirac observables but with $\tau \to -\tau$. These are the ‘evolving’ observables in a frozen time formulation. 

\[ \]
In the quantum description, one quantizes the $\tau, \pi$ in the usual manner and the constraint equation becomes just the Schrodinger equation. Explicitly, one can write a general vector in $\mathcal{H}_{kin}$ in the form:

$$|\Psi\rangle = \int d\tau |\tau\rangle \otimes |\Phi(\tau)\rangle$$

The kinematical inner product is then given by,

$$\langle \Psi'|\Psi\rangle_{kin} = \int d\tau \langle \Phi'(\tau)|\Phi(\tau)\rangle_0$$

The suffix 0 refers to the inner product in $\mathcal{H}_0$.

Thus physical states are those $|\Psi\rangle$ whose $|\Phi(\tau)\rangle$ satisfy the usual time dependent Schrodinger equation. Introducing $U(\tau) := e^{-i\tau \hat{H}}$, we denote the solutions of the Schrodinger equation as $|\Phi(\tau)\rangle = U(\tau)|\Phi(0)\rangle$. The corresponding $|\Psi\rangle$’s are not normalizable with respect to the kinematical inner product since the integrand is independent of $\tau$ rendering $\tau$ integration divergent.

Dirac observables are usually defined as those observables which commute with the constraints. It may be sufficient to require that the physical observables commute only weakly with the constraints. In this case the factor ordering must ensure that the constraint operators act first i.e. are to the right. Weak commutation then amounts to physical observables acting invariantly on the physical states. As an example one can define ‘evolving observables’ as follows [2]. Corresponding to a usual operator, $\hat{O}$ on $\mathcal{H}_0$, define a family of operators on the space of physical states by,

$$[\hat{O}(\tau)|\Phi\rangle](\tau') := U(\tau')U(-\tau)\hat{O}|\Phi\rangle(\tau)$$

These ‘evolving observables’ are physical in the sense they act invariantly on the space of physical states. In general, they do not commute with the constraint operator in the full $\mathcal{H}_{kin}$. Since physical states are not kinematically normalizable, one has to define a physical inner product on the space of solutions of the constraint. A natural definition suggests itself as:

$$\langle \Psi'|\Psi\rangle_{phy} := \langle \Phi'(\tau_0)|\Phi(\tau_0)\rangle_0 \quad \tau_0 \text{ is some fixed time}$$

The kinematical inner product is just the integral of the physical inner product over $\tau_0$. It is obvious that the physical inner product is independent of the particular $\tau_0$ chosen and
of course coincides with the usual inner product in $\mathcal{H}_0$.

It is easy to see that the physical matrix elements of these evolving observables between physical states are given by,

$$\langle \Psi' | \hat{O}(\tau) | \Psi \rangle_{phy} = \langle \Phi'(0) | U(-\tau) \hat{O} U(\tau) | \Phi(0) \rangle_0$$  \hspace{1cm} (5)

Hence, the physical matrix elements are obtained as the usual matrix elements of operators on $\mathcal{H}_0$. We see thus that the usual description of quantum dynamics in terms of a continuous time can be recast as a frozen time presentation. This is of course well known.

We will now introduce a discrete time description which mimics all the features seen in the loop quantum cosmology.

B. Discrete case

Instead of choosing the usual Schrodinger representation for $\tau, \pi_\tau = -i\hbar \frac{\partial}{\partial \tau}$, let us introduce a number representation. Define $a := \alpha \tau + i \beta \pi_\tau$ and $a^\dagger$ its hermitian conjugate. $\alpha, \beta$ are real and satisfy $2\alpha \beta \hbar = 1$. Hence we have a one parameter family of creation-annihilation operators labeled by $\beta$, say. This parameter is expected to play a role analogous to that played by the Immirzi parameter in LQC. We will choose the eigenvalues of the number operator, $N := a^\dagger a$ as our discrete time label. Notice that these eigenvalues are independent of $\beta$. For future use in continuum limit we note that,

$$N = \left( \frac{1}{2\hbar \beta} \right)^2 \tau^2 + \beta^2 \pi_\tau^2 - \frac{1}{2} \sim \frac{1}{4\hbar^2 \beta^2} \tau^2 \quad \text{as } \beta \to 0$$  \hspace{1cm} (6)

This will justify the eigenvalues of the number operator being identified with $\tau$ at least for large eigenvalues and small $\beta$ and of course $n$ is monotonic in $\tau^2$.

