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Dynamics and entanglement in spherically symmetric quantum gravity

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The gravity-scalar field system in spherical symmetry provides a natural setting for exploring gravitational collapse and its aftermath in quantum gravity. In a canonical approach, we give constructions of the Hamiltonian operator, and of semiclassical states peaked on constraint-free data. Such states provide explicit examples of physical states. We also show that matter-gravity entanglement is an inherent feature of physical states, whether or not there is a black hole.

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I. INTRODUCTION

Black hole thermodynamics, cosmology and, more generally, unification have all provided strong impetus for developing a theory of quantum gravity. There appears to be agreement on at least two features such a theory should have regardless of the details of the approach. These are background (or metric) independence and fundamental discreteness. It may be that other ideas such as holography arise as a consequence of the first two but this is far from clear at the present level of understanding.

Progress in quantum gravity has been limited to models where a complete quantization can be performed, such as the work on mini-superspace cosmology in the early seventies [1] and its later incarnations in the Hartle-Hawking approach [2] and loop quantum cosmology [3]. These are all quantum mechanical systems arrived at by the assumption of spatial homogeneity of spacetime. The extent to which such models can reveal insights into quantum gravity is not clear [4], although recent developments on singularity avoidance may be one such feature. More generally, the hope is that such smaller systems will ultimately become absorbed in a full theory of quantum gravity in the same way that the Bohr atom has in quantum electrodynamics.

Going beyond mini-superspace models significantly enlarges the problem to a true field theory of a constrained system. The first step in this direction is to a two-dimensional field theory, where the metric and matter variables depend on time and one spatial coordinate. There are a few models of interest in this category, namely, the Gowdy cosmology, cylindrical gravitational waves, and the asymptotically flat gravity-scalar field theory. The quantum theories of the first two models have been studied in the simplified approximation of one local degree of freedom [5,6]. These are vacuum models so they are less interesting physically than the last one, which has the potential to reveal much about gravitational collapse and black hole formation in quantum gravity [7–9]. Furthermore, this model is the natural next step beyond just the quantum mechanics of the Schwarzschild black hole, on which much has been written [10–15].

This system has a true Hamiltonian that forms a part of its asymptotic Poincaré symmetries. The model provides the setting for two important physical scenarios: numerical studies of gravitational collapse [16,17] and the so-called information loss paradox, whose origin involves an assumption on the large scale structure of an evaporating black hole based on semiclassical physics [18]. It concerns a collapsing low-entropy (or even pure-state) matter that forms a black hole, which subsequently evaporates within a finite time, resulting in a highly entropic Hawking radiation [19]. If the correlations between the inside and the outside of the black hole are not restored during the evaporation process, then the corresponding increase in entropy is interpreted as a lost ‘‘information.’’ Various arguments have been advanced to justify or dismiss this phenomenon [20], as well as possible consequences of either option [21]. There is the possibility that the existence of a quantum theory of gravity automatically removes the information loss ‘‘paradox,’’ since a complete quantization of the true Hamiltonian would result in the unitary evolution of the combined matter-gravity system [22], while the entropy flow between subsystems can be interpreted with the help of quantum information theory [23].

In this paper we build on recent developments [7,8] aimed at obtaining a compete quantum theory of the asymptotically flat gravity-scalar field theory in spherical symmetry. These earlier works used a gauge appropriate for Painleve-Gullstrand (PG) coordinates (because of their regularity at the horizon), and provided a construction of the Hamiltonian and null expansion operators. Not addressed in these works are the problems of finding physical states and addressing their dynamics. This is what we study in this paper.

The outline of this paper is as follows. We first review the model and its quantization. We then give a prescription for constructing semiclassical physical states that are peaked on classical data, and give a new form of the Hamiltonian operator. (An earlier version of this operator utilized a Dirac-like trick to write a square root operator.) Using these we show that physical states exhibit matter-gravity entanglement. We argue that this may be a robust

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model-independent feature of nonlocality in quantum gravity.

