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Self-adjointness in the Hamiltonians of deparameterized totally constrained theories: a model

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Several proposals to deal with the dynamics of general relativity involve gauge fixings or the introduction matter fields in terms of which the theory is deparameterized. The resulting theories have true Hamiltonians for their evolution that usually involve square roots, and this poses certain challenges for their implementation as self-adjoint quantum operators. We show in the context of a simple model of totally constrained theory that one can introduce related, well defined operators that reproduce semiclassically the same physics as the original ones, at least for states peaked in the regions of phase space where their associated classical quantities are well defined.

I. INTRODUCTION

Two important problems in the canonical approach to quantum gravity are the issue of the constraint algebra and of the physical interpretation of the dynamics of the theory. In the usual canonical formulations, general relativity has constraints that close a first class algebra in the Dirac sense. It is not a Lie algebra as it has structure functions. In particular the Poisson bracket of two Hamiltonian constraints is proportional to a diffeomorphism constraint with the proportionality factor a function of the canonical variables. This poses problems at the time of quantizing the theory. In particular it is easy to show that one cannot implement the constraints as self adjoint operators and hope to close the algebra at a quantum level. The physical interpretation of the dynamics of the theory also requires to disentangle the resulting "frozen" formalism, since there is no non-vanishing true Hamiltonian for the theory, in terms of Dirac observables. However, for the case of pure gravity in vacuum we do not know a single Dirac observable in closed form (apart from certain formal constructions [1]). One can expect that approximate treatments may yield expressions for Dirac observables, but only in certain regimes [2].

The previously listed problems have led to various proposals to deal with them. One possibility is to gauge fix the theory. Gauge fixing eliminates the constraints, the issue of the constraint algebra, and reveals the true dynamics of the theory. The quantization should therefore presumably be straightforward. But it turns out it is not. An example is given by recent proposals to gauge fix spherically symmetric gravity coupled to a scalar field [3]. Although a gauge fixing in which the true Hamiltonian is the integral of a local scalar density has recently been achieved, its definition involves square roots. In this particular case there is no reason why generically what appears under the square root should be a positive quantity. This just shows that one cannot find a single gauge fixing that works generically for all types of initial data (in the proposal of [3] one can find different gauge fixings for different types of initial data that yield positive quantities inside the square roots). This example is particularly revealing of the limitations one faces when gauge fixing since in it all things are analytically under control. Nevertheless, promoting the resulting Hamiltonian to a self-adjoint operator is challenging due to the presence of square roots.

Another proposal is to consider the inclusion of matter in the theory as a tool to deparameterize it and construct Dirac observables, starting with the pioneering work of Brown and Kuchař [4] (see [5] for a recent review). In a sense, this is very natural, since in the real world we rely on matter to construct reference frames in terms of which we describe physics. With the introduction of a certain kind of matter, one can use it as as clock to deparameterize the theory and have a true Hamiltonian. In many of these proposals the diffeomorphism constraint remains, but the true Hamiltonian is diffeomorphism invariant. However, since most forms of matter (see [6] for an exception) have Hamiltonians that are quadratic in the fields and momenta, when one uses them to deparameterize the theory one is again led to expressions for the Hamiltonian that involve square roots. One can show in many cases that the expression under the square root is classically positive definite on-shell. However, when one quantizes there have been arguments put forward [7, 8] saying that one needs to consider negative values.

Motivated by these occurrences of square roots, we would like to analyze a simple model where square roots occur, and to study the consequences of one procedure to deal with them upon quantization. The model is the one considered by Rovelli [9] and can be thought of as two harmonic oscillators with a constant sum of their energies. The quantization of this model is challenging since the phase space is compact and it therefore does not admit a Hamiltonian structure. Nevertheless global Dirac observables exist and a full quantization is possible [10]. It is therefore a good arena to compare the full quantization with the types of "truncated" quantizations obtained by using the techniques one uses to deal with square roots.

II. THE MODEL AND ITS QUANTIZATION

The model [9] has a four dimensional phase space q_1, q_2, p_1, p_2 with a constraint given by

$$C = \left[-\frac{1}{2}\left(p_1^2+p_2^2+q_1^2+q_2^2\right)+M\right], \tag{1}$$

with M a constant. The surface $C=0$ is a pre-symplectic space without a true Hamiltonian structure since it is compact.

The reduced phase space due to the constraint $C=0$ can be parameterized as,

$$q_1 = \sqrt{2A}\sin\tau, \tag{2}$$

$$q_2 = \sqrt{2M-2A}\sin(\tau+\phi). \tag{3}$$

A and ϕ constants that can later be identified as Dirac observables of the theory. If we choose the lapse as $N=1$ then $\dot{q}_1=-p_1$ and $p_1=-\sqrt{2A}\cos\tau$ and similarly $\dot{q}_2=-p_2$ and $p_2=-\sqrt{2M-2A}\cos(\tau+\phi)$.

