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Quantum scalar field in quantum gravity: the vacuum in the spherically symmetric case

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We study gravity coupled to a scalar field in spherical symmetry using loop quantum gravity techniques. Since this model has local degrees of freedom, one has to face "the problem of dynamics", that is, diffeomorphism and Hamiltonian constraints that do not form a Lie algebra. We tackle the problem using the "uniform discretization" technique. We study the expectation value of the master constraint and argue that among the states that minimize the master constraint is one that incorporates the usual Fock vacuum for the matter content of the theory.

I. INTRODUCTION

Loop quantum gravity is being explored in model situations of increasing complexity. There has been steady advance in treating homogeneous cosmologies [1], an area of activity that has come to be known as loop quantum cosmology. There has also been progress in spherical symmetry in vacuum [2]. However, in all these cases one did not have to face the "problem of dynamics", i.e. dealing with the non-Lie algebra of constraints of general relativity. In homogeneous cosmologies there is only one constraint and it therefore has a trivial algebra. In spherical symmetry special gauges were chosen that resulted in an Abelian algebra. In this paper we would like to study spherically symmetric gravity coupled to a spherically symmetric scalar field using loop quantum gravity techniques. It is not known in this situation how to formulate the problem in a way that one ends up with a Lie algebra of constraints. A total gauge fixing was introduced by Unruh [3], but it leads to a non-local expression for the Hamiltonian. Here we will fix partially the gauge to eliminate the diffeomorphism constraint in order to simplify things. This still leads to a Hamiltonian constraint that has a non-Lie Poisson bracket with itself, involving structure functions. To treat this problem we will use the "uniform discretization" technique [4]. We will introduce a variational technique adapted to the minimization of the master constraint (in the context of uniform discretizations one should probably refer to it as "master operator" since it only vanishes in the continuum limit). In the case that zero is in the kernel of the master constraint the technique yields the correct physical state in model situations.

The inclusion of scalar fields in spherical symmetry opens a rich set of possibilities to be studied including the formation of black holes, critical collapse, the emergence of Hawking radiation, among others. Here we will have much more modest goals: to see how the complete theory approximates the vacuum state of the scalar field living on a flat space-time. An outstanding problem in a full quantum gravity treatment involving matter fields is the emergence of a vacuum state for the fields and what relation it may have to the ordinary Fock vacuum of quantum field theory in curved space-time. We will apply the variational technique in the case of spherically symmetric gravity coupled to a scalar field and show that it yields a vacuum state that is closely related to the Fock one.

The organization of this paper is as follows: in section II we review the classical theory. In section III we discuss the quantization of a spherical scalar field in a classical flat space-time in order to have something to compare with the full case. In section IV we study the full quantization of gravity and the scalar field, using a variational technique to minimize the master constraint. We end with a discussion.

II. SPHERICALLY SYMMETRIC GRAVITY WITH A SCALAR FIELD: THE CLASSICAL THEORY

Spherically symmetric gravity with the Ashtekar new variables has been studied in detail in [5] and [6]. Here we present only a brief summary. One assumes that the topology of the spatial manifold is of the form $\Sigma = R^+ \times S^2$. We will choose a radial coordinate x and study the theory in the range $[0, \infty]$. The invariant connection can be written as,

$$A = A_x(x)\Lambda_3 dx + (A_1(x)\Lambda_1 + A_2(x)\Lambda_2)\, d\theta + ((A_1(x)\Lambda_2 - A_2(x)\Lambda_1)\sin\theta + \Lambda_3\cos\theta)\, d\varphi, \quad (1)$$

where A_x, A_1 and A_2 are real arbitrary functions on R^+, the Λ_I are generators of $su(2)$, for instance $\Lambda_I = -i\sigma_I/2$ where σ_I are the Pauli matrices or rigid rotations thereof. The invariant triad takes the form,

$$E = E^x(x)\Lambda_3 \sin\theta \frac{\partial}{\partial x} + \left(E^1(x)\Lambda_1 + E^2(x)\Lambda_2\right)\sin\theta \frac{\partial}{\partial\theta}$$

$$+\left(E^1(x)\Lambda_2 - E^2(x)\Lambda_1\right)\frac{\partial}{\partial\varphi}, \tag{2}$$

where again, E^x, E^1 and E^2 are functions on R^+.

As discussed in our recent paper[5] and originally by Bojowald and Swiderski[6], it is best to make several changes of variables to simplify things and improve asymptotic behaviors. It is also useful to gauge fix the diffeomorphism constraint to simplify the model as much as possible. It would be too lengthy and not particularly useful to go through all the steps here. It suffices to notice that one is left with two pairs of canonical variables E^φ, K_φ and E^x, K_x, and that they are related to the traditional canonical variables in spherical symmetry $ds^2 = \Lambda^2 dx^2 + R^2 d\Omega^2$ by $\Lambda = E^\varphi/\sqrt{|E^x|}$, $P_\Lambda = -\sqrt{|E^x|}K_\varphi$, $R = \sqrt{|E^x|}$ and $P_R = -2\sqrt{|E^x|}K_x - E^\varphi K_\varphi/\sqrt{|E^x|}$ where P_Λ is the momentum canonically conjugate to Λ.

In terms of these variables the diffeomorphism and Hamiltonian constraints for gravity minimally coupled to a massless scalar field are [7],

$$\begin{aligned} C_r &= (|E^x|)' K_x - E^\varphi (K_\varphi)' - P_\phi \phi' \qquad (3)\\ H &= \frac{1}{G}\left[-\frac{E^\varphi}{2\sqrt{|E^x|}} - 2K_\varphi\sqrt{|E^x|}K_x - \frac{E^\varphi K_\varphi^2}{2\sqrt{|E^x|}} + \frac{((|E^x|)')^2}{8\sqrt{|E^x|}E^\varphi}\right.\\ &\left. - \frac{\sqrt{|E^x|}(|E^x|)'(E^\varphi)'}{2(E^\varphi)^2} + \frac{\sqrt{|E^x|}(E^x)''\mathrm{sgn}(E^x)}{2E^\varphi}\right] + \frac{P_\phi^2}{2\sqrt{|E^x|}E^\varphi} + \frac{(|E^x|)^{3/2}(\phi')^2}{2E^\varphi} \qquad (4)\end{aligned}$$

and since the variables are gauge invariant there is no Gauss law. We have taken the Immirzi parameter equal to one. We now proceed to partially fix the gauge by choosing $E^x = x^2$ ($R = x$ in terms of the metric variables). One can solve the diffeomorphism constraint for K_x,

$$K_x = \frac{E^\varphi (K_\varphi)' + P_\phi \phi'}{2x}, \tag{5}$$

which yields the Hamiltonian constraint for the partially gauge fixed model as,

$$\begin{aligned} H &= \frac{1}{G}\left[-\frac{E^\varphi}{2x} - \frac{E^\varphi K_\varphi^2}{2x} + \frac{3x}{2E^\varphi} - \frac{x^2(E^\varphi)'}{(E^\varphi)^2} - E^\varphi K_\varphi (K_\varphi)'\right]\\ &+\frac{P_\phi^2}{2xE^\varphi} + \frac{x^3(\phi')^2}{2E^\varphi} - K_\varphi P_\phi \phi'. \end{aligned} \tag{6}$$

We now rescale the Lagrange multiplier $N_{\rm old} = N_{\rm new} G (E^x)'/E^\varphi$, the rescaled Hamiltonian constraint is,

$$H = H_{\rm vac} + 2G\, H_{\rm matt} \tag{7}$$

where

$$H_{\rm vac} = \left(-x - xK_\varphi^2 + \frac{x^3}{(E^\varphi)^2}\right)' = \partial H_v(x)/\partial x, \tag{8}$$

$$H_{\rm matt} = \frac{P_\phi^2}{2(E^\varphi)^2} + \frac{x^4(\phi')^2}{2(E^\varphi)^2} - \frac{xK_\varphi P_\phi \phi'}{E^\varphi}. \tag{9}$$

This form of the Hamiltonian constraint allows an easy identification of the required boundary term if one assumes asymptotically flat conditions. The total Hamiltonian is given by,

$$H_T = \int_0^{x^+} dx N(x)(H_{\rm vac}(x) + 2G\, H_{\rm matt}(x)) + H_B \tag{10}$$

where $N(x)$ is the rescaled lapse $N_{\rm new}$ and H_B is the boundary term at the asymptotic region x^+. Integrating by parts we get

$$\begin{aligned} H_T &= -\int_0^{x^+} dx \frac{dN(x)}{dx}\left(H_v(x) + 2G\int_0^x dy H_{\rm matt}(y)\right) + N(x^+)\left(-2GM + 2G\int_0^{x^+} dy H_{\rm matt}(y)\right) + H_B\\ &= -\int_0^{x^+} dx \frac{dN(x)}{dx}\left(H_v(x) - 2G\int_x^{x^+} dy H_{\rm matt}(y) + 2GM\right) - 2GM\dot{\tau}. \end{aligned} \tag{11}$$

The boundary term $H_B = -2GM\dot{\tau}$ has been introduced in order to ensure that M is a constant and τ the proper time in the asymptotic region. This is the standard boundary term in the spherically symmetric case. M is the space time mass while the Schwarzschild radius is given by $R_S = 2G(M - \int_0^{x^+} dy H_{\rm matt}(y)))$. In the case of a space time with a black hole the radial coordinate is given by $R = x + R_S$. M is a Dirac observable. In the case of weak fields therefore, so is the integral from 0 to ∞ of $H_{\rm matt}$ that we shall cal H_M. Even in presence of black holes H_M is an observable if the black hole is isolated. We will treat H_M as an energy in order to define the vacuum and the excited states of the theory in the case of interest in this paper, weak fields without the presence of black holes.

