Thermal fluctuations in loop cosmology

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Quantum gravitational effects in loop quantum cosmology lead to a resolution of the initial singularity and have the potential to solve the horizon problem and generate a quasi scale-invariant spectrum of density fluctuations. We consider loop modifications to the behavior of the inverse scale factor below a critical scale in closed models and assume a purely thermal origin for the fluctuations. We show that the no-go results for scale invariance in classical thermal models can be evaded even if we just consider modifications to the background (zeroth order) gravitational dynamics. Since a complete and systematic treatment of the perturbed Einstein equations in loop cosmology is still lacking, we simply parameterize their expected modifications. These change quantitatively, but not qualitatively, our conclusions. We thus urge the community to more fully work out this complex aspect of loop cosmology, since the full picture would not only fix the free parameters of the theory, but also provide a model for a non-inflationary, thermal origin for the structures of the Universe.

I. INTRODUCTION

The possibility that primordial thermal fluctuations might seed the structure of our Universe is an intriguing alternative to quantum fluctuations in a deSitter phase [1,2,3,4]. Unfortunately a number of obstacles present themselves to such an enterprise. Firstly any thermal scenario should necessarily be based on a solution of the horizon problem. This is so that the assumption of thermalization itself makes sense: modes must start off in causal contact to thermalize and then leave the horizon. (This is in fact true of any scenario where the fluctuations are “passive” [5,6,7]) A number of solutions to the horizon problem have been proposed [8,9,10] and in this paper we use in effect a combination of two.

But more importantly thermal scenarios run against an apparent wall: the well known fact that thermal fluctuations have a white-noise spectrum, i.e. spectral index $n_S = 0$, rather than the observed near-scale-invariance, $n_S \approx 1$. Thus any scenario where the primordial fluctuations result from a “snap-shot” of a thermal bath at a fixed temperature is doomed. This discouraging result, however, may be circumvented by noting that the white-noise nature of thermal fluctuations follows from the extensive nature of the energy. Reasonable and general as this assumption might be, it could be violated in the early Universe, during a phase ruled by new physics at the Planck or string energy scale. This has been suggested by at least two lines of research. In one a gauge of strings at the Hagedorn phase is employed [8]. Another invokes a holographic phase in loop quantum gravity [10].

Yet another solution is to ensure that different modes leave the horizon and freeze-out at different temperatures. Then, the equal-temperature spectrum of thermal fluctuations is still white-noise, but the spectrum of frozen-in fluctuations imprinted outside the horizon isn’t. The actual form of that spectrum depends on the balance between the size of the mode leaving the horizon at a given time and the temperature (and thus the mode’s amplitude) at the time the mode is picked out of the thermal bath, leaves the horizon and freezes-in. There is some controversy over whether this mechanism may lead to a scale-invariant spectrum and one of the purposes of this paper is to clarify the matter.

In Section II we provide a model calculation based on a minimally modified thermal scenario, in which thermal matter is allowed to have a different equation of state with $w = p/\rho < -1/3$, but where nothing else is changed. We show that unless new physics comes into play, modifying the Einstein equations, the thermodynamical relations, or some other standard assumption, in all such scenarios the spectral index is $n_S = 4$. This is true regardless of $w$, the only free parameter of the model. This section is supplemented by Appendix A which provides all relevant definitions of measures of structure.

Of course it is natural that new physics does come into play in the early Universe, and the rest of this paper is focused on the potential of loop quantum cosmology (LQC) to reverse this negative result (for an up to date introductory review see [11] and for early developments in the field see [12]). Modifications to the the Einstein equations in LQC originate from two sources: the field strength (curvature) of the Ashtekar connection which is expressed in terms of holonomies and the inverse powers of volume in the constraint. These are quantified by two parameters in the theory. Firstly, the $j$ parameter, which appears due to tracing over holonomies of the SU(2) connection in both gravitational and matter parts of the constraint. This parameter also determines the scale at which modifications to inverse volume become significant. Secondly, the $l$ parameter, which arises due to the inverse volume term in the matter part and quantifies the functional form of this modification.

So far a complete and consistent quantization of LQC with the knowledge of physical Hilbert space has only been performed for $j = 1/2$. It shows a physical resolu-
ne of the singularity and leads to the correct classical limit \[ 13, 14, 15, 16, 17 \]. Nevertheless, these investigations have provided valuable insights on existence of effective Hamiltonian which is an excellent approximation to the underlying quantum dynamics and which can be generalized to higher \( j \) in particular for the regime where \( w \approx -2/3 \). This can be obtained by a suitable choice of the \( l \) parameter.

Since work on inclusion of inhomogeneities in loop cosmology is at a very early stage of development \[ 19 \] (and various technical aspects, in particular those relevant for the regime of interest, are yet to be understood) we adopt a phenomenological approach and parameterize the expected modifications to the perturbed Einstein equations. We show that expected corrections in fact make the above result stronger.

More work needs to be carried out by the community until our calculations may be converted into specific constraints. But, as we summarize in Section \[ V \] in this paper we are able to provide a list of what exactly needs to be worked out so that \( n_S \approx 1 \) is converted into a constraint upon the free parameters of LQC.

II. THE BASE CALCULATION AND THE NO-GO RESULT IN CLASSICAL PHYSICS

Let us consider a thermal scenario in which the only effect of new physics is to change the equation of state of thermal matter. This certainly happens in theories with deformed dispersion relations \[ 2, 3 \], and also in LQC \[ 20 \]. We then assume that statistical physics, the gravitational equations and a few basic thermodynamical relations are not modified. This won’t necessarily happen in loop cosmology, but the way in which the modifications arise is not yet fully understood. It is therefore interesting to provide a base calculation, assuming no changes, as a blueprint for further work.

The calculation follows three steps.