II. GRAVITY-SCALAR FIELD MODEL

Our starting point is the Arnowitt-Deser-Misner (ADM) Hamiltonian formulation for general relativity. The phase space of the model is defined by prescribing a form of the gravitational phase space variables q_{ab} and $\tilde{\pi}^{ab}$, together with falloff conditions for these variables, and for the lapse and shift functions N and N^a. The ADM 3 + 1 action for general relativity minimally coupled to a massless scalar field is

$$S = \frac{1}{16\pi G}\int d^3xdt[\tilde{\pi}^{ab}\dot{q}_{ab} + \tilde{P}_\phi\dot{\phi} - NH - N^aC_a]. \tag{1}$$

The pair (ϕ, P_ϕ) are the scalar field canonical variables, and

$$H = \frac{1}{\sqrt{q}}\left(\tilde{\pi}^{ab}\tilde{\pi}_{ab} - \frac{1}{2}\tilde{\pi}^2\right) - \sqrt{q}R(q) + 8\pi G\left(\frac{1}{\sqrt{q}}\tilde{P}_\phi^2 + \sqrt{q}q^{ab}\partial_a\phi\partial_b\phi\right) \simeq 0, \tag{2}$$

$$C_a = D_c\tilde{\pi}^c_a - 8\pi G\tilde{P}_\phi\partial_a\phi \simeq 0, \tag{3}$$

where $\tilde{\pi} = \tilde{\pi}^{ab}q_{ab}$.

This action (together with the boundary terms; see e.g. [8,24]) is well defined and determines the falloff conditions on canonical variables. Below (Sec. II A) we outline the structure that results from imposition of spherical symmetry and use of the flat-slice partial gauge fixing. (This is a summary of the work in [8].) The reason for utilizing this gauge is that the horizon is not located at a coordinate singularity. In Sec. II B we present a family of initial data that will illustrate, in a later section, a construction of semiclassical physical states of the model.

A. Hamiltonian theory in the flat-slice formalism

The reduction to spherical symmetry utilizes an auxiliary flat Euclidean metric e_{ab} and unit radial normal $s^a = x^a/r$, where $r^2 = e_{ab}x^ax^b$. The parametrization of the reduced phase space we use is given by the matrices

$$q_{ab} = \Lambda(r,t)^2 s_a s_b + \frac{R(r,t)^2}{r^2}(e_{ab} - s_a s_b), \tag{4}$$

$$\tilde{\pi}^{ab} = \frac{P_\Lambda(r,t)}{2\Lambda(r,t)}s^a s^b + \frac{r^2 P_R(r,t)}{4R(r,t)}(e^{ab} - s^a s^b). \tag{5}$$

As a line element the spatial metric is therefore

$$ds^2 = \Lambda^2(r,t)dr^2 + R(r,t)^2 d\Omega^2, \tag{6}$$

where the solid angle $d\Omega^2$ arises from the second term in these expressions.

The PG coordinates are those where equal coordinate time slices are spatially flat [8,24]. However, it is sufficient to use the partial gauge fixing $\Lambda = 1$ to obtain the feature of nonsingular coordinates at the horizon, which is the feature of PG coordinates we desire. This is what is summarized in the remaining part of this section.

Substituting (5) into the ADM 3 + 1 action with a minimally coupled scalar field leads to the reduced action

$$S_R = \frac{1}{4G}\int dtdr(P_R\dot{R} + P_\Lambda\dot{\Lambda} + P_\phi\dot{\phi}) - \frac{1}{4G}\times\int dtdr(NH + N^rC_r) - \int dt(N^r\Lambda P_\Lambda)|_{r=\infty}, \tag{7}$$

where N, N^r are the lapse and radial shift functions, and the reduced Hamiltonian and (radial) diffeomorphism constraints H and C^r are

$$H = \frac{1}{R^2\Lambda}\left[\frac{1}{8}(P_\Lambda\Lambda)^2 - \frac{1}{4}(P_\Lambda\Lambda)(P_R R)\right] + \frac{2}{\Lambda^2}[2RR''\Lambda - 2RR'\Lambda' - \Lambda^3 + \Lambda R'^2] + \left[\frac{P_\phi^2}{2\Lambda R^2} + \frac{R^2}{2\Lambda}\phi'^2\right] \simeq 0, \tag{8}$$

$$C_r = P_R R' - \Lambda P'_\Lambda + P_\phi\phi' \simeq 0. \tag{9}$$

These constraints are first class with an algebra that is similar to that for the full theory.