III. QUANTIZATION OF THE MATTER FIELD ON A FIXED FLAT BACKGROUND

Since we wish to understand in which way loop quantum gravity recovers results from ordinary quantum field theory in curved spacetime, we would like to outline some of those results for later comparison. If the space-time is flat it is convenient to fix the gauge $K_\varphi = 0$ to obtain explicitly the background metric in the usual spherical coordinates. In this case one solves $H_{\rm vac} = 0$ one gets that $E^\varphi = x$. Solving the evolution equation yields the Lagrange multiplier and one recovers the full flat space-time metric. The matter portion of the Hamiltonian constraint becomes,

$$H_{\rm matt} = \frac{P_\phi^2}{2x^2} + \frac{x^2(\phi')^2}{2}. \tag{12}$$

The evolution equation obtained from this Hamiltonian corresponds to spherical waves,

$$\phi'' - \ddot{\phi} + 2\frac{\phi'}{x} = 0. \tag{13}$$

This can be solved by separation of variables,

$$\phi(x,t) = \int_0^\infty d\omega \frac{\left(C(\omega)\exp(-i\omega t) + \bar{C}(\omega)\exp(i\omega t)\right)\sin(\omega x)}{\sqrt{\pi\omega}x}, \tag{14}$$

which corresponds to spherical waves that are regular at the origin. From Hamilton's equation we can get an expression for P_ϕ,

$$P_\phi(x,t) = \int_0^\infty d\omega \frac{\left(-iC(\omega)\omega\exp(-i\omega t) + i\bar{C(\omega)}\omega\exp(i\omega t)\right)x\sin(\omega x)}{\sqrt{\pi\omega}}. \tag{15}$$

From the standard commutation relations, $[\hat{\phi}(x,t), \hat{P}_\phi(y,t)] = i\delta(x-y)$, one gets the $[\hat{C}(\omega), \hat{\bar{C}}(\omega')] = \delta(\omega - \omega')$. One can proceed to define a vacuum state $|0\rangle$ as the state that is annihilated by $\hat{C}$. If one evaluates the expectation value of $H_{\rm matt}$ on the vacuum state one finds that it has an ultraviolet divergence. The usual resolution of this problem is to introduce a cutoff. It should be noted that when one treats this problem in loop quantum gravity this type of divergence does not appear because the well defined objects are holonomies associated to finite paths. In our treatment this aspect is lost since we have gauge fixed the radial variable which therefore becomes a c-number. As we usually proceed when we use the uniform discretization technique, we regularize the expression by placing it on a lattice. We will discuss later on the issue of taking the lattice spacing to zero.

We will assume that the radial direction is bounded with a spatial extent L and consists of discrete points x_i separated by a coordinate distance ϵ, and in particular we take x_i as ϵ times an integer. We reinterpret the integrals as sums, Dirac deltas as Kronecker deltas, functional derivatives as partial derivatives, and partial derivatives in the radial directions as finite differences. Specifically [8]

$$\int dx \;\to\; \epsilon\sum_x \tag{16}$$

$$\delta(x-y) \;\to\; \frac{\delta_{x,y}}{\epsilon} \tag{17}$$

$$\frac{\delta}{\delta\phi(x)} \;\to\; \frac{1}{\epsilon}\frac{\partial}{\partial\phi} \tag{18}$$

$$\phi(x)' \;\to\; \frac{\phi(x_{i+1}) - \phi(x_i)}{\epsilon} \tag{19}$$

$$(\omega)^2 \;\to\; \frac{\sum_i\left(2 - 2\cos(\epsilon\omega_i)\right)}{\epsilon^2} \tag{20}$$

If the spatial direction is discrete, the associated momentum space is bounded with extent $2\pi/\epsilon$. To the first nontrivial order in in epsilon, all formulae involving momenta ω are unchanged except that momentum integrals are now sums over a momentum space of finite extent.

The expectation value of $\hat{H}_{\rm matt}$ can be computed replacing the quantum version of the expressions given above for $\phi(x,t)$ and $P_\phi(x,t)$ in $\hat{H}_{\rm matt}$. Computing the expectation value on the vacuum state one is only left with contributions proportional to $\hat{C}\hat{\bar{C}}$. On the lattice the result may be approximated in the limit of large L by the integral,

$$\langle 0|\hat{H}_{\rm matt}(x)|0\rangle = \int_0^{2\pi/\epsilon} d\omega \frac{\omega^2 x^2 - 2x\omega\cos(\omega x)\sin(\omega x) + \sin^2(\omega x)}{2x^2\pi\omega}. \tag{21}$$

The integral can be computed in closed form in terms of integral cosine functions. It is more useful to give an approximation for its value as an expansion in ϵ,

$$\langle 0|\hat{H}_{\rm matt}(x)|0\rangle = \frac{\pi}{\epsilon^2} - \frac{\sin^2(2\pi x/\epsilon)}{\pi x^2} + \frac{\ln(x/\epsilon)}{4x^2\pi} + O(\epsilon^0). \tag{22}$$

The leading order in the energy density expansion is π/ϵ^2 which has the correct dimensions for an energy density in one spatial dimension, since we are only considering the radial mode of the scalar field.

As in four dimensions, the energy of the vacuum gives rise to a cosmological constant if one allows the field to back-react on gravity. The nature of this constant is different, however in two dimensions [9]. First of all, notice that if one had started from four dimensional gravity with a cosmological constant and imposed spherical symmetry, one can view the model as a $1+1$ dimensional theory with a dilaton with a mass given by the four dimensional cosmological constant. That is, it does not produce a term that behaves like a cosmological constant in $1+1$ dimensions. The vacuum energy, by contrast produces a constant term in the Hamiltonian constraint. Second, notice that even in vacuum $H_{\rm vac}$ already has a constant term in it. So the energy of the vacuum essentially operates as a rescaling of that constant term, which in turn can be absorbed by a rescaling of the radial coordinate. In four dimensions, if one chooses a Planck scale cutoff it implies that the radius of curvature of space-time becomes of the order of Planck length, which is clearly unphysical. In spherical symmetry the presence of the constant can be reabsorbed in a redefinition of the coordinates. This redefinition however, has consequences when one wishes to reinterpret the model as an approximation to a four dimensional space-time. The redefinition of the radial coordinate implies that the spheres do not have $4\pi R^2$ area anymore. The four dimensional universe modeled contains a topological defect, a "global texture" [10]. Notice that this immediately precludes taking the lattice spacing to zero, since already when the lattice spacing is of the order of $\ell_{\rm Planck}$ one will have a solid deficit angle that exceeds 4π and does not allow to interpret the model as a four dimensional space-time.

There are two avenues to handle the situation: either one rescales the radial variable and accepts that the model approximates four dimensional space-times with (large) topological defects, or one can modify the two dimensional model by adding a constant to the Hamiltonian constraint (a cosmological constant in $1+1$ dimensional gravity). Such a model will not stem from a dimensional reduction of four dimensional gravity, but upon quantization will turn out to approximate four dimensional spherical gravity around a flat background without a topological defect.

We will take the first point of view and write the Hamiltonian constraint as, $H = H_{\rm vac} + G\, H_{\rm matt}$, where

$$H_{\rm vac} = \left(-x(1-2\Lambda) - xK_\varphi^2 + \frac{x^3}{(E^\varphi)^2}\right)', \tag{23}$$

$$H_{\rm matt} = \frac{P_\phi^2}{(E^\varphi)^2} + \frac{x^4(\phi')^2}{(E^\varphi)^2} - 2\frac{xK_\varphi P_\phi \phi'}{E^\varphi} - \rho_{\rm vac}, \tag{24}$$

where $\Lambda = \frac{G}{2}\rho_{\rm vac}$ and $\rho_{\rm vac}$ is the vacuum energy density. We choose $\hbar = c = 1$ units. This rewriting of the constraint has the property that the expectation value of $H_{\rm matt}$ will be zero in the vacuum.

IV. FULL QUANTIZATION OF THE MODEL

We would like to write the master constraint based on the Hamiltonian constraint of the model we introduced in the last section. Although the discrete Hamiltonian constraint fails to close a first class algebra, we have showed in [11] that with the uniform discretization technique one can consistently treat the problem by minimizing the resulting master constraint. To write the master constraint at a quantum level we will polymerize the expression of the gravitational part of the constraint. We will not use a polymer representation in the scalar sector for simplicity and because we want to make contact with the usual treatments based on a Fock quantization. It is known that the Fock quantization for fields can be recovered from the polymer quantization [12, 13].