In terms of creation-annihilation operators, the constraint equation becomes,

$$\left( \frac{a - a^\dagger}{2i\beta} + \hat{H} \right) |\Psi\rangle = 0.$$  \hspace{1cm} (7)

Writing $|\Psi\rangle = \sum_{n=0}^{\infty} |n\rangle \otimes |\Phi_n\rangle$ one obtains the kinematical inner product as,

$$\langle \Psi' | \Psi \rangle = \sum_{n=0}^{\infty} \langle \Phi'_n | \Phi_n \rangle.$$  \hspace{1cm} (8)
The physical states are then those $|\Psi\rangle$ whose $|\Phi_n\rangle$’s satisfy,

$$|\Phi_{n+2}\rangle = \frac{-2i\beta}{\sqrt{n+2}}\hat{H}|\Phi_{n+1}\rangle + \sqrt{\frac{n+1}{n+2}}|\Phi_n\rangle \quad \forall \, n \geq -1 \quad (9)$$

This is our discrete time evolution (discrete Schrodinger equation). We notice that the difference equation is an operator difference equation of order two implying that two vectors (in $\mathcal{H}_0$) have to be specified to determine a solution i.e. has ‘two independent’ solutions. However exactly as in the case of loop quantum cosmology, we have a consistency condition (since spectrum of $N$ is bounded below) which fixes $|\Phi_1\rangle$ in terms of $|\Phi_0\rangle$ implying a unique solution for every given $|\Phi_0\rangle$. By contrast, in the continuum description, there is no such condition but the equation is of course a first order differential equation.

For subsequent analysis, it is convenient to convert the vector equation into infinitely many scalar equations by expanding the $|\Phi_n\rangle = \sum_\alpha C_\alpha^n |E_\alpha\rangle$ in the eigenbasis of the $\hat{H}$. For simplicity we have assumed that spectrum of $\hat{H}$ in $\mathcal{H}_0$ is discrete. The discrete equation then becomes,

$$C_\alpha^{n+2} = \frac{-2i\beta E_\alpha}{\sqrt{n+2}}C_\alpha^{n+1} + \sqrt{\frac{n+1}{n+2}}C_\alpha^n \quad \forall \, n \geq -1, \, \forall \, \alpha. \quad (10)$$

Let us now turn to the “continuum limit”. This can be understood in various ways. A simple way is to ask whether one can find continuous variable $t$ and a function $C^\alpha(t)$ which will interpolate a solution of the discrete equation for large $n$. To explore this let us look for a function $C(t)$ and a function $t(n)$ such that in a suitable large $n$ limit one has (suppressing the label $\alpha$),

$$C_{n+k} = C(t(n + k)) := C(t(n) + k\delta t) \approx C(t) + k\delta t \frac{\partial C}{\partial t}. \quad (11)$$

where, $k\delta t = t(n + k) - t(n)$ has been used. Treating $\delta t$ small is equivalent to requiring $t(n)$ to be slowly varying with $n$. Substitution in the difference equation and keeping terms to leading order in $n$ (treating $\delta t$ also as small), leads to $C^{-1}\frac{\partial C}{\partial t} = -iE_n^{\frac{\beta}{\delta t\sqrt{n}}}$. The left hand side is a function of $t$ by assumption so we must have $\frac{\beta}{\delta t\sqrt{n}}$ to be a function of $t$. Since the limit is to be considered for all $C^\alpha$, we have excluded $E$. Simplicity and dimensional considerations then suggest that we choose $t$ such that $\frac{\beta}{\delta t\sqrt{n}} := \hbar^{-1}$. The variable $t$ so specified will be denoted by $\tau$. It follows that $\tau(n) = 2\hbar\beta\sqrt{n}$. Observe that $\delta\tau \sim n^{-1/2}$ and thus vanishes for large $n$ without having to take $\hbar\beta$ to be vanishingly small. This is different
from the LQC. To get a finite $\tau$ for arbitrarily large $n$ however, we must consider a joint limit $n \to \infty, \beta \to 0$ keeping $\tau$ fixed. We could have taken $\hbar \beta$ to zero but presently we are interested in a continuum limit instead of a semi-classical limit. It follows that in the above joint limit $C(\tau)$ satisfies the usual Schrödinger equation and so does the full $|\Phi(\tau)\rangle$. Thus we see that continuous functions that interpolate solutions of the difference equation asymptotically are solutions of the usual Schrödinger equation with a suitable identification of $\tau(n)$.