A. The fixed temperature power spectrum

The first step is to compute the fixed temperature power spectrum. This turns out to depend only on the specific heat at constant volume (a result that has been known since the XIX century, and is now textbook material \[ 21 \]). The spectrum is generally white noise, a fact that can be directly traced to the extensive nature of the energy, i.e. to the fact that the energy inside a given region is proportional to its volume.

The derivation is very general. Consider the partition function

\[
Z = \sum_r e^{-\beta E_r},
\]

where \( \beta = T^{-1} \). The total (matter) energy \( U \) inside a volume \( V \) is given by:

\[
U = \langle E \rangle = \frac{\sum_r E_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}} = -\frac{d\log Z}{d\beta}
\]

and its variance by

\[
\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2 = \frac{d^2 \log Z}{d\beta^2} = -\frac{dU}{d\beta} = T^2 c_V
\]

where \( c_V \) is the specific heat at constant volume. If the energy is extensive then \( U = \rho V \), with energy density \( \rho = \rho(T) \), that is \( U \) is proportional to the volume. The spectral index and amplitude may now be found by means of the following tools (for the closed model we will be interested in the regime where intrinsic curvature terms can be neglected):

- The Poisson equation

\[
k^2 \Phi = 4\pi Ga^2 \delta \rho = 4\pi Ga^2 \delta \rho,
\]

relating the gravitational potential \( \Phi \) and the density fluctuations. Outside the horizon there may be gauge issues, but this relation certainly holds for subhorizon modes.

- The proportionality between the variance \( \sigma_g^2(R) \) in a quantity \( g \) defined in position space and smeared on a scale \( R \), and the “dimensionless power spectrum”:

\[
\sigma_g^2(R) = \langle \delta g^2 \rangle_R \approx P_g(k_R = a/R)
\]

(see Appendix \[ A \] for definitions; note that here \( k \) is comoving, but \( R \) is a proper size). The spectral index \( n_S \) is defined from \( P_\Phi = A^2 k^{n_S-1} \). Formula \[ 22 \] has not been questioned for \( n_S < 1 \); but see \[ 23 \].
Then using (3) we have
\[ \langle \delta \rho^2 \rangle_R = \frac{1}{R^6} \langle \delta E^2 \rangle_R = \frac{\sigma^2_E(R)}{R^6} = \frac{T^2}{R^6} \cdot \]
Combining this result with (4) and (5) (for \( g = \delta \rho \)) we thus conclude
\[ \mathcal{P}_\Phi \sim \frac{a^4 \mathcal{P}_\delta}{k^3} \sim \frac{a^4}{k^3} \left[ \frac{T^2}{R^6} \right]_{R=R_0} \sim \frac{k^2}{a^2} T^2 \left[ \mathcal{C}_V \right]_{R=R_0} . \] (7)
Using the extensive nature of the energy we have \( \mathcal{C}_V = \rho' \mathcal{P}_\rho \), so finally
\[ \mathcal{P}_\Phi \sim \frac{a}{k} T^2 \rho' . \] (8)
The fluctuations are therefore white noise \((n_S = 0)\), and have an amplitude that only depends on the Stephan-Boltzmann law, relating energy density and temperature. We shall assume a Stephan-Boltzmann law of the type \( \rho \propto \rho'(T)R^3 \), so finally
\[ \mathcal{P}_\Phi \sim \frac{a}{k} T^2 \rho' . \]

B. Frozen-in power spectrum

We assume that comoving scales \( k \) start thermalized and inside the horizon, and then leave the horizon, with (first) crossing defined by \( k = aH \). This requires either accelerated expansion [1], a loitering phase [2], a decreasing speed of light [3], a bouncing scenario, or a combination thereof. We use the first mechanism, so that the equation of state satisfies \( w < -1/3 \).

As the \( \Phi \) modes leave the horizon their amplitude gets fixed at whatever thermal amplitude they have at crossing, that is:
\[ \mathcal{P}_\Phi(k) \sim \frac{a^4}{k^3} \left[ \frac{T^2}{R^6} \right]_{k=aH} . \] (9)
Since different modes freeze at different temperatures the spectrum left outside the horizon won’t be white noise.

Using the Friedman equation \( H^2 \propto \rho \) we can rewrite (9) as
\[ \mathcal{P}_\Phi(k) \sim \left[ \frac{T^2 \rho'}{\sqrt{\rho}} \right]_{k=aH} . \] (10)
where \( k = aH \) specifies a relation between a given comoving \( k \) leaving the horizon at a given time, and the temperature, thereby allowing the inversion of the right hand side as a function of \( k \). Eqn. (10) implies:
\[ \frac{d \ln \mathcal{P}_\Phi}{d \ln T} = 1 + \frac{\zeta}{2} . \] (11)
The relation between \( k = aH \) and the temperature, however, depends on both the equation of state \( p = w \rho \) and \( \rho \propto T^\zeta \). Using the Friedman equation we have \( k = aH \propto a\sqrt{\rho} \), and since \( \rho \propto 1/a^{3(1+w)} \), we may derive
\[ a \propto T^{\frac{\zeta}{3(1+w)}} . \] (12)
Therefore:
\[ \frac{d \ln k}{d \ln T} = -\frac{\zeta}{3(1+w)} + \frac{\zeta}{2} = \frac{\zeta(1+3w)}{6(1+w)} . \] (13)
We can now compute the spectral index as
\[ n_S - 1 = \frac{d \ln \mathcal{P}_\Phi}{d \ln k} = \frac{d \ln \mathcal{P}_\Phi}{d \ln T} \frac{d \ln T}{d \ln k} = 3\frac{2 + \zeta}{\zeta - 1} + 3w . \] (14)
but note that the condition \( w < -1/3 \) (or that \( k = aH \) increases in time) is necessary for this formula to make sense.