A. Variational technique to study the expectation value of the master constraint

Here we will introduce a variational technique to minimize the master constraint. The technique is general, it is not restricted to the model we study in this paper. We start by considering a fiducial Hilbert space $\mathcal{H}_{\rm aux}$ in which the master constraint is a well defined self-adjoint operator. We will then use a variational technique to find approximations to the minimum value of the expectation value of the master constraint within this space. In many cases of interest, the minimum expectation value will not be zero, but will be small (the master constraint has units of action squared, so normally one would require it to be much smaller than $\hbar^2$, in order to have a good approximation of the physical space, in our units that translates into much smaller than one). As we will see in the examples, the resulting quantum theory will therefore not reproduce exactly the symmetries of the continuum theory but it will approximate them, even at the quantum level. We will see that if zero is in the spectrum of the operator the corresponding eigenstates in many cases will be distributional with respect to the fiducial space we are considering.

To implement the variational method, we consider trial states in $\mathcal{H}_{\rm aux}$ that are Gaussians centered around the classical solution of the model of interest in phase space. That means that as functions of $\mathcal{H}_{\rm aux}$ these will generically be Gaussians times phase factors such that the resulting state is centered around the classical solution in both configuration variables and momenta. The states are parameterized by the values of the standard deviations of the Gaussians in either configuration or momentum space. A caveat is that in gauge theories one may choose to work with a classical solution that is not in a completely determined gauge. Such a solution will be a trajectory in phase space. Such a trajectory will determine some of the canonical variables as functions of others, which will remain free. In that case one has to allow such variables to be free in the trial solution by considering Gaussians centered around a value that is a free parameter. If one chooses to work with a classical solution in a completely specified gauge one just considers Gaussians around the point in phase space represented by the classical solution of interest and extremizes the expectation value of the master constraint with respect to the standard deviations of the Gaussians. It can happen that the extremum occurs as a limit in the parameter space in which case the resulting state does not belong in $\mathcal{H}_{\rm aux}$ but in its dual (after a suitable rescaling, it becomes a distribution).

Before attacking the problem of interest, it is useful to see the technique we just described in action in a couple of simple examples. The first example we choose is a system with two degrees of freedom q_1, p_1 and q_2, p_2, and two constraints $p_1 = 0$ and $p_2 = 0$. The total Hamiltonian for the system is $H_T = N_1 p_1 + N_2 p_2$ with $N_{1,2}$ Lagrange multipliers. The states annihilated by the constraints are trivial and given by the distribution $\delta(p_1)\delta(p_2)$. We fix a gauge $q_1 - q_2 = 0$. Fixing the gauge is not needed in a simple model like this, but may be a necessity to simplify things in more complicated models. So we will choose a gauge fixing here to show that in the end the process loses all information about the gauge fixing and recovers the correct physical state. This requires fixing the Lagrange multipliers so there is only one (N) left and the total Hamiltonian becomes $H_T = N(p_1 + p_2)$. The conjugate variable to the gauge fixing, $p_1 - p_2$ is strongly zero. We start with a two parameter family of states in $\mathcal{H}_{\rm aux}$ choosing as configuration variables $q_1 - q_2$ and $p_1 + p_2$,

$$\psi_{\sigma_\pm,\beta} = \frac{1}{\sqrt{\pi\sqrt{\sigma_+\sigma_-}}} \exp\left(-\frac{(q_1-q_2)^2}{2\sigma_-}\right) \exp\left(-\frac{(p_1+p_2)^2}{2\sigma_+}\right) \exp\left(i\beta\left(p_1+p_2\right)\right), \tag{25}$$

with β an arbitrary parameter associated with the fact that the variable $q_1 + q_2$ is pure gauge. One could choose to work in a completely gauge fixed solution in which $q_1 + q_2$ is zero, in that case there is no need to introduce the parameter β. The choice of this family of states is based on the fact that they describe wave-packets centered around the classical solutions of the constraints, $q_1 - q_2 = 0$, $p_1 - p_2 = 0$ and $p_1 + p_2 = 0$. We now define the master constraint $\mathbb{H} = p_1^2 + p_2^2$ and act on this space of states. The expectation value is,

$$\langle\psi_{\sigma_\pm,\beta}|\mathbb{H}|\psi_{\sigma_\pm,\beta}\rangle = \frac{1}{4\sigma_-} + \frac{1}{4}\sigma_+ \tag{26}$$

where $\sqrt{(\sigma_\pm)}$ are the standard deviations of the Gaussians, $\sigma_\pm$ taken to be positive. One therefore sees that the expectation value cannot be zero for any finite value of the σ's. However, if one takes $\sigma_- = \frac{1}{2\epsilon^2}$ and $\sigma_+ = 2\epsilon^2$ then in the limit $\epsilon \to 0$, $<\mathbb{H}>= O(\epsilon^2)$. The states $|\psi_\epsilon\rangle$ become,

$$\langle q_1 - q_2, p_1 + p_2|\psi_\epsilon\rangle = \frac{1}{\sqrt{\pi}} \exp\left(-\left(q_1-q_2\right)^2\epsilon^2\right) \exp\left(-\frac{(p_1+p_2)^2}{4\epsilon^2}\right) \exp\left(i\beta\left(p_1+p_2\right)\right), \tag{27}$$

And their Fourier transform

$$\langle p_1 - p_2, p_1 + p_2|\psi_\epsilon\rangle = \frac{1}{\epsilon\sqrt{2\pi}} \exp\left(-\frac{(p_1-p_2)^2}{4\epsilon^2}\right) \exp\left(-\frac{(p_1+p_2)^2}{4\epsilon^2}\right) \exp\left(i\beta\left(p_1+p_2\right)\right), \tag{28}$$

These states are normalized in $\mathcal{H}_{\rm aux}$ but they vanish (in the sense of distributions) in the limit $\epsilon \to 0$. They need to be rescaled in order to end up with well defined distribution on some suitable subspace of $\mathcal{H}_{\rm aux}$.

So the physical states would be

$$\langle p_1 - p_2, p_1 + p_2|\psi\rangle_{\rm ph} \equiv \lim_{\epsilon\to 0} \frac{1}{\sqrt{2\pi\epsilon}}\langle p_1 - p_2, p_1 + p_2|\psi_\epsilon\rangle = 2\delta(p_1 + p_2)\delta(p_1 - p_2) = \delta(p_1)\delta(p_2) \quad (29)$$

Notice that the parameter β is free at the end of the process since it corresponds to the value of a variable that is pure gauge in this model.

There is an additional element that the above example does not capture and we would like to discuss. When we apply this technique in situations of interest, we will be discretizing the theories we analyze. Usually, discretization turns first class constraints into second class ones. The uniform discretization procedure tells us that we do not need to concern ourselves with the second class nature of the constraints (for a discussion see [11]). We can still consider the master constraint and seek the minimization of its eigenvalues, but the presence of second class constraints in the discrete theory usually implies that the minimum eigenvalue of the master constraint will not be zero. The best one can hope for is that it will be small and the resulting quantum theory will approximate the symmetries of the theory one started with. This is a point of view that has been held as natural for some time in the context of quantum gravity, where one expects that some level of fundamental discreteness will emerge. We would like to illustrate this with a modification of the previous example. Instead of taking $p_1 = 0$ and $p_2 = 0$ as the constraints we will take $p_1 + \alpha q_2 = 0$ and $p_2 = 0$ with α a small parameter (in realistic theories the small parameter is related to the lattice spacing in the discretization). We will still take the same set of $\psi_{\sigma_\pm,\beta}$ as before, that is, for the trial solution we have chosen Gaussians centered around classical solutions of the gauge theory where the anomalous term vanishes. We do this because one usually knows solutions to the continuum theory one wishes to approximate (e.g. flat space or the Schwarzschild solution in the case of gravity) whereas the discrete theories have complicated solutions that usually cannot be treated in analytic form. The master constraint now becomes,

$$\mathbb{H} = p_1^2 + p_2^2 + 2\alpha p_1 q_2 + \alpha^2 q_2^2, \quad (30)$$

and using the same ansatz (25) for the states one finds that

$$\langle\psi_{\sigma_\pm,\beta}|\mathbb{H}|\psi_{\sigma_\pm,\beta}\rangle = \alpha^2\beta^2 + \frac{1}{4\sigma_-} + \frac{1}{4}\sigma_+ + \frac{\alpha^2}{2\sigma_+} + \frac{\alpha^2\sigma_-}{2}. \quad (31)$$

We would like to identify a limit in the variables $\sigma_\pm$ such that this quantity vanishes. As was to be expected, this is not possible. We can attempt to find values of the parameters $\sigma_\pm$ and β that minimize this expression. The result is $\beta = 0$ and $\sigma_+ = \sqrt{2}\alpha$ and $\sigma_- = \frac{1}{\sqrt{2}\alpha}$. which yields $\langle\psi_{\rm min}|\mathbb{H}|\psi_{\rm min}\rangle = \sqrt{2}\alpha$. The state is,

$$\langle p_1, p_2|\psi_{\rm min}\rangle = \exp\left(-\frac{\left({p_1}^2 + {p_2}^2\right)\sqrt{2}}{\alpha}\right)\sqrt{\frac{\sqrt{2}}{\alpha\pi}}. \quad (32)$$