Can we obtain $C(\tau)$ as a limiting function from the joint limit of $C_n$? The answer is yes. Consider the difference equation for large $n$ but with fixed $\beta$,

$$C_{n+2}^{\alpha} - C_n^{\alpha} = -\frac{2i\beta \mathcal{E}_n}{\sqrt{n}} C_{n+1}^{\alpha} + o\left(\frac{1}{n}\right).$$

(12)

The left hand side of this equation equated to zero is an equation with constant coefficients (Poincare type) [10]. The asymptotic behaviour of its solutions is given in terms of its characteristic roots obtained by substituting $C_n^{\alpha} \sim \lambda^n$. The characteristic roots are just $\lambda = \pm 1$, independent of the label $\alpha$. Evidently, the root $\lambda = -1$ can not correspond to a solution which has limiting value in the joint limit. Furthermore, even for $\lambda = 1$, one can not see the limit to be a solution of the continuum Schrodinger equation. One needs a more refined ansatz: $C_n \sim \lambda^n \mu \sqrt{n}$. Substitution determines $\lambda = \pm 1$ from the $n$ independent term and also gives $\ell n \mu = -2i\lambda \beta \mathcal{E}_n$ from the sub-leading $n^{-1/2}$ term. For $\lambda = 1$ we see that $C_n^{\alpha}$ goes over to the solution of the continuum Schrodinger equation. By contrast, $\lambda = -1$ does not have a limit. A generic asymptotic solution will be a linear combination of these two asymptotic solutions and it will not have a limiting value in the joint limit. There is then a unique solution that does have limiting value. This is very similar to the arguments [8].

So far the steps are completely analogous to those taken in loop quantum cosmology. However here we run in to a problem. **No exact solution of the difference equation can possibly have a non-zero and finite limiting value in the joint limit.** This follows because the ratio of the $C_n^{\alpha}$ for $n$ odd and $n$ even is necessarily purely imaginary as is evident from the difference equation. Thus although the assumptions we made about a conceivable continuum limit do admit a corresponding ansatz for the asymptotic solution of the difference equation, no exact solution can in fact support such an ansatz. The notion of pre-classical limit as articulated in LQC [9, 10], is not realized by any exact solution even...
though a continuum limit in the sense of difference equation going over to a differential
equation is valid. One has only asymptotic solutions i.e. solutions of asymptotic equation as
distinct from asymptotic form of solutions of the exact equation, which have a pre-classical
limit but no exact solution has this property. It seems that the continuum solutions can at
best be thought of as approximating the exact solution that too only asymptotically i.e. for
large $n$.

Is not having any pre-classical solutions a disaster for getting a continuum picture? Not
necessarily. For emergence of a continuum description from an underlying discrete one what
is needed is a mapping to continuous description and not necessarily a continuum limit. The
next sub-section shows how this can happen.

C. Relating the continuum and the discrete descriptions

The evolution equations have been derived by writing:

$$ |\Psi\rangle \in \mathcal{H}_{\text{kin}} = \int_{-\infty}^{\infty} d\tau |\tau\rangle \otimes |\Phi(\tau)\rangle \quad \text{continuous case} $$

$$ = \sum_{n=0}^{\infty} |n\rangle \otimes |\Phi_n\rangle \quad \text{discrete case} \quad (13) $$

Imposing the constraint in the Schrodinger representation and the Fock representation
respectively leads to the usual Schrodinger equation for $|\Phi(\tau)\rangle$ and the difference equation
for $|\Phi_n\rangle$. The two basis vectors $|\tau\rangle$ and $|n\rangle$ are related as:

$$ |\tau\rangle = \sum_{n=0}^{\infty} |n\rangle \langle n|\tau\rangle = \sum_{n} f_n^*(\tau) |n\rangle, $$

$$ |n\rangle = \int_{-\infty}^{\infty} d\tau |\tau\rangle \langle \tau|n\rangle = \int d\tau f_n(\tau) |\tau\rangle \quad (14) $$

The transformation functions, $f_n(\tau)$ are easily determined and are given by,

$$ f_n(\tau) := \langle \tau|n\rangle = \mathcal{N}_n H_n(\xi)e^{-1/2\xi^2} \quad \xi := \frac{\tau}{\sqrt{2} \hbar \beta}, $$

$$ \mathcal{N}_n = \left( \frac{(2\pi)^{1/4} \sqrt{\hbar \beta} \sqrt{2^n n!}}{\sqrt{\hbar \beta} \sqrt{2^n n!}} \right)^{-1} \quad (15) $$

and $H_n(\xi)$ are the Hermite polynomials. The vectors $|\Phi(\tau)\rangle$ and $|\Phi_n\rangle$ are easily seen to
be related as:
\[ |\Phi(\tau)\rangle = \sum_n f_n(\tau)|\Phi_n\rangle \]
\[ |\Phi_n\rangle = \int d\tau f_n^*(\tau)|\Phi(\tau)\rangle. \] (16)