The exact theory for this model was developed in [10]. One can define[1] three angular momentum Dirac observables,

$$L_x = -\frac{1}{2}\left(p_1q_2-p_2q_1\right) = -\sqrt{A(M-A)}\sin\phi, \tag{4}$$

$$L_y = \frac{1}{2}\left(p_1p_2+q_1q_2\right) = \sqrt{A(M-A)}\cos\phi, \tag{5}$$

$$L_z = \frac{1}{4}\left(p_1^2-p_2^2+q_1^2-q_2^2\right) = A-\frac{M}{2}, \tag{6}$$

such that $L^2=\frac{M^2}{4}$. One can define an angular momentum basis $|j,m\rangle$ with j integer or half-integer such that $\hat{L}_z|j,m\rangle = m|j,m\rangle$. Notice that in the constant M cannot take arbitrary values in the quantum theory, $M^2_{\text{Full}} = j(j+1)$. We use "full" to refer to the full quantization since later we will compare with the truncated quantization.

The exact expression for the observable $\hat{A}$ is given by,

$$\hat{A}_{\text{Full}}|j,m\rangle = \left(\hat{L}_z+\frac{M}{2}\right)|j,m\rangle = \left(m+\sqrt{j(j+1)}\right)|j,m\rangle. \tag{7}$$

For the observable L_x, L_x we introduce the usual notation of raising and lowering operators $L_x=(L_++L_-)/2$ and $L_y=(L_+-L_-)/(2i)$, in terms of which we have,

$$\hat{L}_x^{\text{Full}}|m\rangle = \frac{\hat{L}_++\hat{L}_-}{2}|m\rangle = \frac{\sqrt{j(j+1)-m(m+1)}}{2}|j,m+1\rangle + \frac{\sqrt{j(j+1)-m(m-1)}}{2}|j,m-1\rangle, \tag{8}$$

and we will find convenient to compare with the truncated theory to redefine $m=j-n$, for a given j,

$$\hat{L}_x^{\text{Full}}|j,m\rangle = \hat{L}_x^{\text{Full}}|n\rangle = \frac{\sqrt{(n+1)(2j-n)}}{2}|n+1\rangle + \frac{\sqrt{n(2j-n+1)}}{2}|n-1\rangle. \tag{9}$$

A similar construction can be carried out for $\hat{L}_y^{\text{Full}}$.

III. GAUGE FIXING

Let us now consider a gauge fixed treatment of the model. To this aim we will proceed locally in phase space, and introduce a total Hamiltonian $H_T=NC$ with N a Lagrange multiplier in order to fix the gauge. We choose a gauge $q_1=t$, with t the time parameter associated with the evolution generated by the total Hamiltonian. This leads to $\dot{q}_1=1$ and therefore,

$$1 = \{q_1, H_T\} = -Np_1, \tag{10}$$

[1] The definition chosen differs from that of [9] and [10]. What we call L_y would correspond to L_x of those references and what we call L_x would be $-L_y$. Both satisfy the algebra of angular momenta. The truncated theory we will consider later does not have such symmetry and only approximates well the choice we make in this paper.

which fixes the lapse $N=-1/p_1$ with $p_1=-\sqrt{2M-p_2^2-q_2^2-t^2}$ and therefore $N>0$. This already tells us that the Hamiltonian theory is not globally defined as for large enough t the square root is imaginary. The total Hamiltonian now reads,

$$H_T=\frac{1}{p_1}\left[\frac{1}{2}\left(p_1^2+p_2^2+q_1^2+q_2^2\right),-M\right] \tag{11}$$

before the strong imposition of the constraint. We get the equations of motion by computing the Poisson brackets of the variables with the total Hamiltonian,

$$\dot{q}_2 = \frac{p_2}{p_1}, \tag{12}$$

$$\dot{p}_2 = -\frac{q_2}{p_1}. \tag{13}$$

These equations can be obtained from a true Hamiltonian,

$$H_{\rm True}=\sqrt{2M-p_2^2-q_2^2-t^2}. \tag{14}$$

Due to the square root, at a quantum level $H_{\rm True}$ will not become a self-adjoint operator. However, one can define Hamiltonians that approximate well the exact solutions for semiclassical excitations around classical exact solutions for which $H_{\rm True}$ is real. An example could be to take the absolute value of what is inside the square root in $H_{\rm True}$. Or to consider its square and then take the real branch of its fourth root. If one thinks of cases of interest, like gauge fixings in spherically symmetric gravity, this means one could use these techniques to study, for instance, black hole evaporation for large black holes.