We note that this reduction to spherically symmetry is unusual in that the usual ADM mass integral vanishes due to the flat slicing condition. It is therefore important to ensure that the reduced action is functionally differentiable with a consistent set of falloff conditions on the phase space variables, and on the lapse and shift functions. This analysis has been carefully done by one of the authors in Ref. [8], where these details are explicitly given. The asymptotic conditions on the phase space variables are

$$R = r + \mathcal{O}(r^{-1/2-\epsilon}), \qquad P_R = Ar^{-1/2}/2 + \mathcal{O}(r^{-1-\epsilon}), \tag{10}$$

$$\Lambda = 1 + \mathcal{O}(r^{-3/2-\epsilon}), \qquad P_\Lambda = Ar^{1/2} + \mathcal{O}(r^{-\epsilon}) \tag{11}$$

$$\phi = Br^{-1/2} + \mathcal{O}(r^{-3/2-\epsilon}), \qquad P_\phi = Cr^{1/2} + \mathcal{O}(r^{-\epsilon}), \tag{12}$$

and those on the lapse and shift functions are

$$N^r = Ar^{-1/2} + \mathcal{O}(r^{-1/2-\epsilon}), \qquad N = 1 + \mathcal{O}(r^{-\epsilon}), \tag{13}$$

where A, B, C are constants. The leading order terms are solutions of the constraints, so there is no logarithmic divergence of the action at this order. The mass formula is the surface term in Eq. (7); the mass parameter arises in this integral through the momentum P_Λ. It is readily verified that if the scalar field is set to zero the Schwarzschild solution results [8].

B. Partial gauge fixing

We next impose the gauge choice $\Lambda = 1$, which corresponds to a step toward flat-slice coordinates. With this condition imposed, the Hamiltonian constraint is solved (strongly) for the conjugate momentum P_Λ as a function of the phase space variables. This gives

$$P_\Lambda = P_R R + \sqrt{(P_R R)^2 - X}, \tag{14}$$

where

$$X = 16R^2(2RR'' - 1 + R'^2) + 16R^2 H_\phi \tag{15}$$

and

$$H_\phi = \frac{P_\phi^2}{2R^2} + \frac{R^2}{2}\phi'^2. \tag{16}$$

This effectively eliminates the conjugate pair (Λ, P_Λ) in favor of the remaining phase space variables. We must however obtain the consequence of this for the lapse and shift functions in the standard way: the evolution equation for Λ [8] and the requirement that the gauge $\Lambda = 1$ be preserved under evolution lead to the equation

$$N = -\frac{4R^2(N^r)'}{\sqrt{(P_R R)^2 - X}}. \tag{17}$$

We note that this relation does not lead to any restriction on the phase space variables, since it is merely a relation between the lapse N and the shift N^r, neither of which is absolutely fixed at this stage. We also note that on the classical space of solutions, the argument of the square root is positive; in quantum theory, it is, in principle, possible that fluctuations may make this negative. This, however, is an issue that is present, in general, in the ADM variable approach to quantum gravity because the Hamiltonian constraint contains a factor of $\sqrt{q}$, which may fluctuate such that the argument is negative. The issue hinges on how the corresponding operator is defined. We discuss this below, where we set up the Dirac quantization problem.