It is interesting to compare this state and the corresponding expectation value of $\mathbb{H}$ obtained from our variational technique with the exact minimum of this model. A naive analysis would tell us that the minimum corresponds to an exact eigenstate with zero eigenvalue for $\mathbb{H}$. However, that solution is not well behaved. It is known that one can find solutions of the master constraint that do not solve the constraints if one does not impose regularity in the solutions found [14]. The master constraint is an operator in the Hilbert space and one can analyze its spectral resolution. The spurious solutions do not belong in the spectral resolution of the master constraint. In this case one can solve exactly the eigenvalue problem $\mathbb{H}|\psi\rangle = E|\psi\rangle$. The solutions with minimum eigenvalue are of the form $\delta(p_1)\psi_0(p_2)$ where $\psi_0(p_2)$ is the fundamental state of the Hamiltonian of a harmonic oscillator in the momentum representation. The minimum eigenvalue for such exact solution is α (compare with the variational one in which the eigenvalue was slightly higher $\sqrt{2}\alpha$). It is also interesting to note that if instead of choosing the gauge $q_1 - q_2 = 0$ we had chosen $q_1 = 0$ and proceeded with the variational technique, one obtains the exact state directly. This illustrates that the method approximates well the state of interest in situations where zero is not in the kernel of the master constraint. The solution that minimizes the master constraint admits a very simple interpretation that shows that the uniform discretization of the theory with the anomalous term α small but non-vanishing, approximately reproduces the invariances of the theory with first class constraints $p_1 = P_2 = 0$. In fact q_1 and q_2 are gauge variables and the physical space is independent of these variables. The physical state is constant in q_1 and q_2. For a small but non vanishing alpha the physical states are independent of q_1 and weakly dependent on q_2. A final comment is that in this case the parameter β, which was not determined in the case with first class constraints, gets determined here. That is, in the case where β was associated with an exact gauge symmetry, the minimization of the master constraint was insensitive to the value of β. In the case where the constraints are second class and we do not get zero as minimum of the master constraint there is some dependence on β, but it is weak, since the term in the master constraint is $\beta^2\alpha^2$ and α is small (in the quantum state one has approximately $\delta(p)\exp(ip\beta)$). The theory where one does not exactly annihilate the master constraint only has approximate gauge symmetries and therefore has slightly "preferred" gauges from the point of view of minimizing the master constraint.

B. The discrete master constraint

Let us now consider the complete Hamiltonian constraint. We wish to discretize it and to polymerize the gravitational variables. The Hamiltonian gets rescaled in the discretization $H(x_i) \to H(i)/\epsilon$,. We also rescale the expression multiplying the continuum Hamiltonian constraint times G. The resulting discrete expression is,

$$\begin{aligned} H(i) \;=\; & -(1-2\Lambda)\epsilon - x(i+1)\frac{\sin^2\left(\rho K_\varphi(i+1)\right)}{\rho^2} + x(i)\frac{\sin^2\left(\rho K_\varphi(i)\right)}{\rho^2} + \frac{x(i+1)^3\epsilon^2}{(E^\varphi(i+1))^2} - \frac{x(i)^3\epsilon^2}{(E^\varphi(i))^2} \\ & +G\left(\epsilon\frac{(P^\varphi(i))^2}{(E^\varphi(i))^2} + \epsilon\frac{x(i)^4\left(\phi(i+1)-\phi(i)\right)^2}{(E^\varphi(i))^2} - 2x(i)\frac{\sin\left(\rho K_\varphi(i)\right)}{E^\varphi(i)\rho}(\phi(i+1)-\phi(i))P^\phi(i) - \rho_{\rm vac}\epsilon\right). \end{aligned} \tag{33}$$

We need to construct the master constraint. Since the Hamiltonian is a density of weight one, we define the master constraint associated with the Hamiltonian constraint in the full theory as,

$$\mathbb{H} = \frac{1}{2}\int dx \frac{H(x)^2}{\sqrt{g}}\ell_{\rm P}, \tag{34}$$

or, in terms of the variables of the model, up to a constant factor,

$$\mathbb{H} = \frac{1}{2}\int dx \frac{H(x)^2}{(E^\varphi)\sqrt{E^x}}\ell_{\rm P}, \tag{35}$$

and in the discretized theory $\mathbb{H}^\epsilon = \sum_i \mathbb{H}(i)$ with

$$\mathbb{H}(i) = \frac{1}{2}\frac{H(i)^2\ell_{\rm P}}{\sqrt{E^x(i)}E^\varphi(i)}. \tag{36}$$

The constant $\ell_{\rm P}$ must be introduced so that $\mathbb{H}$ is dimensionless with $\hbar = c = 1$, one could use $\sqrt{G}$ instead of it. It is convenient to rescale the Hamiltonian constraint by $\sqrt{E^\varphi/(E^x)'}$. This does not change the density weight. If one does not rescale things it turns out $\mathbb{H}$ is proportional to $1/E^\varphi$. In the polymer representation this implies that the vacuum is the "zero loop" state, which is degenerate (it corresponds to zero volume space-times). To eliminate this unphysical possibility one exploits the fact that the Hamiltonian constraint is defined up to a factor given by a scalar function of the canonical variables without changing the first class nature of the classical constraint algebra. The rescaling factor in the discrete theory after the gauge fixing is $\sqrt{E^\varphi(i)/(2x(i)\epsilon)}$. So (33) has to be multiplied times that factor when constructing the master constraint (36).

Let us focus on the matter portion of the Hamiltonian, we will write it as,

$$H_{\rm matt}(i) = \frac{H^{(1)}_{\rm matt}(i)}{(E^\varphi)^2(i)} + \frac{H^{(2)}_{\rm matt}(i)\sin\left(\rho K_\varphi(i)\right)}{\rho E^\varphi(i)} - H^{(3)}_{\rm matt}(i). \tag{37}$$

The master constraint can be written as,

$$\begin{aligned} \mathbb{H}(i) \;=\; & \ell_{\rm P}\left[c_{11}(i)\left(H^{(1)}_{\rm matt}(i)\right)^2 + c_{22}(i)\left(H^{(2)}_{\rm matt}(i)\right)^2\right. \\ & + c_1(i)H^{(1)}_{\rm matt}(i) + c_2(i)H^{(2)}_{\rm matt}(i) + c_{33}(i)\left(H^{(3)}_{\rm matt}(i)\right)^2 + c_3(i)H^{(1)}_{\rm matt}(i) \\ & \left. + c_{12}(i)H^{(1)}_{\rm matt}(i)H^{(2)}_{\rm matt}(i) + c_{13}(i)H^{(1)}_{\rm matt}(i)H^{(3)}_{\rm matt}(i) + c_{23}(i)H^{(2)}_{\rm matt}(i)H^{(3)}_{\rm matt}(i) + c_{00}(i)\right], \end{aligned} \tag{38}$$

where,

$$H^{(1)}_{\rm matt}(i) \;=\; \left(\epsilon\left(P^\varphi(i)\right)^2 + \epsilon x(i)^4\left(\phi(i+1)-\phi(i)\right)^2\right)\ell_P^2 \tag{39}$$

$$H^{(2)}_{\rm matt}(i) \;=\; \left(-2x(i)\left(\phi(i+1)-\phi(i)\right)P^\varphi(i)\right)\ell_P^2 \tag{40}$$

$$H^{(3)}_{\rm matt}(i) \;=\; 2\rho_{\rm vac}\epsilon\ell_P^2. \tag{41}$$

To economize space, we will not give the classical expressions for the coefficients, since they can be readily obtained from the quantum expressions.

In order to quantize the master constraint we need to choose a factor ordering. The expression of the master constraint is a sum of symmetric operators consisting of polynomials in $\hat{E}^\varphi$ and $\sin(\rho\hat{K}_\varphi)$, $\hat{P}^\phi$ and $\hat{\phi}$. We choose a factor ordering with the factors of $\hat{E}^\varphi$ are distributed symmetrically to the right and the left of the factors of $\sin(\rho\hat{K}_\varphi)$. For the factors $\hat{P}^\phi$ and $\hat{\phi}$ we follow a similar strategy, putting the $\hat{P}^\phi$ symmetrically to the left and to the right of $\hat{\phi}$'s. The coefficients in the above expression of the master constraint with this factor ordering are,

$$\hat{c}_{11}(i) = \frac{1}{4x(i)^2\epsilon\hat{E}^\varphi(i)^4}, \tag{42}$$

$$\hat{c}_{12}(i) = \frac{1}{2x(i)^2\rho\epsilon}\frac{1}{\hat{E}^\varphi(i)^{3/2}}\sin(\rho K_\varphi(i))\frac{1}{\hat{E}^\varphi(i)^{3/2}}, \tag{43}$$

$$\hat{c}_{13}(i) = -\frac{1}{2x(i)^2\epsilon}\frac{1}{\hat{E}^\varphi(i)^2}, \tag{44}$$

$$\hat{c}_{22}(i) = \frac{1}{8x(i)^2\rho^2\epsilon}\left(\frac{1}{\hat{E}^\varphi(i)^2} - \frac{1}{\hat{E}^\varphi(i)}\cos(2\rho K_\varphi(i))\frac{1}{\hat{E}^\varphi(i)}\right), \tag{45}$$

$$\hat{c}_{23}(i) = -\frac{1}{2x(i)^2\rho\epsilon}\frac{1}{\sqrt{\hat{E}^\varphi(i)}}\sin(\rho K_\varphi(i))\frac{1}{\sqrt{\hat{E}^\varphi(i)}}, \tag{46}$$