Two promising regions of parameter space stand out. Firstly \( \zeta = -2 \), that is \( \rho \propto 1/T^2 \); this may lead to scale-invariance because the amplitude of the frozen-in thermal fluctuations does not depend on the temperature in this case (c.f. Eqn.10). Secondly \( w = -1 \); one can see that this could lead to scale-invariance because \( \rho \) does not change (it behaves like a cosmological constant), and so neither does the temperature or amplitude of the fluctuations as they leave the horizon.

However further conditions apply. Regarding the first case we have to check that \( w < -1/3 \) is possible, so that modes do leave the horizon. With respect to the latter, we should additionally have \( \zeta \neq 0 \) (or \( \zeta \neq \infty \)), so that there are fluctuations at all (and they are not infinite). Unfortunately closer inspection shows that these conditions cannot be met.

C. Thermodynamical constraints

It’s been noted [24, 23, 26] that the equation of state \( p = \omega \rho \) and the Stephan-Boltzmann law \( \rho = \rho(T) \) are linked by a thermodynamical relation. The argument assumes that energy and entropy are extensive. Consider the first law of thermodynamics:
\[ dU = -PdV + TdS . \] (15)
If the energy \( U \) and entropy \( S \) are extensive, then \( U(\lambda V, \lambda S) = \lambda U(V, S) \). Taking a derivative with respect to \( \lambda \) at \( \lambda = 1 \), and using (15) we arrive at the Euler relation
\[ U = -PV + TS . \] (16)
so that defining \( \rho = U/V \) and entropy density \( s = S/V \) we have
\[ s = \frac{P + \rho}{T} . \] (17)
We can now prove that \( s = dP/dT \) in a variety of ways, e.g. introducing the free energy \( F = U - TS = F(V, T) \), so that \( dF = -PdV - SdT \). This leads to the integrability condition:
\[ s = \left( \frac{\partial S}{\partial V} \right)_T = \left( \frac{\partial P}{\partial T} \right)_V . \] (18)
Thus the expression
\[
\frac{dP}{dT} = \frac{P + \rho}{T} .
\]  

If \( w \) is a constant we obtain that \( \rho \propto T^w \) with
\[
\zeta = 1 + \frac{1}{w} .
\]  

The trouble is that this relation implies that \( \zeta = 0 \) for \( w = -1 \): “deformed” radiation may behave like a cosmological constant, but then the specific heat vanishes and there are no thermal fluctuations at all. This is an interesting result but kills the second candidate for scale-invariance proposed above.  

The first candidate is killed by noting that \( \zeta = -2 \) implies \( w = -1/3 \), that is a Mink Universe. This is merely a borderline case for solving to the horizon problem: the comoving horizon does not increase but neither does it increase.

One might expect that models near these two can bypass these problems and display if not strict scale-invariance, at least approximate scale-invariance. However this is not the case. Inserting (20) into (14) a simple algebraic calculation shows that \( w \) (or \( \zeta \)) cancel out and we are left with
\[
n_s = 4
\]  

for all model parameters.

Therefore one needs further new physics to bypass this negative result. Presumably the double branched dispersion relations considered in [3] are behind the fact that \( w = -1, \zeta = 1 \) is possible (in contradiction with [20]). We now examine the way modifications to the dynamics in LQC reverse these results.

### III. EFFECTIVE DYNAMICS IN LOOP QUANTUM COSMOLOGY

The phase space in LQC consists of the geometrical variables – the connection \( c \) and the triad \( p \) – and the matter variables, which for a scalar field will be \( \phi \) and its canonical momenta \( p_\phi \). The triad is related to the scale factor as \( p = a^2 = V^{2/3} \). On the classical solutions of GR for closed model, \( c \) is related to the time derivative of scale factor as \( c = \gamma \dot{a} + 1 \) where \( \gamma \approx 0.2375 \) is the Barbero-Immirzi parameter. The connection and triad are canonically conjugate satisfying
\[
\{ c, p \} = \frac{8\pi G \gamma}{3} .
\]  

For the closed model, in the regime where the Hubble rate is small compared to Planck scale we can write an effective Hamiltonian which encodes the modifications to the inverse scale factor below a critical scale \( a_* \) (parameterized by \( j \) [B21]) in terms of functions \( S \) (Eq. [B22]) and \( D_l \) (Eq. [B23]):

\[
H_{\text{eff}} = -\frac{3}{8\pi G \gamma^2} S a ((c - 1)^2 + \gamma^2) + H_m
\]  

where \( H_m \) is the matter Hamiltonian obtained after inverse volume modifications using [B20]. For a massive scalar field it is
\[
H_m = \frac{1}{2} D_l \frac{p_\phi^2}{a^3} + a^3 V(\phi) .
\]  

Dynamics can now be obtained by the use of Hamilton’s equations. In order to obtain the modified Friedman equation we first evaluate
\[
\dot{c} = \{ c, H_{\text{eff}} \} = -\frac{8\pi G \gamma}{3} \frac{\partial H_{\text{eff}}}{\partial \rho}
\]  

and then using it in \( H_{\text{eff}} \approx 0 \):
\[
\frac{\dot{a}^2}{a^2} = \frac{8\pi G}{3} S (H_m - \frac{S^2}{a^2}) - \frac{8\pi G}{3} S \rho_{sc} - \frac{S^2}{a^2}
\]  

where \( \rho_{sc} = H_m/a^3 \) denotes the modified energy density [27] (we follow the conventions of Ref. [20]). It can be easily seen that a bounce occurs for \( a < a_* \) when \( (8\pi G/3) \rho_{sc} = S/a^2 \) which is possible due to form of \( S \) and \( D_l \) in this regime. Also, for \( a \gg a_* \) and \( D_l \) approach unity yielding us the classical Friedman dynamics.