The gauge $\Lambda = 1$ reduced the radial diffeomorphism constraint to

$$C_r = -P'_\Lambda + P_R R' + P_\phi \phi' \simeq 0, \tag{18}$$

with P_Λ given by (14) above. We note that using this constraint the square root in the latter equation can be written as

$$\sqrt{(P_R R)^2 - X} = \int_0^r (P_R R' + P_\phi \phi') - P_R R. \tag{19}$$

To summarize this section, the partially gauged fixed theory is prescribed by the phase space variables (ϕ, P_ϕ) and (R, P_R) and the reduced Hamiltonian

$$\begin{aligned} H_R^G &= \int_0^\infty [(N^r)' P_\Lambda + N^r(P_R R' + P_\phi \phi')] dr \\ &= \int_0^\infty (N^r)' \Big(R P_R + \sqrt{(P_R R)^2 - X} \Big) dr \\ &\quad + \int_0^\infty N^r (P_R R' + P_\phi \phi') dr, \end{aligned} \tag{20}$$

where the surface term in the reduced action (7) has been written as a bulk term and combined with the remaining radial diffeomorphism constraint. Together with the asymptotic conditions given above, the variational principle is well defined. This is the reduced system we study in the rest of the paper.

Finally we note that we have not yet fully fixed the gauge to the flat-slice case since we have not imposed the condition $R = r$. We prefer to retain R as a dynamical variable for developing the quantum theory, since full gauge fixing leads to a reduced Hamiltonian for the scalar field degrees of freedom that is nonlocal [8], and so poses a problem for quantization.

C. Classical data

Finding classical initial data sets is necessary both in numerical calculations and for the construction of semiclassical physical states. As one of our aims in this paper is to present a concrete realization of the latter, it is useful to see what form such data take before we proceed to a construction of such states. The data should be an asymptotically flat solution of the remaining constraints prescribed by functions $\phi(r)$, $P_\phi(r)$ and $R(r)$ and $P_R(r)$. The family of data that we exhibit below depends on two parameters. It is regular at the coordinate origin and may have trapped surfaces, depending on the parameter values.

We shall see, after describing the quantum theory, that semiclassical states corresponding to data with trapped surfaces such as this describe a quantum black hole state. This occurs because states peaked on classical constraint-free data satisfy the condition that the expectation value of the constraint operator vanishes to leading order in a well-defined expansion (see Sec. V below.)

With the partial gauge fixing $\Lambda = 1$ already imposed as described in Sec. II B, we fix gauge fully by imposing $R = r$. This simplifies the constraint to

$$C_r = -P'_\Lambda + P_R + P_\phi \phi' = 0, \tag{21}$$

with

$$P_\Lambda = P_R r + \sqrt{(P_R r)^2 - X}, \tag{22}$$

where X now reduces to

$$X \equiv 16R^2(2RR'' - 1 + R'^2) + 16R^2 H_\phi = 16r^2 H_\phi. \tag{23}$$

To find some explicit solutions of interest, we make the ansatz $\phi = 0$. The constraint then becomes a relation between P_R and P_ϕ, so one of these may be chosen freely.

To obtain an explicit class of solutions, let us set

$$16H_\phi = h^2(r)P_R^2(r), \tag{24}$$

for some function h. Then (22) becomes

$$P_\Lambda = P_R r(1 + \sqrt{1 - h^2}) \equiv P_R r(1 + g), \tag{25}$$

and the auxiliary function $h = \sqrt{1 - g^2}$ satisfies

$$0 \le h^2 \le 1, \qquad \lim_{r\to\infty} h^2 = 0. \tag{26}$$

The constraint is now

$$P_R' r + (P_R r g)' = 0, \tag{27}$$

which can be rewritten as

$$(P_R r)' - P_R + (P_R r g)' = 0. \tag{28}$$

Finally, this may be put into an integrated form by setting

$$P_R = \Pi_R' \tag{29}$$

to give

$$\Pi_R = c \exp\left(\int^r \frac{dx}{(1 + g(x))x}\right). \tag{30}$$

Thus, given suitable functions g, we can find Π_R and hence P_R, followed by P_ϕ from Eq. (24).