$$\hat{c}_{33}(i) = \frac{1}{4x(i)^2\epsilon}, \tag{47}$$

$$\begin{aligned}\hat{c}_1(i) = & -\frac{x(i)\epsilon}{2\hat{E}^\varphi(i)^4} + \frac{1}{4\epsilon x(i)^2\hat{E}^\varphi(i)}\left(-2\epsilon(1-2\Lambda) + \frac{x(i+1)\cos(2\rho K_\varphi(i))}{\rho^2} - \frac{x(i+1)}{\rho^2}\right)\frac{1}{\hat{E}^\varphi(i)} \\ & -\frac{1}{\hat{E}^\varphi(i)}\frac{\cos(2\rho K_\varphi(i))}{4x(i)\rho^2\epsilon}\frac{1}{\hat{E}^\varphi(i)} + \frac{1}{4x(i)\rho^2\epsilon\hat{E}^\varphi(i)^2} + \frac{\epsilon x(i+1)^3}{2x(i)^2}\frac{1}{\left(\hat{E}^\varphi(i)\hat{E}^\varphi(i+1)\right)^2},\end{aligned} \tag{48}$$

$$\begin{aligned}\hat{c}_2(i) = & \left[-\frac{1}{2\rho x(i)^2}(1-2\Lambda) + \frac{x(i+1)}{4\rho^3 x(i)^2\epsilon}(\cos(2\rho K_\varphi(i+1))-1) + \frac{3}{8\rho^3 x(i)\epsilon} + \frac{\epsilon x(i+1)^3}{2\rho x(i)^2\hat{E}^\varphi(i+1)^2}\right]\times \\ & \times\frac{1}{\sqrt{\hat{E}^\varphi(i)}}\sin(\rho K_\varphi(i))\frac{1}{\sqrt{\hat{E}^\varphi(i)}} - \frac{1}{8\rho^3 x(i)\epsilon}\frac{1}{\sqrt{\hat{E}^\varphi(i)}}\sin(3\rho K_\varphi(i))\frac{1}{\sqrt{\hat{E}^\varphi(i)}} \\ & -\frac{x(i)\epsilon}{2\rho}\frac{1}{\hat{E}^\varphi(i)^{3/2}}\sin(\rho K_\varphi(i))\frac{1}{\hat{E}^\varphi(i)^{3/2}}\end{aligned} \tag{49}$$

$$\begin{aligned}\hat{c}_3(i) = & \frac{1}{2x(i)^2}(1-2\Lambda) + \frac{x(i+1)}{4x(i)^2\epsilon\rho^2}(1-\cos(2\rho K_\varphi(i+1))) - \frac{1}{4x(i)\epsilon\rho^2}(1-\cos(2\rho K_\varphi(i))) \\ & +\frac{x(i)\epsilon}{2\hat{E}^\varphi(i)^2} - \frac{\epsilon x(i+1)^3}{2x(i)^2\hat{E}^\varphi(i+1)^2},\end{aligned} \tag{50}$$

$$\begin{aligned}\hat{c}_{00}(i) = & \frac{1}{32\epsilon\rho^4}(3 - 4\cos(2\rho K_\varphi(i)) + \cos(4\rho K_\varphi(i))) \\ & +\frac{\epsilon}{4x(i)^2} + \frac{x(i+1)}{4x(i)^2\rho^2}(1-\cos(2\rho K_\varphi(i+1))) \\ & -\frac{x(i+1)}{8x(i)\epsilon\rho^4}(1 - \cos(2\rho K_\varphi(i)) - \cos(2\rho K_\varphi(i+1)) + \cos(2\rho K_\varphi(i))\cos(2\rho K_\varphi(i+1))) \\ & +\frac{x(i+1)^2}{32\epsilon\rho^4 x(i)^2}(3 + \cos(4\rho K_\varphi(i+1)) - 4\cos(2\rho K_\varphi(i+1))) \\ & -\frac{\Lambda x(i+1)}{2x(i)^2\rho^2}(1-\cos(2\rho K_\varphi(i+1))) \\ & -\frac{1}{4x(i)\rho^2}(1-2\Lambda)(1-\cos(2\rho K_\varphi(i))) - \frac{\epsilon\Lambda}{x(i)^2}(1-\Lambda)\end{aligned}$$

$$
\begin{aligned}
&+\frac{\epsilon x(i+1)^3}{4x(i)\rho^2}\left(\frac{1}{\hat{E}^\varphi(i+1)^2}-\frac{1}{\hat{E}^\varphi(i+1)}\cos(2\rho K_\varphi(i))\frac{1}{\hat{E}^\varphi(i+1)}\right)\\
&-\frac{x(i)\epsilon}{4\rho^2}\left(x(i)\left(\frac{1}{\hat{E}^\varphi(i)^2}-\frac{1}{\hat{E}^\varphi(i)}\cos(2\rho K_\varphi(i))\frac{1}{\hat{E}^\varphi(i)}\right)\right.\\
&\left.-x(i+1)\left(\frac{1}{\hat{E}^\varphi(i)^2}-\frac{1}{\hat{E}^\varphi(i)}\cos(2\rho K_\varphi(i+1))\frac{1}{\hat{E}^\varphi(i)}\right)\right)\\
&-\frac{\epsilon x(i+1)^4}{4x(i)^2\rho^2}\left(\frac{1}{\hat{E}^\varphi(i+1)^2}-\frac{1}{\hat{E}^\varphi(i+1)}\cos(2\rho K_\varphi(i+1))\frac{1}{\hat{E}^\varphi(i+1)}\right)+\frac{x(i)\epsilon^2}{2\hat{E}^\varphi(i)^2}(1-2\Lambda)\\
&-\frac{\epsilon^2 x(i+1)^3}{2x(i)^2\hat{E}^\varphi(i+1)^2}(1-2\Lambda)+\frac{\epsilon^3 x(i+1)^6}{4x(i)^2\hat{E}^\varphi(i+1)^4}-\frac{x(i)\epsilon^3 x(i+1)^3}{2\left(\hat{E}^\varphi(i+1)\hat{E}^\varphi(i)\right)^2}+\frac{x(i)^4\epsilon^3}{4\hat{E}^\varphi(i)^4},
\end{aligned}
\tag{51}
$$

and it should be noted that the coefficients commute with $H^{(1)}_{\rm matt}, H^{(2)}_{\rm matt}$ and $H^{(3)}_{\rm matt}$ so there are no ordering issues with them.

C. Construction of the trial states

Since we are interested in the vacuum solution, that classically corresponds to vanishing scalar fields, we will therefore ignore $H_{\rm matt}$ (24) and only consider the gravitational part (23) in order to construct the classical solution used to build the ansatz states for the variational technique,

$$
H_{\rm vac}=\left(-x(1-2\Lambda)-xK_\varphi^2+\frac{x^3}{(E^\varphi)^2}\right)'. \tag{52}
$$

As we discussed in subsection A we will choose a definite gauge to work in. Our choice is $K_\varphi=0$, and this implies $E^\varphi=x/\sqrt{1-2\Lambda}$. As we claimed before, the presence of the cosmological constant rescales the radial variable (recall that without the constant the solution was $E^\varphi=x$). The resulting four dimensional space-time will be locally flat with a solid deficit angle and described in spherical coordinates.

We construct a polymer representation. As we did in previous papers [5] one sets up a lattice of points $j=0\ldots N$ in the radial direction and writes a "point holonomy" for the K_φ variable at each lattice site,

$$
T_{\vec{\mu}}=\exp\left(i\sum_j \mu_j K_\varphi(j)\right)=\langle K_\varphi|\,\vec{\mu}\,\rangle. \tag{53}
$$

In this expression the quantities μ_i play the role of the "loop" in this one dimensional context. They also are proportional to the eigenvalues of the triad operator $\hat{E}^\varphi(i)$. The quantum state we will choose for the variational method will be centered around the classical solution and therefore we will choose to have the variable μ_i centered at the classical value of $E^\varphi(i)=\epsilon x_1(i)\equiv\epsilon x(i)/\sqrt{1-2\Lambda}$,

$$
\langle\,\vec{\mu}\,|\psi_{\vec{\sigma}}\rangle=\prod_i\sqrt[4]{\frac{2}{\pi\sigma(i)}}\exp\left(-\frac{1}{\sigma(i)}\left(\mu_i-\frac{x_1(i)\epsilon}{\ell_{\rm P}^2}\right)^2\right) \tag{54}
$$

on this state $\langle E^\varphi(i)\rangle=\epsilon x_1(i)$ and $\langle K_\varphi(i)\rangle=0$. Notice that this type of ansatz in general will be too restrictive: we have ignored possible correlations among neighboring points by assuming a Gaussian at each point. This could potentially be problematic when studying excited states and computing propagators. We will not attack those problems in this paper so we will continue with the restrictive ansatz for the moment being.

We will now compute the expectation value of the matter portion of the Hamiltonian constraint on the above state. The result will be an operator acting on the matter fields. We will then construct the vacuum for the resulting operator. What we are doing is to construct a quantum field theory living on the geometry given by the expectation values of the triad and extrinsic curvature on the above state. We proceed in this way for expediency since this is our first approach to the problem. In the future we plan to revisit the problem treating all the variables in a polymerized representation, both gravitational and material ones, with the variational technique. Preliminary results indicate that such an approach is viable. For the matter field one would start by considering a coherent state centered at zero values for the field and then will obtain the vacuum as a limit. This would yield valuable insights into the relation of the usual Fock quantization with the loop quantum gravity techniques, especially when one gets to discuss physical elements like the propagators of fields.