Using the properties of the Hermite polynomials, it is easy to see that \(|\Phi_n\rangle\) satisfy the difference equation iff \(|\Phi(\tau)\rangle\) satisfies the Schrodinger equation. The respective initial states are related as:
\[ |\Phi_0\rangle = \frac{\sqrt{2}}{(2\pi)^{1/4}} \sqrt{\hbar} \left\{ \int_{-\infty}^{\infty} d\xi e^{-\xi^2/2} -i\sqrt{2}\xi \hat{H} \right\} |\Phi(0)\rangle. \] (17)

By expanding \(|\Phi(0)\rangle\) in eigenstates of the Hamiltonian one can show that,
\[ \langle \Phi_0|\Phi_0\rangle_0 \leq 2\sqrt{2}\pi \hbar \beta \langle \Phi(0)|\Phi(0)\rangle_0. \] (18)

This shows that in the limit \(\beta \to 0\) the transform breaks down.

This route, available in the present case, shows that it is possible to define states depending on a continuous variable in a differentiable manner \(\text{without}\) appealing to any ‘pre-classical’ or otherwise limiting procedure.

III. PHYSICAL QUANTITIES

As a first attempt, we will just mimic the steps followed in the continuous time case. For this it is convenient to write the second order difference equation as a first order matrix difference equation. This is easily achieved. The evolution equation can be written as:
\[ \begin{pmatrix} |\Phi_{n+1}\rangle \\ |\Phi_{n+2}\rangle \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{I} \\ \sqrt{\frac{n+1}{n+2}} & -\frac{2i\beta}{\sqrt{n+2}} \hat{H} \end{pmatrix} \begin{pmatrix} |\Phi_n\rangle \\ |\Phi_{n+1}\rangle \end{pmatrix} \quad \iff \quad z_{n+1} = \mathbb{A}(n)z_n \quad n \geq 0 \]
\[ \begin{pmatrix} |\Phi_{n-1}\rangle \\ |\Phi_{n}\rangle \end{pmatrix} = \begin{pmatrix} \frac{2i\beta}{\sqrt{n}} \hat{H} & \sqrt{\frac{n+1}{n}} \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix} \begin{pmatrix} |\Phi_n\rangle \\ |\Phi_{n+1}\rangle \end{pmatrix} \quad \iff \quad z_{n-1} = \mathbb{B}(n)z_n \quad n \geq 1. \] (19)

It follows from the definitions that \(\mathbb{A}(n-1)\mathbb{B}(n) = \mathbb{B}(n+1)\mathbb{A}(n) = \mathbb{I}\). Not all states evolving by the above equations are physical though because the physical states also have to satisfy the consistency condition namely \(|\Phi_1\rangle = -2i\beta \hat{H}|\Phi_0\rangle\).
Let $D_n$ denote the space spanned by the $z_n$’s. It can be viewed as $H_0 \oplus H_0$. To define an evolving observable $\hat{O}(m)$ corresponding to an operator $\hat{O}$ acting invariantly on all $D_n$’s, consider the $z_m$ member of an physical state $\{|\Phi_n\rangle\}$. Operate on it by $\hat{O}_0$ and evolve back to $D_0$. This will not in general satisfy the consistency condition. Let $\mathcal{P}$ be a projection operator which will project any element of $D_0$ on to one corresponding to a physical one. That is, define a new $z_0$ whose components satisfy the consistency condition. Evolve this to any $n > 0$. This clearly defines a physical state. $\hat{O}(m)$ is defined to produce this physical state from the starting physical state. By construction, these operators, defined to act on physical states, produces a new physical state. Introduce the evolution operators $E(0, n) : D_0 \to D_n$ and $E(n, 0) : D_n \to D_0$ given explicitly by,

$$E(0, n) := A(n-1)A(n-2)\cdots A(0)$$

$$E(n, 0) := B(1)B(2)\cdots B(n)$$

(20)

Then $\hat{O}(m)$ is expressible as,

$$[\hat{O}(m)z]_n := E(0, n) \circ \mathcal{P} \circ E(m, 0)\hat{O}z_m.$$  

(21)

The projection operator can be constructed easily and is uniquely given by,

$$\mathcal{P} := \frac{1}{I + 4\beta^2 \hat{H}^2} \begin{pmatrix} I & 2i\beta \hat{H} \\ -2i\beta \hat{H} & 4\beta^2 \hat{H}^2 \end{pmatrix}.$$  

(22)

In analogy with the continuum case, one may naturally define a physical inner product as the $n = 0$ term of the series in equation 8. We can make other possible choices, for example, $z_0^\dagger \mathcal{M}z_0$, where $\mathcal{M}$ is a suitable $2 \times 2$ matrix of operators on $H_0$. $\mathcal{M} = \text{diag}(I, 0)$ will produce the $n = 0$ term of the series. Physical matrix elements of the evolving observables are then given by,

$$\langle \Psi' | \hat{O} | \Psi \rangle = z_0^\dagger \mathcal{P} \mathcal{M} \mathcal{P} E(m, 0) \hat{O} E(0, m) z_0.$$  

(23)

We have used $z_0^\dagger \mathcal{P} = z_0^\dagger$ for physical states to obtain a symmetrical expression. While this looks very similar to the continuum case (apart from the presence of $\mathcal{P} \mathcal{M} \mathcal{P}$), its implications are very different.