We can obtain the modified Raychaudhuri equation using Hamilton’s equation for \( c \):
\[
\dot{c} = \{ c, H_{\text{eff}} \} = \frac{8\pi G \gamma}{3} \frac{\partial H_{\text{eff}}}{\partial \rho}
\]  

and the expression for the modified pressure
\[
P_{sc} = -\frac{\partial H_M}{\partial V} = -\frac{2}{3} S^{-1/2} \frac{\partial H_M}{\partial \rho} .
\]  

These equations lead to
\[
\frac{\dot{a}}{a} = -\frac{1}{2\gamma} ((c - 1)^2 + \gamma^2) \left( \frac{\dot{S}}{S} - \frac{S}{a} \right) - 4\pi G a P_{sc}
\]  

which combined with the time derivative of Eq. [25] result in the modified Raychaudhuri equation:
\[
\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} (3\rho_{sc} + 3 P_{sc}) + \frac{1}{2} \frac{\dot{S}}{S} \left( \frac{\dot{a}}{a} - \frac{S}{a} \right) .
\]  

It is then straightforward to verify, using the Friedman and the Raychaudhuri equations, that \( \rho \) satisfies the conservation law:
\[
\dot{\rho}_{sc} + 3 \frac{\dot{a}}{a} (\rho_{sc} + P_{sc}) = 0 .
\]
Defining the modified equation of state as

$$w_{sc} = \frac{P_{sc}}{\rho_{sc}}$$

we therefore have

$$\rho_{sc} = \frac{\rho_{0sc}}{a^{3(1+w_{sc})}}.$$  \hspace{1cm} (33)

The modified Klein-Gordon equation can be derived by using

$$\dot{\phi} = \{\phi, H_m\} = \frac{\partial H_m}{\partial \phi}$$

and

$$\dot{p}_\phi = \{p_\phi, H_m\} = -\frac{\partial H_m}{\partial p_\phi}.$$  \hspace{1cm} (35)

Taking the time derivative of $\dot{\phi}$ we are led to

$$\ddot{\phi} = -3 \frac{\dot{a}}{a} \left(1 - \frac{1}{3} \frac{d \ln D_l}{d \ln a}\right) \phi - D_l \frac{\partial \mathcal{V}}{\partial \phi}.$$  \hspace{1cm} (36)

For $a \ll a_*$, $D_l \ll 1$ and the dynamics of the massive scalar field just behaves as of the massless scalar field. It is straightforward to verify that the energy density

$$\rho_{sc} = \frac{1}{2} \frac{\ddot{\phi}^2}{D_l} + \mathcal{V}$$

and pressure

$$P_{sc} = \frac{1}{2} \frac{\ddot{\phi}^2}{D_l} \left(1 - \frac{1}{3} \frac{d \ln D_l}{d \ln a}\right) - \mathcal{V}.$$  \hspace{1cm} (38)

lead to above Klein-Gordon equation through the conservation equation \ref{conservation}.

The modified equation of state thus becomes

$$w_{sc} = \frac{P_{sc}}{\rho_{sc}} = \frac{\ddot{\phi}^2 \left(1 - \frac{1}{3} \frac{d \ln D_l}{d \ln a}\right) - 2D_l \mathcal{V}}{\ddot{\phi}^2 + 2D_l \mathcal{V}}.$$  \hspace{1cm} (39)

Using Eq.\ref{modifiedEOS} we obtain $w_{sc}$ for $a \ll a_*$:

$$w_{sc} \approx 1 - \alpha$$

where

$$\alpha = \frac{3 - l}{1 - l}.$$  \hspace{1cm} (41)

The modified equation of state for arbitrary matter can be similarly found by following the procedure in Ref.\ref{mukhanov}. Here one views $\rho_{sc}$ as being obtained from substituting inverse powers of scale factor as appropriate powers of $D_l$. If the classical energy density is given by

$$\rho_c = \frac{\rho_0}{a^{3(1+w_c)}}$$

then it is easy to see that

$$\rho_{sc} = \frac{\rho_0}{a^{3(1+w_{sc})}} D^{w_c}.$$  \hspace{1cm} (43)

Since the latter satisfies a conservation equation, it evolves according to an expression like \ref{modifiedEOS} but with modified equation of state

$$w_{sc} = w_c \left(1 - \frac{1}{3} \frac{d \ln D_l}{d \ln a}\right).$$  \hspace{1cm} (44)

Thus for $a \ll a_*$ we obtain

$$w_{sc} \approx w_c (1 - \alpha).$$  \hspace{1cm} (45)

Since $0 < l < 1$, $w_{sc}$ can be easily less than $-1/3$ for arbitrary matter when $a < a_*$.  

IV. ORIGIN OF THERMAL FLUCTUATIONS IN LOOP COSMOLOGY

In the preceding section we saw that even at the zeroth order there are modifications to the Friedman dynamics in loop cosmology. These are sufficient to possibly overcome the no-go result obtained in classical physics. We start with the simplest possibility where the only change coming from the intrinsic curvature can be ignored in the Friedman equation. We note that immediately after the bounce, $\rho_{sc}$ becomes dominant over $S/a^3$ term and for a proper choice of initial conditions for matter such a regime can coexist with $a \ll a_*$.