In order to take the expectation value of the matter portion of the Hamiltonian constraint, (37) on the state (54) we need to realize two quantum operators. The first one is,

$$\frac{1}{\left(\hat{E}^\varphi(i)\right)^2}\langle\,\mu(i)\,|\psi_{\sigma(i)}\rangle \;=\; \left(\frac{2}{3}\right)^{12}|\mu(i)|\left((|\mu(i)+\rho|)^{3/4}-(|\mu(i)-\rho|)^{3/4}\right)^{12}\sqrt[4]{\frac{2}{\pi\,\sigma(i)}}\exp\left(-\frac{\left(\mu(i)-\frac{\epsilon\,x_1(i)}{\ell_{\rm P}^2}\right)^2}{\sigma(i)}\right) \tag{55}$$

where we have considered the action on one of the factors of (54). To derive this expression we consider $\left(\hat{E}\right)^{-3/2}\hat{E}\left(\hat{E}\right)^{-3/2}$ and use the realization of $\left(\hat{E}\right)^{-3/2}$ that was discussed in the context of loop quantum cosmology in [15]. The reason we can use the loop quantum cosmology results is that our Hilbert space is a direct product of loop quantum cosmology Hilbert spaces each at one of the lattice sites in the radial direction. With the above result one can compute the expectation value,

$$\langle\,\psi_{\vec{\sigma}}|\frac{1}{\left(\hat{E}^\varphi(i)\right)^2}|\psi_{\vec{\sigma}}\rangle = \frac{1-2\,\Lambda}{\epsilon^2 x(i)^2}+\frac{5}{8}\,\frac{{\ell_{\rm P}}^4\,(1-2\,\Lambda)^2\,\rho^2}{\epsilon^4 x(i)^4}+\frac{3}{4}\,\frac{\sigma\,{\ell_{\rm P}}^4\,(1-2\,\Lambda)^2}{\epsilon^4 x(i)^4}. \tag{56}$$

The calculation is done by integrating in $\vec{\mu}$ and the result is lengthy, here we just show it in the approximation $\epsilon > \ell_{\rm P}$. The first term is the classical value, the others are quantum corrections, the first one comes from the polymerization, the second from fluctuations in $\vec{\mu}$. The second operator we need is the one arising in the second term of the Hamiltonian,

$$\langle\,\psi_{\vec{\sigma}}|\frac{1}{\sqrt{\hat{E}^\varphi(i)}}\frac{\sin(\rho\hat{K}_\varphi(i))}{\rho}\frac{1}{\sqrt{\hat{E}^\varphi(i)}}|\,\psi_{\vec{\sigma}}\rangle = 0. \tag{57}$$

To quickly see why this is zero keep in mind that the state is a Gaussian centered at $K_\varphi = 0$ and the sine is an odd function. With these results the expectation value of the Hamiltonian (the "effective Hamiltonian") is,

$$\hat{H}^{\rm eff}_{\rm matt} = \langle\,\psi_{\vec{\sigma}}|\hat{H}_{\rm matt}(x,t)|\,\psi_{\vec{\sigma}}\rangle = \frac{(1-2\,\Lambda)\left(\hat{P}^\phi(x,t)\right)^2}{x^2 g(x)^2}+\frac{x^2\,(1-2\,\Lambda)\left(\hat{\phi}'(x,t)\right)^2}{g(x)^2}-\rho_{\rm vac}. \tag{58}$$

In this equation we have pursued the unusual approach of taking the continuum limit in the terms that involve derivatives and the terms that involve the momenta of the scalar field. This simplifies calculations since we will be dealing with differential equations rather than difference equations. The idea is that the solutions to the differential equations, suitably discretized, will be a good approximation (at least to $O(\epsilon)$ corrections) to the solutions of the difference equations. In the above expression the quantity $g(x)$ is given by,

$$g(x) = 1-\frac{5}{16}\,\frac{{\ell_{\rm P}}^4\rho^2(1-2\Lambda)}{x^2\epsilon^2}-\frac{3}{8}\frac{\sigma(x)\,\ell_{\rm P}^4(1-2\Lambda)}{x^2\epsilon^2}. \tag{59}$$

From the effective Hamiltonian we get the "wave equation" for the fields living on the curved semiclassical background,

$$\frac{2}{x}\,\frac{\partial\phi(x,t)}{\partial x}-\frac{2}{g(x)}\frac{\partial\phi(x,t)}{\partial x}\frac{\partial g(x)}{\partial x}+\frac{\partial^2\phi\,(x,t)}{\partial x^2}-\frac{1}{4}\frac{g(x)^4}{(1-2\Lambda)^2}\frac{\partial^2\phi(x,t)}{\partial t^2} = 0. \tag{60}$$

Since the background is time-independent, positive and negative frequency modes can be introduced by going to Fourier space in t. The resulting equation can be cast in Sturm–Liouville form as,

$$(2B(x)\phi'(x,\omega))'+\frac{\omega^2}{2}\phi(x,\omega)A(x) = 0 \tag{61}$$

where

$$A(x) \;=\; \frac{x^2}{1-2\,\Lambda}-\frac{5}{8}\,\frac{{\ell_{\rm P}}^4\rho^2}{\epsilon^2}-\frac{3}{4}\,\frac{\sigma\,{\ell_{\rm P}}^4}{\epsilon^2}, \tag{62}$$

$$B(x) \;=\; x^2\,(1-2\,\Lambda)+\frac{5}{8}\,\frac{{\ell_{\rm P}}^4\rho^2}{\epsilon^2}+\frac{3}{4}\,\frac{\sigma\,{\ell_{\rm P}}^4}{\epsilon^2} \tag{63}$$

The solution to this Sturm–Liouville problem is

$$\phi(x,w) = \frac{1}{x}\sin\left(\frac{\omega\, x}{2\,(1-2\Lambda)}\right) \tag{64}$$
$$-\frac{1}{3x^3}\left[x^2\omega^2\cos\left(\frac{\omega x}{2}\right)\mathrm{Si}\,(\omega x)-\frac{x}{2}\omega\cos\left(\frac{\omega x}{2}\right)-x^2\omega^2\sin\left(\frac{\omega x}{2}\right)\mathrm{Ci}(\omega x)+\sin\left(\frac{\omega x}{2}\right)\right]\frac{\ell_{\mathrm{P}}^4}{4\epsilon^2}\left[\frac{5\rho^2}{2}+3\sigma\right]$$

and this solution neglects terms with higher powers than $\ell_{\mathrm{P}}^4/(\epsilon x)^2$. Where $\mathrm{Si}(x) \equiv \int_0^x dt \sin(t)/t$, and $\mathrm{Ci}(x) \equiv \gamma + \ln(x) + \int_0^x dt(\cos(t)-1)/t$ are the sine integral and cosine integral functions respectively and Euler's Gamma is given by $\gamma = 0.5772156649$. The first term in the bracket in (64) corresponds to the standard spherical mode decomposition in (locally) flat space-time. The next parenthesis includes two terms that are corrections, the first due to polymerization and the next, involving σ is a quantum correction. These terms would not be present in a treatment of quantum field theory on a classical space-time. Using the Hamilton equations we can compute P^φ,

$$P^\varphi(x,t) = \frac{x^2 g(x)^2}{2\sqrt{\omega}(1-2\Lambda)}\frac{\partial\phi(x,t)}{\partial t} \tag{65}$$

and use it to compute the effective Hamiltonian (58),

$$\hat{H}^{\mathrm{eff}}_{\mathrm{matt}} = (1-2\Lambda)\int_0^{2\pi/\epsilon} d\omega\omega\hat{\bar{C}}(\omega)\hat{C}(\omega). \tag{66}$$

To obtain this expression we note that the solution (64) can be written as $\phi(x,t) = \int_0^\infty d\omega u(x,\omega)h(\omega,t)$ where $h(\omega,t)$ is the last parenthesis in (64). Notice that we have introduced a lattice cutoff for the frequency $2\pi/\epsilon$. Then one uses the lattice version of the closure relation $\int_0^\infty d\omega u(x,\omega)u(x',\omega) = 2\delta(x-x')/A(x)$ and the orthogonality relation $\int_0^\infty dx A(x)u(x,\omega)u(x,\omega')/2 = \delta(\omega-\omega')$.

We have therefore concluded the computation of the state that we will use as a trial in the variational method. It will be given by a direct product of the vacuum of the matter part of the Hamiltonian (66) and the Gaussian (54) on the gravitational variables.

$$|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = |\psi_{\vec{\sigma}}\rangle \otimes |0\rangle \tag{67}$$

The parameters $\vec{\sigma}$ will be varied to minimize the master constraint. Notice that the state is a direct product because we are considering the vacuum. If we were to consider excitations then there might be entanglement between the matter and gravitational variables [16].