These definitions, while plausible, are unsatisfactory. We have focussed on the operators which act invariantly on the space of physical states. However to be of use for measurements, such operators must satisfy further properties such as self-adjointness. This of
course needs to be defined relative to the physical inner product. The non-unitarity of evolution however implies that even if have a self-adjoint operator at \( n = 0 \), the other members of the family are not self-adjoint in general. The presence of the projection operator implies that algebraic relations among operators are not preserved by the evolution. For example, an operator associated with an \( \hat{O}^2(0) \) is not the square of the corresponding operator associated with \( \hat{O}(0) \) and like wise for commutation relations. In the present case of Fock representation, the condition arises due to the spectrum of number operator being bounded below. In LQC, although the state label \( n \) takes all integral values, there is still the consistency condition which should cause similar difficulties.

One could have dealt with the second order equation it self. Now there is no need for any explicit projection operator. The evolution is still non-unitary but in addition, one can not evolve a given \( |\Phi_n\rangle \) back to a \( |\Phi_0\rangle \) since the equation is second order. The first order formulation avoids this but introduces explicit projection operator. Thus our attempt to mimic the steps followed in the continuous time case do not lead to satisfactory definitions.

However, we can appeal to the relations between the continuum and the discrete description discussed before. Then the physical inner product and matrix elements as defined in the continuous case can be expressed as,

\[
\langle \Phi'(\tau)|\Phi(\tau) \rangle = \sum_{m,n} f_m^*(\tau) f_n(\tau) \langle \Phi'_m|\Phi_n \rangle \\
\langle \Phi'(\tau)|A|\Phi(\tau) \rangle = \sum_{m,n} f_m^*(\tau) f_n(\tau) \langle \Phi'_m|A|\Phi_n \rangle
\]

These are very different from the physical inner products and matrix elements we attempted previously! The right hand sides involve infinite sums and are highly non-local in the discrete time label. Note that the apparent \( \tau \) dependence on the right hand sides is consistent with that implied by the left hand sides of the above equations. Thus, if we somehow invented these inner products and matrix elements, we could construct a continuum description from the discrete one. In the case of quantum mechanical example we are discussing, we have the advantage of knowing a continuum description ab initio but for LQC also something similar can be conceivable. This however is not attempted in the present work. In the next section we make some general remarks regarding viability of a ‘dynamical’
interpretation and attempt to arrive at an interpretation of $\beta$.

IV. ‘EVOLUTION’ IN QUANTUM MECHANICS

Unlike classical mechanics, quantum mechanics permits two notions of evolution which are not equivalent due to the uncertainty relation. The two notions correspond to evolution at the level of states i.e. a continuous or a discrete family of rays (or vectors) and evolution at the level of observed quantities i.e. family of expectation values of observables. To appreciate the non-equivalence of these two let us quickly recall the derivation of time-energy uncertainty relation. One can do this quite generally.

Let $G$ be a self adjoint operator on a Hilbert space. Consider the one parameter group of unitary operators generated by $G$, $U(\xi) := \exp(-i\xi G)$, $\xi \in \mathbb{R}$. Define a family of normalized state vectors $|\psi(\xi)\rangle := U(\xi)|\psi(0)\rangle$. For any self adjoint operator, $A$, corresponding to an observable define $f_\psi(\xi) := \langle \psi(\xi)|A|\psi(\xi)\rangle$. Assume $A$ to be independent of $\xi$ for simplicity. Then it follows that,

$$\delta f_\psi(\xi) := \delta \xi \frac{\partial f_\psi}{\partial \xi} = i\delta \xi \langle \psi(\xi)|[G,A]|\psi(\xi)\rangle, \quad \delta \xi > 0 \ (\text{say}) \quad (25)$$