Using Eq.\ref{modifiedEOS}, Eq.\ref{basis} modifies to

$$\mathcal{P}_\Phi(k) \sim \frac{\frac{T^2 \rho_{sc}'}{S \rho_{sc}^2}}{1 + \frac{\dot{S}}{S}}.$$  \hspace{1cm} (46)

Since $\rho_{sc} \propto a^{-3(1+w_{sc})}$ and $\rho \propto T^2$, we obtain

$$a \propto T^{\frac{2}{3(1+w_{sc})}}.$$  \hspace{1cm} (47)

Using Eq.\ref{modifiedEOS} we find that for $a \ll a_*$, $S \propto a^3$ and hence

$$\frac{d \ln \mathcal{P}_\Phi}{d \ln T} = \frac{(1 + w_{sc})(2 + \zeta) + \zeta}{2(1 + w_{sc})}.$$  \hspace{1cm} (48)

Also $k = aH \propto a\sqrt{\rho_{sc}}$ leads to

$$\frac{d \ln k}{d \ln T} = \frac{\zeta(1 + 3w_{sc}) - 3\zeta}{6(1 + w_{sc})}.$$  \hspace{1cm} (49)

The modifications to the spectral index thus become

$$n_S - 1 = \frac{d \ln \mathcal{P}_\Phi}{d \ln k} = \frac{3(1 + w_{sc})(2 + \zeta) + \zeta}{\zeta(1 + 3w_{sc}) - 3\zeta}.$$  \hspace{1cm} (50)

In addition if we use a semi-classical density for the entropy,

$$s_{sc} = \frac{S}{V} = \frac{S}{a^3}.$$  \hspace{1cm} (51)
the thermodynamical argument presented in Section II relating $\zeta$ and $w$, is also valid, for the semi-classical values of these parameters. Thus,

$$\zeta = 1 + \frac{1}{w_{sc}}. \tag{52}$$

On substituting this in Eq. (50), the condition for near scale invariance $n_S \approx 1$ translates to the requirement that $w_{sc} \approx -2/3$ which can be obtained by an appropriate choice of $l$ parameter and $w_{sc}$. Therefore we find that at the zeroth order the no-go conditions for scale invariance of thermal fluctuations can be overcome by modifications to the gravitational dynamics in loop cosmology.

However, the calculation presented above is incomplete, because very little is known about the perturbed Einstein’s equations in loop cosmology, in particular for $a \ll a_\ast$. Preliminary work on flat models and the regime $a \gg a_\ast$ suggests that modifications to the gravitational dynamics influence the growth of fluctuations in a very non-trivial way. Based on these calculations we classify below some possible modifications:

- In a simplified setting the Poisson equation inside the horizon could become

$$k^2 \Phi = 4\pi Ga^2 D^l(a)\delta \rho, \tag{53}$$

where $I$ is an unknown exponent.

- It could be that the scale where the fluctuations become dominated by gravity (and not pressure) is not simply proportional to the horizon scale $k \sim aH$. For simplicity we shall ignore this possibility: it relates to varying speed of sound scenarios to be explored elsewhere.

- It could be that beyond the gravity-driven “freeze-out” scale the potential $\Phi$ continues to evolve and does not freeze-out as usual. This was proved explicitly in [19] for $a > a_\ast$. Here we shall model the evolution of the horizon outside the horizon for $a < a_\ast$ as

$$\Phi \propto a^N \tag{54}$$

where $N$ is an exponent to be computed.

There are positive indications for this hope from [19], [20], [21] and [28]. Therefore we have assumed in this paper that physics learned in the mini-superspace approximation (in the sense of modifications to inverse volume terms) will not change qualitatively. There are positive indications for this hope from ongoing work [20], but we stress this important caveat in our analysis.

We stress that these modifications parameterize our ignorance of the theory but they should be derivable in terms of $j$ and $l$ alone, from first principles.

Given these novelties we find that formula (49) gets modified to

$$P_\Phi(k) \sim \left[ \frac{a}{k} D^H T^2 \rho_{sc} \right]_{k=aH} \tag{55}$$

and since $H \propto \sqrt{S \rho_{sc}}$ we have at horizon crossing

$$P_\Phi(k) \sim \left[ T^2 D^H \rho_{sc} \right]_{k=aH}. \tag{56}$$

But because the potential continues to evolve outside the horizon this is not enough to read off a condition for scale invariance. Indeed the spectrum left after $a = a_\ast$ will be processed into

$$P_\Phi(k) = \left[ \frac{T^2 D^H \rho_{sc}}{\sqrt{S \rho_{sc}}} \right]_{k=aH} \tag{57}$$

where all the quantities on the right-hand side are to be computed when the mode left the horizon, for $k = aH$. The relation between temperature and $a$ is unmodified (apart from replacing $\zeta$ and $w$ by their semi-classical values). Therefore we can deduce the counterpart of (11) as

$$\frac{d \ln P_\Phi}{d \ln T_H} = 1 + \frac{\zeta}{2} \left( 1 + \frac{1}{3(1 + w_{sc})} (3 - 12I \alpha + 4N) \right) \tag{58}$$

where $T_H$ is the temperature when the mode left the horizon.

Using Eq. (49) we then obtain

$$n_S - 1 = \frac{3(1 + w_{sc})(\zeta + 2) + \zeta(3 - 12I \alpha + 4N)}{\zeta(1 + 3w_{sc}) - 3\zeta}. \tag{59}$$

The condition for near scale invariance ($n_S \approx 1$) then implies $3(1 + w_{sc})(\zeta + 2) \approx -\zeta(3 - 12I \alpha + 4N)$ leading to

$$w_{sc} \approx -\frac{2}{3} - \frac{4}{9}(N - 3I \alpha). \tag{60}$$

This equation can be viewed as a first order improvement over our zeroth order calculation which led to $w_{sc} \approx -2/3$.

V. CONCLUSIONS

Loop quantum cosmology has the potential to relate observational physics and quantum gravity, allowing concrete calculations to be made in the quantum gravity regime as long as a minisuperspace approximation is assumed to be valid. The approach is known to modify the equation of state of ordinary matter, thereby permitting a solution of the horizon problem without resorting to exotic scenarios thermal fluctuations could be behind the observed structure of the Universe. In order to analyze this issue we have assumed in this paper that physics learned in the mini-superspace approximation (in the sense of modifications to inverse volume terms) will not change qualitatively. There are positive indications for this hope from ongoing work [20], but we stress this important caveat in our analysis.