D. Minimizing the master constraint

The realization of the master constraint (38) as a quantum operator depends on the realization of six key operators. We proceed to present their expectation values here. We start by the operators involving the cosine of $\hat{K}_\varphi$,

$$\langle\psi^{\mathrm{trial}}_{\vec{\sigma}}|\cos\left(2\rho\hat{K}_\varphi(i)\right)|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = \exp\left(-\frac{2\rho^2}{\sigma(i)}\right), \tag{68}$$
$$\langle\psi^{\mathrm{trial}}_{\vec{\sigma}}|\cos\left(4\rho\hat{K}_\varphi(i)\right)|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = \exp\left(-\frac{8\rho^2}{\sigma(i)}\right). \tag{69}$$

We then consider the powers of the inverse of $\hat{E}^\varphi$. We already computed the expectation value of the square in (56). Here we list the other needed powers,

$$\langle\psi^{\mathrm{trial}}_{\vec{\sigma}}|\frac{1}{\left(\hat{E}^\varphi(i)\right)^4}|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = \frac{(1-2\,\Lambda)^2}{\epsilon^4 x(i)^4} + \frac{5}{4}\frac{{\ell_{\mathrm{P}}}^4\,(1-2\,\Lambda)^3\,\rho^2}{\epsilon^6 x(i)^6} + \frac{5}{2}\frac{\sigma\,{\ell_{\mathrm{P}}}^4\,(1-2\,\Lambda)^3}{\epsilon^6 x(i)^6}, \tag{70}$$

$$\langle\psi^{\mathrm{trial}}_{\vec{\sigma}}|\frac{1}{\hat{E}^\varphi(i)}\cos\left(2\rho\hat{K}_\varphi(i)\right)\frac{1}{\hat{E}^\varphi(i)}|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = \frac{1-2\Lambda}{\epsilon^2 x(i)^2\exp(\frac{2\rho^2}{\sigma})}\left(1+\frac{5}{2}\frac{\rho^2 l_p^4}{\epsilon^2 x(i)^2}+\frac{3}{4}\frac{\sigma l_p^4}{\epsilon^2 x(i)^2}\right), \tag{71}$$

$$\langle\psi^{\mathrm{trial}}_{\vec{\sigma}}|\frac{1}{\left(\hat{E}^\varphi(i)\right)^{3/2}}\sin\left(\rho\hat{K}_\varphi(i)\right)\frac{1}{\left(\hat{E}^\varphi(i)\right)^{3/2}}|\psi^{\mathrm{trial}}_{\vec{\sigma}}\rangle = 0, \tag{72}$$

$$\langle\psi^{\rm trial}_{\vec\sigma}|\frac{1}{\sqrt{\hat E^\varphi(i)}}\sin\left(\rho\hat K_\varphi(i)\right)\frac{1}{\sqrt{\hat E^\varphi(i)}}|\psi^{\rm trial}_{\vec\sigma}\rangle=0, \tag{73}$$

$$\langle\psi^{\rm trial}_{\vec\sigma}|\frac{1}{\sqrt{\hat E^\varphi(i)}}\sin\left(3\rho\hat K_\varphi(i)\right)\frac{1}{\sqrt{\hat E^\varphi(i)}}|\psi^{\rm trial}_{\vec\sigma}\rangle=0. \tag{74}$$

With these results we can proceed to compute the expectation value of the master constraint on the gravitational state. The result will be an operator acting on the matter part. The calculation of the expectation values of the coefficients $\hat c_i$ and $\hat c_{ij}$ (42)-(51) is straightforward, but lengthy. We will not list the results here. What is more challenging is the computation of the expectation value of the matter part of the expansion of (38). It helps that some of the coefficients vanish. The non-vanishing contributions are,

$$\begin{aligned}\langle\psi_{\vec\sigma}|\hat{\mathbb{H}}(i)|\psi_{\vec\sigma}\rangle &= \ell_{\rm P}\Bigg[\langle\hat c_{11}(i)\rangle\left(\widehat{H^{(1)}_{\rm matt}(i)}\right)^2+\langle\hat c_{22}(i)\rangle\left(\widehat{H^{(2)}_{\rm matt}(i)}\right)^2+\langle\hat c_1(i)\rangle\widehat{H^{(1)}_{\rm matt}(i)}+\langle\hat c_{33}(i)\rangle\left(\widehat{H^{(3)}_{\rm matt}(i)}\right)^2\\ &\quad+\langle\hat c_3(i)\rangle\widehat{H^{(1)}_{\rm matt}(i)}+\langle\hat c_{13}(i)\rangle\widehat{H^{(1)}_{\rm matt}(i)}\widehat{H^{(3)}_{\rm matt}(i)}+\langle\hat c_{00}(i)\rangle\Bigg].\end{aligned} \tag{75}$$

We now need to compute the expectation value of this operator on the matter vacuum. To do this we again use the procedure of going to the continuum limit in the matter terms involving derivatives and momenta and integrating in the frequencies with an ultraviolet cutoff. Let us start with $H^{(1)}_{\rm matt}(i)$. The continuum limit expression is $H^{(1)}_{\rm matt}(x,t)=\ell_{\rm P}^2\left(\left(P^\phi(x,t)\right)^2+x^4\left(\phi'(x,t)\right)^2\right)$. We now substitute P^ϕ and ϕ by their mode decomposition and one gets a quadratic expression in the $\hat C$'s and $u's$. The expectation value only gets contributions from the $\hat C\hat{\bar C}$ terms. The result is,

$$\langle 0|\hat H^{(1)}_{\rm matt}|0\rangle=l_p^2\int_0^{\frac{2\pi}{\epsilon}}d\omega\frac{1}{8\omega(1-2\Lambda)}[A(x)^2u^2(x,\omega)\omega^2(1-2\Lambda)^2+4x^4(\partial_x u(x,\omega))^2], \tag{76}$$

and substituting $u(\omega,x)$ and $A(x)$ we obtain,

$$\begin{aligned}\langle 0|\hat H^{(1)}_{\rm matt}(x)|0\rangle &= l_p^2(1-2\Lambda)A(x)^2\left(\frac{\pi^2}{8x^2\epsilon^2}+\frac{1}{8x^4}-\frac{\cos^2(\frac{\pi x}{\epsilon})}{8x^4}-\frac{\pi\sin(\frac{\pi x}{\epsilon})\cos(\frac{\pi x}{\epsilon})}{4x^3\epsilon}\right)\\ &\quad+\frac{l_p^2}{(1-2\Lambda)}\left(\frac{\pi^2x^2}{8\epsilon^2}+\frac{\ln(2)}{4}+\frac{x\pi\cos(\frac{\pi x}{\epsilon})\sin(\frac{\pi x}{\epsilon})}{4\epsilon}-\frac{5}{8}\sin^2(\frac{\pi x}{\epsilon})+\frac{1}{4}{\rm Cin}(\frac{\pi x}{\epsilon})\right),\end{aligned} \tag{77}$$

where ${\rm Cin}(x)=\gamma+\ln x-{\rm Ci}(x)$. One can get a more manageable expression, which we will use in the rest of the paper by ignoring corrections of $\ell_{\rm P}^4$ and neglecting the highly oscillating terms that involve $\sin(\pi x/\epsilon)$ or cosines and the integral cosines. The result is,

$$\langle 0|\hat H^{(1)}_{\rm matt}(x)|0\rangle=\frac{l_p^2}{4(1-2\Lambda)}\left(-2+\frac{\pi^2x^2}{\epsilon^2}+\ln(2)+\gamma+\ln(\frac{\pi x}{\epsilon})\right), \tag{78}$$

and the dominant term is π^2x^2/ϵ^2. Reverting to the discrete theory, it reads,

$$\langle 0|\hat H^{(1)}_{\rm matt}(i)|0\rangle=\frac{l_p^2\epsilon^3}{4(1-2\Lambda)}\left(-2+\frac{\pi^2x(i)^2}{\epsilon^2}+\ln(2)+\gamma+\ln(\frac{\pi x}{\epsilon})\right). \tag{79}$$

The procedure to compute the expectation value of the other terms in (75) is exactly the same, but the size of the expressions involved is quite large. We will not display them here for reasons of space.

The result for the expectation value of the integrand of the master constraint is,

$$\begin{aligned}\langle\hat{\mathbb{H}}(x)\rangle &= \frac{\sigma_0\,{\ell_{\rm P}}^3}{\epsilon\,x^2}+\Bigg(8\,\frac{\pi^2}{\epsilon^3x^2}+\frac{32}{\epsilon x^4}\,\ln\left(\frac{L}{\epsilon}\right)-\frac{\left(\gamma-2+\ln\left(\frac{2\pi x}{\epsilon}\right)\right)\pi}{\epsilon\,x^4(1-2\Lambda)}+\frac{1}{96}\,\frac{\pi^3}{\epsilon^5x^2\sigma_0\,(1-2\Lambda)^2}\\ &\quad-\frac{1}{48}\,\frac{\Lambda\,\pi^3}{\epsilon^5x^2\sigma_0\,(1-2\Lambda)^2}-\frac{43}{128}\,\frac{\Lambda\,\pi}{\epsilon^3x^4\sigma_0\,(1-2\Lambda)^2}\\ &\quad+\frac{\epsilon\,(\gamma-2+\ln\left(\frac{2\pi x}{\epsilon}\right))\pi}{x^4(1-2\Lambda)\,L^2}+8\,\frac{\epsilon\,\pi^2}{x^2L^4}-\frac{2\,\pi}{\epsilon x^4(1-2\Lambda)}\,\ln\left(\frac{L}{\epsilon}\right)-16\,\frac{\pi^2}{\epsilon\,x^2L^2}+\frac{1}{32}\,\frac{\pi}{\epsilon\,x^4(1-2\Lambda)^2}\end{aligned} \tag{80}$$

