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Uniform discretizations: a quantization procedure for totally constrained systems including gravity

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Abstract. We present a new method for the quantization of totally constrained systems including general relativity. The method consists in constructing discretized theories that have a well defined and controlled continuum limit. The discrete theories are constraint-free and can be readily quantized. This provides a framework where one can introduce a relational notion of time and that nevertheless approximates in a well defined fashion the theory of interest. The method is equivalent to the group averaging procedure for many systems where the latter makes sense and provides a generalization otherwise. In the continuum limit it can be shown to contain, under certain assumptions, the "master constraint" of the "Phoenix project". It also provides a correspondence principle with the classical theory that does not require to consider the semiclassical limit.

1. Introduction

The issue of the dynamics is perhaps the central problem in canonical quantization approaches to totally constrained theories like quantum general relativity [1, 2]. There are three salient aspects of the problem that have prevented from advancing in the quantization. The first one is how to construct a space of physical states for the theory that are annihilated by the quantum constraints and that is endowed with a proper Hilbert space structure. The second issue is related to the introduction of a correspondence principle with the classical theory, in particular to check the constraint algebra at a quantum level. The third problem is how to address the "problem of time" [3] that is, to introduce a satisfactory picture for the dynamics of the theory in terms of observable quantities.

We have proposed in previous papers [4] a paradigm to deal with the above issues that consists in describing the theory in terms of a discrete evolution. This is analogous for instance to lattice QCD, where one uses a discrete theory to approximate and define the continuum quantum theory as a suitable limit. In our approach the discretization is carried out in such a way that the dynamics of the discrete theory is unconstrained. We call this approach "consistent discretizations". The lack of constraints in the discrete theory bypasses almost automatically the three issues mentioned above for the discrete theory, but leaves open the problem of how to define a continuum limit. One of the important points of our proposal is that the discretization is carried out in a way that the discretization step is dynamically determined and therefore one does not have a direct control on how to take the continuum limit as one does in ordinary discretizations.

In this article we want to spell out a constructive technique to define properly the quantum continuum limit. Our procedure can therefore be viewed as an alternative to the Dirac quantization procedure for a continuum theory in the sense that at the end of the day it yields a quantum continuum theory. We will see that the procedure has attractive advantages with respect to the Dirac procedure.

2. Uniform discretizations

A key element is the introduction of a set of discretizations for a given continuum theory called "uniform discretizations". These are such that the evolution steps are bounded by a value that one chooses in the initial data. The value of the constraints of the continuum theory (which are not exactly satisfied in the discrete theory) are also bounded throughout the evolution. This is of interest in itself since it is quite non-trivial to find discretizations of general relativity for which the constraints remain bounded. The important aspect is that since one controls the discretization step through the initial data, one can define properly a continuum limit just by choosing data that has a step as small as is desired.

We start by considering a canonical theory with a phase space with canonical variables q_i, p_i that is totally constrained, by this meaning that the total Hamiltonian H_T is a linear combination of N constraints ϕ_i which we will assume are first class. We are assuming we are dealing with a mechanical system with a finite number of degrees of freedom. This is of interest in the context we are discussing since field theories when formulated on the discrete space —as is common, for instance, in loop quantum gravity—, become such systems (although there are subtleties, as we discuss later on).

We will now introduce a discrete evolution given by the flux of a Hamiltonian H that is constructed from the constraints of the theory in a way we will soon discuss and such that the evolution of any dynamical variable A is given by

$$A_{n+1} = e^{\{\bullet,H\}}(A_n) \equiv A_n + \{A_n, H\} + \frac{1}{2}\{\{A_n, H\}, H\} + \cdots \quad (1)$$

As is obvious, H is a constant of the motion of the discrete evolution.

The uniform discretizations are given by a family of Hamiltonians H constructed in the following way. Consider a smooth function of N variables $f(x_1, \ldots, x_N)$ such that the following three conditions are satisfied: a) $f(x_1, \ldots, x_N) = 0 \iff x_i = 0 \forall i$ and otherwise $f > 0$; b) $\frac{\partial f}{\partial x_i}(0, \ldots, 0) = 0$; c) $\det \frac{\partial^2 f}{\partial x_i \partial x_j} \neq 0 \ \forall x$ and d) $f(\phi_1(q,p), \ldots \phi_N(q,p))$ is defined for all q, p in the complete phase space. Given this we define $H(q,p) \equiv f(\phi_1(q,p), \ldots \phi_N(q,p))$.

A particularly simple example is $H(q,p) = 1/2 \sum_{i=1}^{N} \phi_i(q,p)^2$, a choice that has interesting parallels with the "master constraint" of the "Phoenix project" [2] as we shall discuss later.