The exact evolution (2,3) written in this gauge, since $q_1=t$, and $\tau=\sin^{-1}\left(\frac{t}{\sqrt{2A}}\right)$, is given by

$$q_2(t) = \sqrt{\frac{M}{A}-1}\left[t\cos\phi+\sqrt{2A-t^2}\sin\phi\right] \tag{15}$$

$$p_2(t) = \sqrt{\frac{M}{A}-1}\left[\sqrt{2A-t^2}\cos\phi-t\sin\phi\right]. \tag{16}$$

This solution can also be obtained by integrating the evolution equation stemming from the Hamiltonians H_T (11) and $H_{\rm True}$ (14). Notice that the gauge fixed solution is not globally defined as is readily seen from the presence of the inverse trigonometric function, so not all values of τ are obtained from t. The solution therefore covers a portion of phase space until for some values of t the solution becomes complex.

IV. QUANTIZATION OF THE TRUNCATED THEORY

The quantization of the Hamiltonian $H_{\rm True}$ (14) has the problem of the square root. In fact, one can show [8] that the operators obtained by a straightforward quantization of $H_{\rm True}$ are not normal. The strategy will to substitute another expression for $H_{\rm True}$ such that they both coincide in the region of the phase space where the argument of the square root is positive, for instance [11],

$$\tilde{H}_{\rm True}=\sqrt{|2M-p_2^2-q_2^2-t^2|}=\left[\left(2M-p_2^2-q_2^2-t^2\right)^2\right]^{1/4}. \tag{17}$$

This Hamiltonian ensures that the equations of motion reproduce those of the classical theory in the region in which $A>t^2/2$. So $\tilde{H}_{\rm True}$ and $H_{\rm True}$ lead to the same solutions in the region in which $H_{\rm True}$ is real. We call the resulting theory "truncated" since it will differ from the original one for large values of $p_2^2+q_2^2$.

In order to quantize we notice that $p_2^2+q_2^2$ is the Hamiltonian of a harmonic oscillator, and therefore one can use the quantization technique of creation and annihilation operators. In particular the Hamiltonian will be a function of the number operator.

As usual we define the classical quantities,

$$a = \frac{1}{\sqrt{2}}\left(q_2+ip_2\right) \tag{18}$$

$$a^* = \frac{1}{\sqrt{2}}\left(q_2-ip_2\right). \tag{19}$$

These quantities can be readily quantized. We introduce the number operator $\hat{N} = \hat{a}^\dagger \hat{a}$, so we have,

$$\hat{p}_2^2 + \hat{q}_2^2 = 2\hat{a}^\dagger \hat{a} + 1 = 2\hat{N} + 1, \tag{20}$$

and we have that $\left[\hat{N}, \hat{H}_{\rm True}\right] = 0$. Introducing the number basis $\hat{N}|n\rangle = n|n\rangle$, we have that

$$2\hat{A}^{\rm Truncated} = 2M_{\rm Truncated} - \hat{p}_2^2 - \hat{q}_2^2 = 2M_{\rm Truncated} - 2\hat{N} - 1, \tag{21}$$

with the Dirac observable becoming the self-adjoint operator,

$$\hat{A}^{\rm Truncated}|n\rangle = \left(M_{\rm Truncated} - n - \frac{1}{2}\right)|n\rangle = A_n|n\rangle. \tag{22}$$

Notice that in this quantization the value of $M_{\rm Truncated}$ is arbitrary, unlike in the full quantization.

V. COMPARISON OF THE FULL AND TRUNCATED THEORIES

The Hilbert space of the truncated theory $|n\rangle$ with $n \in [0,\infty]$ is infinite dimensional. The Hilbert space of the full theory $|j,m\rangle$ with j either a given integer or semi-integer and $-j < m < -j$ and m differing from j by an integer is finite dimensional with dimension $2j+1$. However, it is clear that if one admits arbitrary values of n in the truncated theory this will not correspond to real solutions of the theory one started from since $A < 0$ in that case. To compare the full and truncated theories we need to identify a correspondence between their Hilbert spaces. The best way to see the correspondence is to identify $|j,m\rangle$ with $|n\rangle$ with $n = j - m$. We will see also that $M_{\rm Truncated} = 2j + 1$ in order to reproduce the eigenvalues of $\hat{A}_{\rm Full}$.

We would like to compare the Hilbert space of $\hat{\tilde{H}}$ with that of the full theory. We will see that $\mathcal{H}_{\rm Full} \subset \mathcal{H}_{\rm Truncated}$. Since all quantities of the theory can be written in terms of the Dirac observables, it suffices to study their action. We will see that their action coincides for $t^2/2 < A_n$.