Defining $G' := G - \langle \psi(\xi)|G|\psi(\xi)\rangle$ and like wise for $A$ one gets,

$$|\delta f_\psi(\xi)| = | \delta \xi \langle \psi(\xi)|[G',A']|\psi(\xi)\rangle | \leq 2\delta \xi |\text{Im}(G'\psi,A'\psi)|$$

$$\leq 2\delta \xi |\langle G'\psi,A'\psi \rangle|$$

$$\leq 2\delta \xi ||G'|\psi|| \cdot ||A'|\psi||$$

$$\leq 2\delta \xi \Delta G_\psi \Delta A_\psi \quad (26)$$

Clearly in order to detect a change in the expectation value $f_\psi(\xi)$, the change computed above must be at least as large as the uncertainty, $\Delta A_\psi$. This immediately gives the uncertainty relation:

$$\delta \xi \Delta G_\psi \geq \frac{1}{2} \quad (27)$$

Note that this derivation is independent of canonical commutation relations and thus is not tied to a phase space $\sim \mathbb{R}^{2N}$, $\delta \xi \neq \Delta \xi_\psi$ although it could be. The above
derivation has also assumed \( \delta \xi \) to be small enough so that the higher order terms can be neglected. If these are also included, then the uncertainty relation will assume a different form.

Taking \( G \) to be the Hamiltonian and \( \xi = \tau / \hbar \) we get the usual time-energy uncertainty relation while for \( G \) equal to the momentum (say) and \( \xi = q / \hbar \) we get the position-momentum uncertainty relation. Its meaning is that we cannot observationally resolve values between \( \xi \) and \( \xi + \delta \xi \). The fact that there is a non-zero lower bound and \( \Delta G_\psi \), in a physical situation is always finite (though it could be very large) implies that continuum values for \( \xi \) are strictly mathematical idealizations. This distinguishes the two notions of ‘evolution’ in quantum mechanics, mentioned above. The states can be thought of as evolving continuously but observationally, continuous evolution is necessarily an idealization. The absence of a non-zero lower bound in classical mechanics permits continuum values of \( \xi \) to be taken more literally. Note that this applies not just to ‘time’ but also to ‘space’.

The notion of observationally detectable evolution can be articulated as follows. We can meaningfully say that a system has changed its state provided we can measure at least one of its properties and detect a change. Any such measurements will give expectation values together with uncertainties for the corresponding observable. Thus to conclude that a system in some given state has changed ‘over a period of time’ one must be able to find at least one observable whose expectation value in that state changes more than the uncertainty. Note that this must be understood at the level of an ensemble of identically prepared systems since a single measurement on a single system will just produce some eigenvalue of the observable according to the standard interpretation of quantum mechanics. To account for ‘over a period of time’, one must assume a family (discrete or continuous) of states in which the expectation values are to computed.

Thus, for the observational notion of an evolution, the central quantities are expectation values. Given a discrete family of vectors and self adjoint operators (or a family thereof) one can construct a corresponding family of expectation values. Such a family could be usefully interpreted as an ‘evolution’ provided that the difference between consecutive members of the family of expectation values is larger than the corresponding uncertainties, at least for some observable and for generic states. Such a criterion of detectable evolution is
independent of how the family of vectors is chosen and whether the members of this family are connected by unitary operators. This is also independent of whether the sequence of vectors is obtained from solutions of some (Hamiltonian) constraint of a constrained system.

As seen in the example of quantum mechanical system, the net result of imposing constraint in the kinematical arena is to produce a family of vectors in $\mathcal{H}_0$. Since such families are uniquely determined by $|\Phi_0\rangle$ (or $|\Phi(0)\rangle$), the space of ‘physical states’ is isomorphic to $\mathcal{H}_0$. A natural choice of physical inner product is then simply the inner product in $\mathcal{H}_0$ and ‘physical observables’ are naturally self adjoint operators on this Hilbert space. We can now construct a sequence of ‘physical’ expectation values:

$$\langle A \rangle_n := \frac{\langle \Phi_n | A | \Phi_n \rangle}{\langle \Phi_n | \Phi_n \rangle}$$

Expanding the states in terms of eigenstates of the Hamiltonian (assuming discrete spectrum for simplicity), $|\Phi_n\rangle = \sum_\rho C_{n,\rho} |\epsilon_\rho\rangle$, we get,

$$\langle A \rangle_n = \frac{\sum_\rho,\sigma C_{n,\rho}^* C_{n,\sigma} \langle \epsilon_\rho | A | \epsilon_\sigma \rangle}{\sum_\rho |C_{n,\rho}|^2}$$

If $|\Phi_0\rangle$ is an eigenstate of the Hamiltonian, then so are $|\Phi_n\rangle \forall n$. The expectation values defined above are then independent of $n$. Thus eigenstates of the Hamiltonian are ‘stationary’ states even with respect to the discrete ‘evolution’.