3. Continuum limit and relation to consistent discretizations

An important point is that if we choose initial data such that $H < \epsilon$ then ϕ_i remain bounded throughout the evolution and will tend to zero in the limit $\epsilon \to 0$. Let us see that in this limit one recovers the evolution equations given by the total Hamiltonian H_T in the constrained continuum theory. Let H as in the simple example above and take its initial value to be $H_0 = \delta^2/2$. We define $\lambda_i = \phi_i/\delta$, and therefore $\sum_{i=1}^{N} \lambda_i^2 = 1$. The evolution of the dynamical variable q is given by,

$$q_{n+1} = q_n + \sum_{i=1}^{N} \{q_n, \phi_i\} \lambda_i \delta + O(\delta^2) \quad (2)$$

and if we define $\dot{q} \equiv \lim_{\delta\to 0}(q_{n+1} - q_n)/\delta$, where we have identified the "time evolution" step with the initial data choice for δ, one then has $\dot{q} = \sum_{i=1}^{N}\{q, \phi_i\}\lambda_i$, and similarly for other dynamical variables. The specific values of the multipliers λ_i depend on the initial values of the constraints ϕ_i. Notice that taking the continuum limit requires that the Lagrange multipliers be determined as is usual in the consistent discretization approach, but are well defined bounded real functions of phase space, bypassing an important objection to the original approach.

One could recast the current proposal in terms of the original approach to consistent discretizations. There one started from an action and noted that the Lagrangian could be viewed as a the generating function of a canonical transformation between instants n and $n+1$. To be concrete, let us analyze a system with N Abelian constraints. We introduce the Lagrangian

$$L(q_n, q_{n+1}, \lambda_1, \ldots, \lambda_N) = S(q_n, q_{n+1}, \lambda_1, \ldots, \lambda_N) + g(\lambda_1, \ldots, \lambda_N) \tag{3}$$

where L is a type 1 generating function of a canonical transformation between canonical variables q_n, p_n and q_{n+1}, p_{n+1}, S is Hamilton's principal function for a given set of Lagrange multipliers $\lambda_1, \ldots, \lambda_N$ (they are evaluated at instant n, we omit the subscript for simplicity), g is such that $g(0) = 0$ and the mappings $\lambda_i \to \frac{\partial g}{\partial \lambda_i}$ and $x_i \to \frac{\partial f}{\partial x_i}$ are inverse where f is the function used to define the Hamiltonian. The generating function yields the canonical momenta in the usual way $p_{n+1} = \partial L/\partial q_{n+1}$, $p_n = -\partial L/\partial q_n$. One also has that $\partial L/\partial \lambda_i = 0$ and this determines the the Lagrange multipliers, $\lambda_i = h_i(\phi)$, where h_i is the inverse function of the mapping defined by $\lambda_i \to \frac{\partial g}{\partial \lambda_i}$. This evolution corresponds to a Hamiltonian $H = f(\phi_1, \ldots, \phi_N)$, with $\partial_i f = h_i$. In particular, the simplest case is when $g = \sum_{i=1}^{N} x_i^2/2$ and then $H = \sum_{i=1}^{N} \phi_i^2/2$. The generating function L allows to determine the discrete evolution that preserves exactly the value of the constraints of the continuum theory and recovers the continuum limit when all $\phi_i \to 0$ in the initial data. We therefore see that the approach proposed here is a particular case of the consistent discretizations. We have just chosen to discretize things in a way that the Hamiltonian is simple —rather than the action— and this guarantees a good continuum limit.

The constants of the motion of the discrete theory are quantities that have vanishing Poisson bracket with the Hamiltonian, $\{O_i^D, H\} = 0$ and in the continuum limit $H_0 \to 0$ reproduce, as functions of phase space, the "perennials" of the continuum theory: $O_i^C = \lim_{H_0\to 0} O_i^D$. This can be immediately seen from the fact that the discrete equations reproduce the continuum equations for any dynamical variable in the continuum limit. Conversely, for every perennial of the continuum theory there exists a constant of the motion (in general many constants) of the discrete theory that reduce to the given perennial in the continuum limit. We have therefore shown that uniform discretizations recover the constraints and the perennials of the continuum theory and therefore provide a good starting point for a quantization of the continuum theory.

4. Quantization

We now turn our attention to the quantum theory. We will introduce a Heisenberg quantization for the discrete theory (this is more natural given that one has an explicit evolution). To quantize the theory we follow several steps. We start with the classical discrete system constructed as in the previous section, we eliminate the canonical variables at level $n+1$ in terms of the variables at level n, $q_{n+1} = q_{n+1}(q_n, p_n)$, $\quad p_{n+1} = p_{n+1}(q_n, p_n)$.