We showed that prima facie we are confronted by a no-go result in classical physics, pointing to $n_S = 4$ in all such scenarios. This can be derived assuming only the Einstein equations and a basic thermodynamics relation. The fact that the zeroth order, background, Einstein equations are also modified in loop cosmology allows
us to bypass this negative result, pointing to the region of parameter space where $n_S \approx 1$ is realized. This occurs for the semi-classical equation of state $w_{sc} \approx -2/3$. However, before this requirement can be converted into a constraint upon the free parameters of the theory ($j$ and $l$), a number of important details have to be worked out. We close with an executive summary of what is still missing in the theory:

- A solid quantization in the regime of large $j$, necessary for a full understanding of an extended period with $a < a_*$. This has to be accomplished for closed models as for non-compact flat models the physical meaning of $a_*$ makes little sense.

- A study of the perturbed Einstein equations along the lines of that carried out in [19], but valid for $a < a_*$. This has to be accomplished for closed models and for non-compact flat models the physical meaning of $a_*$ makes little sense.

- A concrete prediction for the spectrum of gravitational waves (tensor modes) completely ignored in this paper.

We believe that once this task list is completed we shall be able to place solid observational constraints upon loop quantum cosmology.

We conclude with a final remark on the role of higher $j$ terms in both the gravitational and the matter parts of the Hamiltonian. In various LQC phenomenology papers one has often ignored the modification to the gravitational part (constituted by $S$). Such an ad-hoc analysis is similar to taking different metrics in the gravity and matter parts of the Einstein equations in GR. As a purely academic exercise we can perform such an analysis and it turns out that the zeroth order calculation in Section IV does not go through; instead one reproduces the no-go result for scale invariance of classical physics [31]. But by consistently incorporating modifications arising for high values of $j$ in both the gravitational and matter parts of the constraint, the no-go obstacle is removed even at the zeroth level of calculation. This is an important lesson for loop cosmology phenomenology, showing the non-trivial features of high $j$. We believe this opens an interesting avenue for re-examining various interesting ideas (e.g., Refs. [19, 30]).

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APPENDIX A: MEASURES OF STRUCTURE

For discrete Fourier modes we define, for any quantity $g$, the dimensionless (or curly) power spectrum $P_\delta(k)$ as:

$$P_\delta(k) = \frac{V}{2\pi^3} k^3 \langle |g_k|^2 \rangle \quad (A1)$$

or occasionally the non-curly one as:

$$P_\delta(k) = V \langle |g_k|^2 \rangle = \frac{2\pi^2}{k^3} P_\delta(k) \, . \quad (A2)$$

The latter is often only used for $\delta$ and using the Poisson equation we have the following alternative definition of the spectral index

$$P_\delta(k) = A^2 k^n \, . \quad (A3)$$

The Fourier transform can be introduced noting that $\Delta k = 2\pi/L$ so that:

$$\int d^3k \approx \frac{(2\pi)^3}{V} \sum_k \, . \quad (A4)$$

Then with:

$$g(x) = \frac{1}{(2\pi)^{3/2}} \int dk \, g(k)e^{ikx} \quad (A5)$$

$$\delta(k) = \frac{1}{(2\pi)^3} \int dx \, e^{ikx} \quad (A6)$$

$$g(k) = \frac{1}{(2\pi)^{3/2}} \int dx \, g(x)e^{-ikx} \quad (A7)$$

we have

$$g_k \approx g(k) \frac{(2\pi)^{3/2}}{V} \quad (A8)$$

$$\delta_{kk'} \approx \frac{(2\pi)^3}{V} \delta(k-k') \quad (A9)$$

and so we find the alternative and equivalent definition for the power spectrum:

$$\langle g(k)g^*(k') \rangle = \frac{2\pi^2}{k^3} P_\delta(k) \delta(k-k') \, . \quad (A10)$$

The position space variance, with either definition, can be written:

$$\sigma_g^2 = \langle g^2(x) \rangle = \int \frac{dk}{k} P_\delta(k) \, . \quad (A11)$$

The filtered position-space variance is also used. It’s based on the smoothed field

$$g(R, x) = \frac{1}{V_R} \int g(x') W(|x-x'|/R) d^3x' \quad (A12)$$

$$V_R = \int d^3x W(x/R) = 4\pi R^3 \int y^2 W(y) dy \quad (A13)$$

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where $R$ is the smoothing scale and $W$ can be, say, a Gaussian or a top hat. (Do not confuse $V_R$ with the large $V$ used in the discrete Fourier series.) Then the “sigma-squared” on scale $R$ is

$$\sigma^2_R = \langle g^2(R, x) \rangle = \int \frac{dk}{k} W(kR) \mathcal{P}_g(k)$$  \hspace{1cm} (A14)

where we used the convolution theorem and $W(kR)$ is the Fourier transform of $(2\pi)^{3/2} W(x/R)/V_R$, that is, it’s normalized so that $W(kR) = 1$ at $k = 0$, then falling off at $kR \sim 1/R$. We can then write approximately

$$\sigma^2_R \approx \mathcal{P}_g(kR)$$  \hspace{1cm} (A15)

for $kR = 1/L$, since that’s where the integrand peaks.

**APPENDIX B: SOME BASICS OFLOOP QUANTUM COSMOLOGY**

This appendix aims to summarize some key features of loop quantization of cosmological models (for details see for example Refs. [14, 16]). We first demonstrate the way the classical constraint is cast in terms of elementary loop variables – holonomies of connection $h_c(A) = \mathcal{P} \exp(\int_c A)$ and triads $E^i_c$. We also show the way $j$ and $l$ parameters and the resulting modifications in the improved quantization of LQC [14] to classical GR originate.