The coefficients $C_{n,\rho}$ above, satisfy the difference equations and are $n^{th}$ order polynomials in $(-2i\beta\epsilon_\rho)$. The expectation values and the uncertainties are thus rational functions of $\beta$.

Applying the reasoning to the simplest two level system brings out further possibilities. Let $\mathcal{H}_0$ be two dimensional and let the Hamiltonian be $\hat{H} = \epsilon_3$. Let a generic observable be a Hermitian $2 \times 2$ matrix. Then it is easy to see that all expectation values (and hence also the uncertainties) are independent of $\beta$! Explicitly, let

$$|\Phi_0\rangle := \begin{pmatrix} \cos \theta \\ \sin \theta e^{i\phi} \end{pmatrix}, \quad A := \begin{pmatrix} a & b \\ b^* & c \end{pmatrix}, \quad a, c \text{ real.}$$

Putting $|\Phi_n\rangle := \frac{P_n}{\sqrt{n!}}|\Phi_0\rangle$, $\forall n \geq 0$ and $Q := -2i\beta \hat{H}$, one can see that the $P_n$’s satisfy the equation,

$$P_{n+2} = QP_{n+1} + (n+1)P_n, \quad \forall n \geq -1, P_0 := 1, P_{-1} := 0$$

$$P_{n+2} = QP_{n+1} + (n+1)P_n, \quad \forall n \geq -1, P_0 := 1, P_{-1} := 0$$
By inspection, $P_n$’s are $n^{th}$ order polynomials in $Q$. Furthermore, for even (odd) $n$, only even (odd) powers of $Q$ occur. Since $Q^2$ is a multiple of the identity matrix, $P_{2m}$ is a polynomial in $(-4\beta^2E^2)$ times the identity matrix while $P_{2m+1}$ is another polynomial in the same variable times $\sigma_3$. In computing the expectation values, these polynomials cancel out in the ratios and all the $\beta$ dependence disappears leaving us with,

$$[A]_n = a\cos^2\theta + c\sin^2\theta + (-1)^n\sin\theta\cos\theta(b^*e^{-i\phi} + be^{i\phi})$$

$$[\Delta A]_n^2 = |b|^2 + \sin^2\theta\cos^2\theta\{(a-c)^2 - (be^{i\phi} + b^*e^{-i\phi})^2\}$$

$$+ (-1)^n\sin\theta\cos\theta\cos^2\theta(c-a)(be^{i\phi} + b^*e^{-i\phi})$$

From these it follows that change in the consecutive expectation values depends only on $b$ as it should since the diagonal part of $A$ commutes with the Hamiltonian. Taking $a = c = 0$ for simplicity and requiring that the change be at least as large as the uncertainty leads to,

$$\left|\frac{\sin\theta\cos\theta(be^{i\phi} + b^*e^{-i\phi})}{|b|}\right| \geq \frac{1}{\sqrt{5}}$$

This simple example illustrates that a discrete evolution of the type being considered could be independent of $\beta$, could have an oscillatory $n$-dependence and there could be a sub-class of states which are not eigenstates of the Hamiltonian and yet will not exhibit detectable evolution. These are of course special properties of the particular system.

More generically, one could try to see the $\beta$ dependence in the limit $\beta \to 0$. The expectation values can then be expressed as a power series in $\beta$. It turns out that,

$$[A]_{2m} \approx [A]_0 + o(\beta^2)$$

$$[A]_{2m+1} \approx \frac{[HAH]_0}{[H^2]_0} + o(\beta^2)$$

$$[\Delta A]_{2m}^2 \approx [\Delta A]_0^2 + o(\beta^2)$$

Thus the difference of expectation values at $n = 2m + 1$ and $n = 2m - 1$ is of order $\beta^2$ while the uncertainty at $n = 2m$ is the uncertainty at $n = 0$ plus a term of order $\beta^2$. For detectability then the uncertainty at $n = 0$ must be comparable to $\beta^2$. This gives a hint about the role of $\beta$. If we select a set of observables with respect to which we wish to detect an evolution then $\beta$ should be chosen to be of the order of (or larger than) the square root of the uncertainty of the observable with the smallest uncertainty. Note that this gives a
**lower limit** on the value of $\beta$. In this manner, the criterion of detectable evolution can be used to get some condition(s) on $\beta$. However there does not seem to be a simple way of obtaining an analogue of uncertainty relation. For continuous family $|\Phi(\tau)\rangle$, there is no $\beta$, the evolution is unitary and the usual results follow.