We then define the kinematical space of states of the quantum theory, $\mathcal{H}_k$, as the space of functions of N real variables $\psi(q)$ that are square integrable. In this space we define operators $\hat{Q}$ and $\hat{P}$ as usual. To construct the operators at other time levels (in the Heisenberg Picture) we introduce a linear invertible operator $\hat{U}$ that we will define later and we take

$$\hat{Q}_n \equiv \hat{U}^{-1}\hat{Q}_{n-1}\hat{U} = \hat{U}^{-n}\hat{Q}_0\,\hat{U}^n\,, \quad \hat{P}_n \equiv \hat{U}^{-1}\hat{P}_{n-1}\hat{U} = \hat{U}^{-n}\hat{P}_0\,\hat{U}^n\,. \tag{4}$$

When the evolution is determined by a discrete Hamiltonian H, as is the case in the uniform discretizations, the evolution operator is given by $\hat{U} = e^{-i\hat{H}/\hbar}$. Notice that $\hat{U}$ may also be determined by requiring that the fundamental operators satisfy an operatorial version of the evolution equations,

$$\hat{Q}_n\hat{U} - \hat{U}Q_{n+1}(\hat{Q}_n, \hat{P}_n) = 0, \quad \hat{P}_n\hat{U} - \hat{U}P_{n+1}(\hat{Q}_n, \hat{P}_n) = 0, \tag{5}$$

and this provides a consistency criterion for the construction of $\hat{U}$.

At a classical level $H = 0$ if and only if the constraints $\phi_i = 0$. There exists a natural definition of the physical space of the continuum theory that does not require that we refer to the constraint. Since we know that $\hat{U} = \exp(-i\hat{H}/\hbar)$, a necessary condition satisfied by the states of the physical space of the continuum theory, $\psi \in \mathcal{H}_{\rm phys}$ is given by $\hat{U}\psi = \psi$. More precisely the states ψ of $\mathcal{H}_{\rm phys}$ should belong to the dual of a space Φ of functions sufficiently regular on $\mathcal{H}_k$. That is, the states $\psi \in \mathcal{H}_{\rm phys}$ satisfy $\int \psi^*\hat{U}^\dagger\varphi dq = \int \psi^*\varphi dq$, where $\varphi \in \Phi$. This condition characterizes the quantum physical space of a constrained continuum theory without needing to implement the constraints as quantum operators by using the discretization technique.

The unitary operators of the discrete theory allow to construct the "projectors" onto the physical space of the continuum theory, which is one of the main goals of any quantization procedure based on Dirac's ideas. It should be noted that these are really generalized projectors in the sense that they project to a set of functions that belong in the dual of a subspace of sufficiently well behaved functions of $\mathcal{H}_k$. All of this is achieved without having to define the quantum constraint. To construct the "projectors" one can compute,

$$\hat{P} \equiv \lim_{M\to\infty} C_M\hat{U}^M. \tag{6}$$

If such a limit exists for some C_M such that $\lim_{M\to\infty}(C_{M+1}/C_M) = 1$ then $\hat{U}\hat{P} = \hat{P}$, and we have that $\hat{U}\hat{P}\psi = \hat{P}\psi$, $\forall\psi \in \mathcal{H}_{\rm k}$.

5. Examples

The limit exists in several examples in which $\hat{H}$ has a continuum spectrum, as we shall see. If the spectrum is discrete with eigenvalues e_i and it contains a vanishing eigenvalue e_{i_0} then a projector is trivially defined as $|e_{i_0}><e_{i_0}|$. A constructive procedure leading to a general definition of the projector in terms of the discrete evolution operator $\hat{U}$ valid for any spectrum, continuum or discrete, is given by:

$$\hat{P} \equiv \lim_{M\to\infty} \sum_{n=M}^{{\rm Int}(rM)} \frac{C_n\hat{U}^n}{{\rm Int}(rM) - M}. \tag{7}$$

where r is a real number greater than one and ${\rm Int}(rM)$ is the integer part of rM. If $\hat{U}$ has a continuum spectrum this definition is a trivial consequence of the previous one. In the case of a discrete spectrum one can check that the definition works recalling the definition of the Kronecker delta in terms of a Fourier series. Notice that the definition of physical space that Thiemann introduces in the "phoenix project" [2], is equivalent to the choice we make if one is considering the Hamiltonian that is quadratic in the constraints. Furthermore, given two states of $\mathcal{H}_{\rm phys}$, $\psi_{\rm ph}$, $\phi_{\rm ph}$, where $\psi_{\rm ph} = \hat{P}\psi$, and $\phi_{\rm ph} = \hat{P}\phi$, the physical inner product is defined by $<\psi_{\rm ph}|\phi_{\rm ph}> = \int dq\phi(q)^*\hat{P}\psi(q)$ and a physical inner product is determined by the projector constructed from the discrete theory.