Therefore in the truncated theory $M/2 = j + 1/2$. Let us start with the observable A

The exact expression for the observable $\hat{A}$ in the full theory is given by,

$$\hat{A}_{\rm Full}|j,m\rangle = \left(\hat{L}_z + \frac{M}{2}\right)|j,m\rangle = \left(m + \sqrt{j(j+1)}\right)|j,m\rangle = A^{\rm Full}_{j,m}|j,m\rangle, \tag{23}$$

whereas the truncated expression is given by

$$\hat{A}_{\rm Truncated}|n\rangle = \left(M_{\rm Truncated} - n - \frac{1}{2}\right)|n\rangle = A^{\rm Truncated}_n|n\rangle. \tag{24}$$

The difference in eigenvalues of $\hat{A}_{\rm Exact}$ and $\hat{A}_{\rm Truncated}$, using the identification of the Hilbert spaces and the choice of $M_{\rm Truncated} = 2j + 1$ is,

$$A^{\rm Full}_{j,j-n} - A^{\rm Truncated}_n = j + \sqrt{j(j+1)} - M + \frac{1}{2} = j + \sqrt{j(j+1)} - 2j - \frac{1}{2}. \tag{25}$$

If $j \gg 1$ then the difference vanishes, it goes as $O(1/j)$. The condition $A > 0$ is equivalent to $2j - n > 0$, so $n < 2j$ and the corresponding subspace of the Hilbert space has the same number of elements as in the full case.

To compare the second observable, let us consider L_x in the Heisenberg representation. In the gauge considered we have that $q_1 = t$, and q_2, p_1, p_2 are given in section III. Substituting them in L_x one recovers expression (4),

$$L_x = -\frac{1}{2}\left(p_1 q_2 - p_2 q_1\right) = -\sqrt{A\left(M - A\right)}\sin\phi \tag{26}$$

and is time independent and therefore its operator representations in the Heisenberg and Schrödinger representations coincide. This expression can be rewritten as,

$$\hat{L}_x = -\frac{1}{2}\sqrt{2\hat{A}^{\rm Truncated}}\hat{q}_2(0). \tag{27}$$

This can be realized in the basis $|n\rangle$ by substituting $\hat{q}_2(0)$ in terms of the creation and annihilation operators. To have a self-adjoint operator we write,

$$\hat{L}_x = \frac{1}{2}\sqrt[4]{\hat{A}^{\rm Truncated}}\left(\hat{a}+\hat{a}^\dagger\right)\sqrt[4]{A^{\widehat{\rm Truncated}}}, \tag{28}$$

which explicitly gives,

$$\hat{L}^H_x|n\rangle = \frac{\sqrt{(n+1)(2j-n)-\frac{1}{4}}}{2}|n+1\rangle + \frac{\sqrt{n(2j-n+1)-\frac{1}{4}}}{2}|n-1\rangle. \tag{29}$$

We can now compare the action of this truncated operator with that of the full theory, which we computed in equation (9). The semiclassical approximation works best when $A \gg t^2/2$ so we are away from the place where the gauge fixing fails and when $A \ll M$ since the expressions obtained were up to order $1/M$. In that regime equations (9) and (29) agree. A similar discussion holds for $\hat{L}_y$.

One can also compute the evolving constants $q_2(t), p_2(t)$ in this space and compare with the exact ones of reference [10]. In the regime discussed they agree.

VI. CONCLUSIONS

We have shown in a totally constrained model that gauge fixing leads to expressions that may be ill defined for certain regions of phase space. This is in analogy with what occurs in gauge fixings in gravity and when one introduces matter to deparameterize the theory. We show that one can introduce a quantization based on a "truncated" version of the theory with well defined self-adjoint operators. It reproduces in the semi-classical limit the correct physics of the original theory in the region of phase-space where the gauge fixing is well defined.

Among the lessons learned from the model is that the Hilbert space of the truncated and full theory can be quite different and one needs to restrict the one of the truncated theory in order to have agreement between them. We also see one does not recover everything of the full theory. In this particular case one of the constants of the model takes a restricted set of values in the full theory and this is not captured by the truncated theory. The approximation gets worse as one gets close in phase space to where the gauge fixing stops being valid.

Another point is that we have considered the observables of the truncated theory for positive A. For negative values of A there exist observables of the truncated theory that coincide for positive values of A with those of the full theory. For negative values of A the comparison makes no sense as the observables of the full theory are not well defined. In particular the algebra of angular momentum does not hold for those observables of the truncated theory. That is the root of having to choose one particular form of the observables of the full theory to approximate, since one does not have present the symmetry $L_x \to L_y$, $L_y \to -L_x$ one has in the angular momentum algebra.

This example suggests a procedure to extract (at least certain) physical predictions from theories that cannot themselves be quantized properly due to the lack of self-adjoint operators.

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