For simplicity we start with quantization of flat isotropic and homogeneous FRW spacetime. In this setting the underlying symmetries lead to simplified connection $c$ and triad $p$:

$$A^i_c = c V_o^{-\frac{1}{2}} \omega^{i}_{a}, \quad E^i_c = p V_o^{-\frac{1}{2}} \sqrt{\stackrel{(a)}{V}} c^i_{a}$$  \hspace{1cm} (B1)

where $(\omega^i_{a}, c^i_{a})$ are a set of orthonormal co-triads and triads compatible with the flat fiducial metric $\stackrel{(a)}{V}$. $V_o$ is the volume of the cell (V) used to define a symplectic structure with respect to $\omega^{i}_{a}$. The variables $c$ and $p$ are canonical conjugate satisfying Eq. (22).

The gravitational and matter parts of the constraint are given by

$$C_{\text{grav}} = -\gamma^{-2} \int d^3x \epsilon_{ijk} e^{-1} E^{ai} E^{bj} F^k_{ab}$$  \hspace{1cm} (B2)

and

$$C_m = 8\pi G \frac{\rho^2}{|p|^{3/2}}$$  \hspace{1cm} (B3)

where for simplicity we consider a massless scalar field. The modulus sign arises because of two possible orientations of the triad, the choice of which has no physical consequences unless we choose spinor fields. $E^a$ denotes the curvature of connection and

$$e = \sqrt{\det E} = \left( \frac{1}{6} \epsilon^{lmn} \epsilon_{ijk} E^a_i E^b_j E^c_k \right)^{1/2}$$  \hspace{1cm} (B4)

To write the constraint in terms of holonomies and triads, the following identities of classical phase space are very useful [32]:

$$\frac{1}{8\pi G \gamma} \{ A^i_c, \epsilon^{ijk} \epsilon_{abc} E^a_i E^b_j E^c_k \} = 3 \epsilon^{ijk} \epsilon_{abc} E^a_i E^b_j ,$$  \hspace{1cm} (B5)

$$\{ A^i_c, V \} = \left[ A^i_c, V^{(1-n)} \right] \frac{1}{1-n}$$  \hspace{1cm} (B6)

and

$$e^i_a = \frac{1}{4\pi G \gamma} \{ A^i_c, V \}.$$  \hspace{1cm} (B7)

Eq. (B5) leads to

$$\epsilon_{ijk} e^{-1} E^{ai} E^{bj} F^k_{ab} = \frac{1}{8\pi G \gamma} e^{-1} \epsilon^{abc} \{ A^i_c, V^2 \} F_{abi} = \frac{1}{4\pi G \gamma} \epsilon^{abc} \{ A^i_c, V \} F_{abi} .$$  \hspace{1cm} (B8)

Here $V = |p|^{3/2} = a^3$ denotes volume of the cell with respect to the physical metric $V = V_o \sqrt{|\det E|}$ (for simplicity we put $V_o = 1$ from now on).

We then express the connection in terms of the holonomy by tracing over the holonomies in a $j$ representation. For $j = 1/2$, using

$$\text{Tr}(\tau_i \tau^j) = -\frac{1}{3} j(j + 1)(2j + 1) \delta^j_i ,$$  \hspace{1cm} (B9)

it is straightforward to obtain

$$\epsilon_{ijk} e^{-1} E^{ai} E^{bj} = \sum_{k} \epsilon^{abc} a_{ijk} \frac{1}{2\pi G \gamma} \text{Tr}(h_k^{(0)} \{ h_k^{(\lambda)} , V \} \tau_i) .$$  \hspace{1cm} (B10)

Here $h_k^{(\lambda)}$ is the holonomy of the connection $c$ along the edge $\lambda a_{c}^{k}$

$$h_k^{(\lambda)} = \cos \frac{\lambda}{2} \mathbb{1} + 2 \sin \frac{\lambda c}{2} \tau_k$$  \hspace{1cm} (B11)

where $\mathbb{1}$ is the identity matrix, $\tau_k = -i \sigma_k / 2$ and $\sigma_k$ are the Pauli spin matrices.

The curvature components can be obtained by considering holonomies around a closed square loop $\Box_{ij}$:

$$F^k_{ab} = -2 \lim_{\lambda \tau \rightarrow 0} \text{Tr} \left[ \left( \frac{h_k^{(\lambda)} - 1}{\lambda^2} \right) x^k \right] a_i^{\lambda} a_j^{\lambda} .$$  \hspace{1cm} (B12)

Due to the inherent quantum nature of geometry in loop quantization the area $\lambda^a |p|$ is shrunk to the minimum eigenvalue of the area operator $\Delta = (2\sqrt{3} \pi) \ell^3_p$ in LQG [13]. This leads to a constraint $\lambda^a |p| = \Delta$. $C_{\text{grav}}$ can then be obtained by combining (B10) and (B12).
The matter part contains inverse powers of $\det E$. To write them in terms of holonomies we use the identity $|\det e^i_a| = |\det E|^{1/2}$ and Eq. (B7)

$$\frac{1}{\sqrt{|\det E|}} = \frac{\det e^i_a}{(\sqrt{|\det E|})^2} = \frac{1}{6} \epsilon^{abc} \epsilon_{ijk} e^i_a e^j_b e^k_c$$

$$(4\pi G\gamma)^3 \epsilon^{abc} \epsilon_{ijk} \{A^j_a, V^{1/3}\} \{A^j_b, V^{1/3}\} \{A^j_c, V^{1/3}\}.$$  

(B13)

Expressing connection in terms of holonomies, in $j = 1/2$ representation inverse scale factor becomes

$$\text{sgn}(p) = \frac{1}{|p|^{1/2}} = \frac{4}{8\pi G\gamma} \text{Tr} \left( \sum_k \tau^h_{k} \{h^\lambda_k, 1, V^{2/3}\} \right)^{1/2(1-l)},$$

where $l = 1 - 1/(2m)$ and $0 < l < 1$.