We now illustrate the technique with a rather general example. We consider a generic mechanical system with a finite dimensional phase space with one constraint $\phi = 0$. We will show that the projector constructed with our technique reproduces the one constructed with group averaging techniques [5]. That is,

$$P = \lim_{M\to\infty} \sqrt{\frac{iM}{\pi}} e^{-iM\phi^2} = \int_{-\infty}^{\infty} \frac{d\mu}{2\pi} e^{i\mu\phi}. \tag{8}$$

To make contact with the group averaging case we need to assume that ϕ is a self-adjoint operator in the kinematical phase space with an eigenbasis given by $\phi|\alpha >= \phi(\alpha)|\alpha >$ and $1 = \int |\alpha >< \alpha| d\alpha$. The proof of the equivalence is,

$$P = P \int |\alpha >< \alpha| d\alpha = \int \lim_{M\to\infty} \sqrt{\frac{iM}{\pi}} e^{-iM\phi^2} |\alpha >< \alpha| \tag{9}$$

and noting that $\lim_{M\to\infty} \sqrt{\frac{iM}{\pi}} e^{-iMx^2} = \delta(x) = \int_{-\infty}^{\infty} \frac{d\mu}{2\pi} e^{i\mu x}$ the proof is complete. For the proof we assumed a quadratic form of the Hamiltonian, but can actually be extended to Hamiltonians of the general form we discussed above, computing the integral by steepest descents. The proof can also be extended to systems with N Abelian constraints by noting that $\lim_{M\to\infty}(\frac{iM}{\pi})^{N/2} e^{-iM\vec{x}.\vec{x}} = \delta(\vec{x}) = \int_{-\infty}^{\infty} d\mu^N e^{i\vec{\mu}.\vec{x}}/(2\pi)^N$. This includes important cases like gravity in $2+1$ dimensions, where one can immediately reproduce the results obtained by Perez and Noui [6] via group averaging. It should be noted that the generic case of a field theory with first class constraints, like general relativity is expected to be involved. The reason is that the discrete version of the constraints will fail to be first class. One can show that the technique we introduced reproduces the correct continuum limit if one uses Dirac brackets to deal with the fact that the constraints are not first class. This suggests that the proposal will be significantly different from others like the master constraint, where the fact that the discrete constraints are not first class is not included. Further details and examples can be found in [9].

6. Conclusions

Summarizing, the method of uniform discretizations allows to tackle satisfactorily the three central problems of the dynamics of quantum general relativity and provides new avenues for studying numerically classical relativity as well. It is based on a set of discretizations generated by Hamiltonians that contain as a particular case the quadratic Hamiltonian of Thiemann's "master constraint programme". The phase space of the continuum theory and the physical inner product can be constructed in a straightforward way from the discrete theory and therefore provides a generalization of the group averaging extension of the Dirac procedure to systems with structure functions in their constraint algebra, like is the case in general relativity. The use of non-quadratic Hamiltonians is possible and adds flexibility to the method. The flexibility is crucial, for instance in tackling in an extremely compact and straightforward way gravity in $2+1$ dimensions (see reference [9]). In other approaches to the dynamics of quantum gravity a major obstacle is the need to define the constraints as quantum operators in an unambiguous way. This may be due to the fact that the constraints are only well defined on a diffeomorphism invariant space of sets where the constraint algebra is trivial, or, as in the case of the "master constraint" since one has only one constraint. This requires an a-posteriori study of each quantization proposal to determine if they can reproduce general relativity in some suitable semi-classical limit. This is complex and difficult to carry out. One is therefore left with proposals that one is not even sure if they have any connection with the theory one desires to quantize. In the discrete approach $\hat{U} = e^{-i\hat{H}/\hbar}$ must implement the discrete classical evolution associated to the canonical transformations and therefore one has a correspondence constructive principle as a guide that requires that the quantum evolution equations reproduce the Heisenberg equations associated with the classical theory. Contrary to other methods, one can construct the continuum theory as approximated by a discrete theory in the kinematical Hilbert space. This allows the use of operators that can be genuinely used as quantum mechanical clocks and is therefore possible to characterize the evolution in a relational way in terms of conditional probabilities [7]. The method is therefore devoid of the usual conceptual problems of canonical quantum gravity.

In conclusion, just like lattice methods did for QCD, the uniform discretizations shift the main problem of the quantization of constrained systems into one of computational nature. The only major hurdles that could stand in the way is that one cannot find a unitary operator that reproduces the classical equations or that the continuum limit may not exist for the case of full general relativity . In the latter case, this will be a strong indication that the theory does not exist. The method allows to incorporate all the benefits of the kinematics of loop quantum gravity [8] and provides an unambiguous avenue to characterize the dynamics and complete the quantum theory.

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