**Remarks:**

1) The possibility of a discrete time arises naturally for a theory presented in a frozen time form. Even conventionally presented theories can be cast in this form and we exploited this in constructing our example. For such theories (always a constrained theory), one needs to choose a suitable degree of freedom as a ‘time degree of freedom’. One can always view the kinematical Hilbert space as a tensor product of Hilbert space of the time degree of freedom and the Hilbert space of the rest of the degrees of freedom. Solutions of the constraint can then be obtained as a families of vectors in the non-time sector. The ‘time’ now appears as a label for each of the family and this could be continuous or discrete. The families themselves are then determined as solutions of differential or difference equation. The form and order of the equations depends on the form of the constraint, the choice of representation (or choice of basis in the Hilbert space of the time degree of freedom) and of course on the choice of the time degree of freedom. Except for these details, a discrete time presentation can be set up generally.

A continuum *approximation* for a discrete presentation can be looked for in the usual manner as indicated in subsection II B. The stronger notion of ‘pre-classicality’ however may not always be realizable. Even in our case, we do have *asymptotic* solutions which do have a pre-classical limit but *exact* solutions do not admit such a limit. Emergence of continuous time however can be sought via a transform instead of a limit.

Note that we did not need to be explicit about the Hilbert space of non-time degrees of freedom. Even the number of degrees of freedom is unimportant for discrete time description. These details are of course crucial in the construction of $\mathcal{H}_0$ and observables.

2) The parameter $\beta$ is a priori completely arbitrary and has dimensions of inverse energy,
$\hbar \beta$ is thus a time scale. What possible interpretation can one ascribe to this parameter? In particular, does it reflect some intrinsic property of the system (and thus is selected by the system) or is it related to the resolutions with which a set of measurements are performed (and thus is to be selected by the experimenter)? Quite independently, there are two time scales: the intrinsic one by which a physical system keeps evolving and the clock scale eg. the least count of an actual clock of an observer.

If $\hbar \beta$ is the intrinsic time scale then logic of continuum approximation would require that the clock scale be much much larger that the intrinsic one so that continuum time description is a very good approximation. Conversely if the clock scale is comparable to the intrinsic scale then one should use the discrete evolution. The schematic argument for small $\beta$ given above would now imply that discrete evolution may still not be observable if the uncertainties in the tracked observables are larger than permitted by the $\beta$.

The intrinsic time scale may be roughly estimated to be of the order of the inverse of the maximum uncertainty in energy measurement that may occur in the system. This need not be infinite, since there would be a maximum energy above which modeling of the physical system breaks down - eg. particle a box would not be a valid description for arbitrarily high energies though the spectrum of the Hamiltonian is of course unbounded.

If however $\hbar \beta$ is not an intrinsic time scale, then it needs to be adjusted depending upon what observables are used for tracking evolution. The small $\beta$ argument gives lower bounds on $\beta$ in terms of the uncertainties of the tracked observables. Unlike the continuous evolution, which is also unitary, the detectability of evolution is directly dependent on particular observables used for tracking.

We are unable to decide between the alternatives. It is possible that $\hbar \beta$ is a scale intermediate to the intrinsic and the clock scales. Considering analogy with the Immirzi parameter in the context of LQC, interpretation of $\beta$ here may also throw some hints about the role of the Immirzi parameter.

3) One of the powerful methods of studying semi-classical limit for systems with
phase space $R^{2N}$, is via the Wigner distribution function [1]. It is essentially a double Fourier transform of expectation value of a certain unitary operator. In the usual continuous time description, the distribution function satisfies the classical Liouville equation to leading order in $\hbar$ when the expectation value is taken with respect to a solution of the Schrodinger equation [12]. It would be interesting to repeat the steps with discrete time though it looks complicated because of the structure of the difference equation.

4) This work has been motivated by the LQC work. So what does it say about discrete time evolution in LQC? As mentioned in the introduction, at present the discussion of physical quantities such as inner products and matrix elements of observables is at a schematic level. The present work points out the possible pitfalls one may encounter. Our analysis of pre-classical limit indicates that such a limit could exist, at the level of states, only for solutions whose asymptotic behaviour has a characteristic root equal to 1. It may still go through at the level of expectation values if the largest root is positive. For the isotropic cosmology with positive spatial curvature (Bianchi-IX), for the expressions given in [3], there is neither a root equal to one nor is the highest root positive. However, independent of whether a pre-classical limit exist or not, one could go ahead with a discrete equation at the level of expectation values. One may then take recourse to Wigner distribution formalism to explore the semi-classical limit. This of course needs the Wigner distribution formalism to be developed in the context of the polymer representation.

While one may construct families of states and even arrange schemes to distinguish corresponding expectation values, it leaves unanswered the question as to why does any system evolve at all?

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