With $C_{\text{grav}}$ and $C_m$ written in form of holonomies and triads, we quantize the theory and are led to a non-singular difference equation with uniform discretization in eigenvalues of volume operator [14]:

$$\hat{V}|v\rangle = \hat{\beta}^3 |v||v\rangle$$

(B16)

with

$$\hat{\beta} = \left(\frac{8\pi G\gamma}{6}\right)^{1/2} K^{-1/3}, \quad K = \frac{2\sqrt{2}}{3\sqrt{3}}.$$  

(B17)

Unlike the old quantization in LQC (where the difference equation was of uniform discretization in eigenvalues of triad [33, 34]), the evolution has the correct classical limit for arbitrary matter content and quantum gravitational effects set in when curvature becomes of the order Planck. Study of backward evolution of semi-classical states peaked at late times on trajectories of a large classical universe shows a generic bounce when $\rho = \rho_{\text{crit}} = 0.82\rho_0$ [14]. In this quantization (for $j = 1/2$) modifications originating from $F_{ab}^i$ terms dominate over those containing $1/\sqrt{|\det E|}$ in both gravitational and matter parts of the constraint. Investigations of closed models yield similar results [16].

We now provide the expressions of the eigenvalues of operators corresponding to $e^{-1} E^a_i E^b_i$ and $1/\sqrt{|\det E|}$ for higher $j$, which can be derived in analogy with (B10) and (B14), using Eq. (B9). We have:

$$s_j = -\frac{9 \hat{\beta}^3 K^{2/3}}{8\pi \ell_p^2 \gamma (j+1)(2j+1)} |v|^{1/3} \sum_{r=-j}^j r|v - 2r|$$

and

$$d_{j,l} = \left[ \frac{27 \hat{\beta}^{2l} K^{2/3}}{16\pi \ell_p^2 \gamma (j+1)(2j+1)} |v|^{1/3} \sum_{r=-j}^j r|v + 2r|^{2l/3} \right]^{1/2(l-1)}.$$  

(B18)

(B19)

For higher $j$, Eqs. (B18) and (B19) can be approximated by

$$s_j = S(q) a, \quad \text{and} \quad d_{j,l}(q) = D_l(q) a^3$$

with

$$q := (a/a_*)^3, \quad a_* = (2j)^{1/3} \hat{\beta},$$

and

$$S(q) = \frac{1}{4} \left[ 2 \left( (q+1)^3 - |q-1|^3 \right) - 3q ((q+1)^2 - \text{sgn}(q-1)|q-1|^2) \right]$$

(B20)

and

$$D_l(q) = \left[ \frac{27 |q|^{1 - \frac{2l}{l+3}}}{8l} \left\{ \frac{1}{l+3} \left( (q+1)^{2(\frac{l+3}{l+3})} - |q-1|^{2(\frac{l+3}{l+3})} \right) - \frac{2q}{2l+3} \left( (q+1)^{2(\frac{l+3}{l+3})} - \text{sgn}(q-1)|q-1|^{2(\frac{l+3}{l+3})} \right) \right\} \right]^{\frac{1}{2(l-1)}}$$

(B21)

(B22)

following the analysis for old quantization [35, 36]. In the regime when $a \ll a_*$

$$S(q) \approx \frac{3}{2} \left( \frac{a}{a_*} \right)^3$$

(B23)

and

$$D_l(q) \approx \left( \frac{9}{2l+3} \right)^{\frac{3}{2(1-l)}} \left( \frac{a}{a_*} \right)^{3(3-l)/(1-l)}.$$  

(B24)

(B25)

For $a \gg a_*$, $S(q) \approx 1$ and $D_l(q) \approx 1$.

Extensive numerical simulations of backward evolution of semi-classical states at late times have shown that in LQC an effective Hamiltonian which provides an excellent approximation to the underlying quantum dynamics can be written. For $j = 1/2$, the effective Hamiltonian for flat [14] and closed model [16] is

$$H_{\text{eff}} = \frac{C_{\text{eff}}}{16\pi G} = -\frac{3s_j \sin^2(\lambda c)}{8\pi G^2 \lambda^2} + d_{j,l} \frac{p_0^2}{2}$$

(B26)

and

$$H_{\text{eff}} = -\frac{3s_j (\sin(\lambda c) \sin(\lambda(c-1)) + (1 + \gamma^2))}{8\pi G^2 \lambda^2} + d_{j,l} \frac{p_0^2}{2}$$

(B27)
respectively. Here $\lambda = \lambda(p) = (\Delta/|p|)^{1/2}$. The $\sin(\lambda c)$ terms arise from field strength part and are responsible for $\rho^2$ modifications of the Friedman equation \cite{14, 16}.

For higher $j$ a quantization procedure has been proposed which indicates resolution of singularity \cite{36}; however, a complete quantization is still lacking. Considering higher values of $j$ in non-compact flat models has the problem of relating the scale at which modifications to $1/\sqrt{\det E}$ terms become important to any physical scale (The scale at which these modifications become important depends on the choice of fiducial cell, for details see Refs. \cite{14, 17}). In the closed models this scale is provided by the intrinsic curvature. If we consider higher $j$ in closed models then, as for $j = 1/2$, modifications arise both from $F_{ab}^j$ and $1/\sqrt{\det E}$ terms. However, in this case we can have a regime in which modifications coming from the latter dominate the former and still lead to a non-singular bounce. When $\sin(\lambda c) \to \Delta^{1/2}c/a$ and $\sin(\lambda c - 1) \to \Delta^{1/2}(c - 1)/a$, the modifications coming from $F_{ab}^j$ can be considered small. In this regime $H = \dot{a}/a \ll \Delta^{-1/2} \sim M_p$ and energy density is small. An effective Hamiltonian \cite{36} can then be obtained by following the procedure outlined for higher $j$ \cite{36}.

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