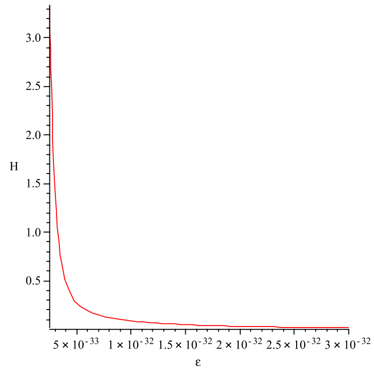

FIG. 1: The expectation value of the master constraint as a function of the lattice spacing. We see that the value of the master constraint is small unless one chooses lattice separations of order Planck length. The figure does not show it, but for separations of the order of 10^{-23}cm the master constraint is very small, of the order of 10^{-20} (we are using units in which $\hbar$ is one and therefore the master constraint is dimensionless).

$$
\begin{aligned}
&+\frac{1}{48}\frac{\pi^3}{\epsilon^3 x^2(1-2\Lambda)^2}+\frac{32\,\epsilon}{x^6\pi^2}\left(\ln\left(\frac{L}{\epsilon}\right)\right)^2-\frac{\pi^3}{\epsilon^3x^2(1-2\Lambda)}+4\,\frac{\pi}{\sigma_0\,\epsilon^3x^2}\\
&-\frac{32}{x^4L^2}\,\epsilon\,\ln\left(\frac{L}{\epsilon}\right)-3\,\frac{\sigma_0\,\pi}{x^3L^2}+\frac{43}{256}\,\frac{\pi}{\epsilon^3x^4\sigma_0\,(1-2\Lambda)^2}+\frac{8}{\sigma_0\epsilon x^4\pi}\,\ln\left(\frac{L}{\epsilon}\right)\\
&-\frac{1}{4(1-2\Lambda)}\,\frac{\left(4x^2\epsilon\sigma_0+4\,x{\sigma_0}^3\epsilon^2+4\,\sigma_0\,\epsilon^2x+7\,{\sigma_0}^3\epsilon^3\right)}{(x+\epsilon)\sigma_0^2x^5\epsilon^4}\times\left(\frac{1}{4}\pi^2x^2+\frac{1}{4}\epsilon^2\left(\gamma-2+\ln\left(\frac{2\pi x}{\epsilon}\right)\right)\right)\\
&-3\,\frac{\sigma_0\,\pi}{(x+\epsilon)\,x^2\epsilon^2}+3\,\frac{\sigma_0\,\pi}{(x+\epsilon)\,x^2L^2}-\frac{6\,\sigma_0}{(x+\epsilon)x^4\pi}\,\ln\left(\frac{L}{\epsilon}\right)-4\,\frac{\pi}{x^2\epsilon\,\sigma_0\,L^2}+\frac{\pi^3}{\epsilon\,x^2(1-2\Lambda)\,L^2}\\
&\left.-2\,\frac{\epsilon}{x^6(1-2\Lambda)\pi}\left(\gamma-2+\ln\left(\frac{2\pi x}{\epsilon}\right)\right)\ln\left(\frac{L}{\epsilon}\right)+3\,\frac{\sigma_0\,\pi}{x^3\epsilon^2}+6\,\frac{\sigma_0}{x^5\pi}\,\ln\left(\frac{L}{\epsilon}\right)-1/16\,\frac{\epsilon}{x^6(1-2\Lambda)^2\pi}\right){\ell_{\rm P}}^5.
\end{aligned}
$$

We have assumed $\sigma=\sigma_0\epsilon^2/\ell_{\rm P}^2$ with σ_0 of order unity and we have neglected terms $O(\ell_{\rm P}^7)$. We have assumed σ to be independent of x in order to simplify the above expression, which otherwise becomes too large. Experiments we have carried out suggest that allowing variations in x leads to the same minimum value of σ approximately independent of x.

We would like to study the minimum of the master constraint as a function of σ_0 for different choices of $\epsilon/\ell_{\rm P}$. Notice that we have assumed σ_0 to be of order one. One can change that by varying the ansatz for σ including other powers $\epsilon/\ell_{\rm P}$ different than 2. We have carried out such experiments. The results can be summarized as follows. In figure 1 we show the value of the master constraint as a function of ϵ (in centimeters) and for $\sigma_0=10$ and $\sigma=\sigma_0\epsilon^3/\ell_{\rm P}^3$. Varying σ_0 while keeping it of order one changes little the shape of the curve. We see that in the approximation studied the theory does not appear to have a continuum limit, but we see that the master constraint quickly drops to zero for lattice spacings larger than Planck scale. Although the figure suggests that the master constraint drops even further for larger lattice spacings, the approximation in which we have handled expressions (in which we have neglected higher powers of $\epsilon/\ell_{\rm P}$) is inadequate for large values of ϵ and the master constraint very likely will increase its value for large values of ϵ. So there exists a genuine preferred value of ϵ that minimizes the master constraint. Even so, the approximation should be reliable up to values of $\epsilon\sim10^{-23}$cm and for such values the master constraint is of the order of 10^{-20}, so one sees that this is a regime where one approximates the continuum theory very well.

We have explored other ranges of σ's (with different powers of $\epsilon/\ell_{\rm P}$). The observation is the following. For lower powers than three we get a curve that looks similar to the one shown in the figure, but that grows faster as one approaches smaller lattice spacings and therefore the minimum occurs farther away from the Planck scale. For powers higher than 10/3 one violates the approximation that $\ell_{\rm P}/\epsilon$ is small and the expressions we derived are not valid. From these considerations and an analysis of the powers involved, we conclude that the minimum for the master constraint is achieved for a power of $\epsilon/\ell_{\rm P}$ in σ close to two and $\epsilon\sim10^{13}\ell_{\rm P}$.

An interesting speculation is that if the minimum of the master constraint happens in the range mentioned, the cosmological constant, which goes as $\Lambda\sim\ell_{\rm P}^2/\epsilon^2$ would not be of Planck scale but several orders of magnitude smaller.

Another observation of interest is to note what would have happened if instead of choosing the state peaked around the flat metric (with a topological defect) one would have chosen the “loop quantum gravity vacuum”, i.e. a state with zero loops which corresponds to a degenerate metric $|\mu(i) = 0\rangle$. Such a state annihilates the matter Hamiltonian in the loop representation and has zero volume. It would be disturbing if this state yielded a lower value for the master constraint than the state we constructed, since it would imply that degenerate geometries dominate. This is not the case, as can be easily seen. For such a state all expectation values (68)-(74) vanish. One can check that the expectation value of the master constraint is,

$$\langle\hat{\mathbb{H}}\rangle = \frac{1}{8}\frac{L\ell_{\rm P}}{\epsilon^2\rho}. \tag{81}$$

That is, the result is very large. For $\epsilon \sim \ell_{\rm P}$ it goes as $L/\ell_{\rm P}$, the size of the universe in Planck lengths. Therefore these degenerate states are heavily suppressed.

V. DISCUSSION

We have studied spherically symmetric gravity coupled to a spherically symmetric scalar field using loop quantum gravity techniques. The problem has a non-Lie algebra of constraints and we used the "uniform discretization" technique to treat the dynamics. We used a variational technique to minimize the discrete master constraint. With the trial states proposed, we were not able to reach a zero eigenvalue for the master constraint, that is, the theory does not seem to have a quantum continuum limit. The lowest eigenstate of the master constraint has the form of a direct product of a Fock vacuum for the scalar field and Gaussian states centered around flat space-time for the gravitational variables. Although the theory does not have a continuum limit, it approximates general relativity well for small values of the lattice separation, which in turn regularizes the cosmological constant. The lattice treatment we have performed diverges when one takes the continuum limit. The reader may wonder why loop quantum gravity has failed to act as the "natural regulator of matter quantum field theories" as claimed, for instance in [17]. The problem arises with the gauge fixing of the diffeomorphism constraint that we performed at the classical level. This leads us to variables that have the structure of a Bohr compactification in the "transverse" φ direction, but the variable in the radial direction is a c-number and therefore is not dynamical and has continuous character. There is no chance therefore that loop quantum gravity based on this gauge fixing could regulate the short distance behavior, which is responsible for the emergence of the cosmological constant. To tackle this issue one would have to allow both the diffeomorphism and Hamiltonian constraint to remain in the theory. The calculational complexity would increase importantly, since one will have to regulate the master constraint in such a way that the resulting states have remnants of diffeomorphism invariance in the discrete theory. This has been successfully accomplished with uniform discretizations in the Husain–Kuchař model [11], but the complexity there was considerably reduced by the lack of a Hamiltonian constraint. It is worthwhile noticing that even if one allowed loop quantum gravity to regulate matter in the proposed way, the resulting cosmological constant is likely to be finite but still very large with respect to the current observed value.

The present paper is a first exploration of a difficult problem, carried out with several assumptions and limitations that we have outlined in the text. Future work will include relaxing the assumption that one has a Fock vacuum for the scalar field and treating both the gravitational and scalar variables on the same footing with the variational technique for the master constraint. In this context it will be interesting to study the excited states of matter and study the modifications in dispersion relations for the matter fields due to the quantum geometry. This will definitely require considering trial states with correlations in the variational method, something we have not done here. One should also relax the gauge fixing of diffeomorphisms to see if the cosmological constant problem becomes better under control. Other future directions would be to consider solutions centered around non-flat geometries, for instance, including a black hole with the aim of studying if the scalar field states involve Hawking radiation.

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