We note that the energy density can be written as

$$16H_\phi = 2\frac{\Pi_R P_R}{r} - \frac{\Pi_R^2}{r^2}. \tag{31}$$

The asymptotic falloff conditions (above) require $P_R \sim 1/\sqrt{r}$, which implies $\Pi_R \sim 2P_R r$ and $g \to 1$. If one wishes to have regular data at $r = 0$, then the expansion $\Pi_R \sim r^\alpha$ leads to

$$0 \le \frac{1}{\alpha} - 1 \le 1, \tag{32}$$

which bounds the power to

$$1/2 \le \alpha \le 1, \tag{33}$$

while the regularity of H_ϕ imposes $\alpha = 1$, so for $r \sim 0$ we get $\Pi_R \sim cr$.

To obtain an explicit asymptotically flat solution, let us consider the choice

$$1 + g = (1 - \tfrac{1}{2}\exp(-a/x^2))^{-1}, \tag{34}$$

which results in

$$\Pi_R = cr \exp\left[-\frac{1}{4}E_1\left(\frac{a}{r^2}\right)\right], \tag{35}$$

where the integral exponential function is defined as

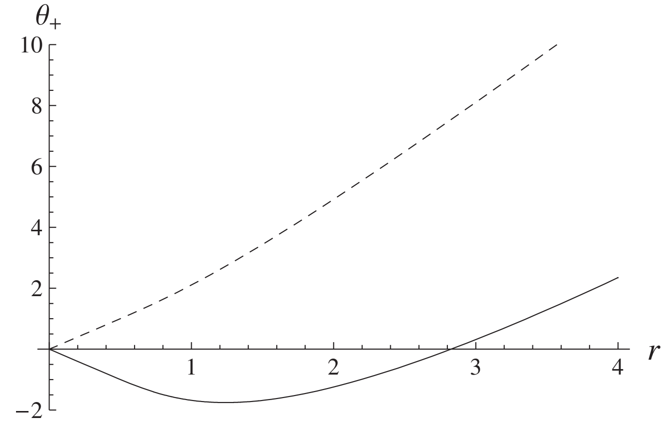

FIG. 1. Expansion of the outgoing null geodesic with (solid line) and without (dashed line) trapped surfaces on the initial hypersurface. The solid line corresponds to $a = 1$, $C = 2$ and the dashed line to $a = 1$, $C = 6$.

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t} dt. \tag{36}$$

The asymptotic behavior of Π_R is as desired,

$$\Pi_R \approx c^4\sqrt{a}e^{\gamma/4}\sqrt{r}, \qquad r \to \infty, \tag{37}$$

where Euler's gamma is $\gamma = 0.57\ldots$, and

$$\Pi_R \approx cr, \qquad r \to 0. \tag{38}$$

From the asymptotic falloff condition

$$P_R = Ar^{-1/2}/2 + \mathcal{O}(r^{-1-\epsilon}), \tag{39}$$

where A is related to the ADM mass as $A = 4\sqrt{2M}$ [8], we see that $c^4\sqrt{a}e^{\gamma/4} = A$.

The next step in the investigation of the classical problem is to check for the presence of apparent horizons. In the gauge we adopted, the expansions of outgoing and ingoing null geodesics are given as [7]

$$\theta_\pm = \pm 4RR' - P_\Lambda, \tag{40}$$

which reduces for the initial data surface to

$$\theta_\pm = \pm 4r - \Pi_R. \tag{41}$$

By varying parameters of Π_R it is possible to generate the regular initial data with or without trapped surfaces, as shown on Fig. 1.

III. QUANTIZATION

In this section we describe an approach to constructing the quantum theory of the system described above. We will be working with the partially gauge fixed theory described in Sec. II B, where we have the pair of phase space variables (R, P_R) and (ϕ, P_ϕ), and the remaining radial diffeomorphism constraint. The quantization we use is a type of polymer quantization where field configuration and translation operators are quantized, but there is no direct quantization of field momenta. Using the basic operators, we shall see that there are well-defined prescriptions for writing the constraint and the Hamiltonian operators.

A. Hilbert space and basic operators

To describe the polymer quantization [25,26] (which may be viewed as the "dual" to that used in loop quantum gravity), we begin with the basic variables

$$R_f = \int_0^\infty dr f(r) R(r), \qquad U_\epsilon(P_R) = \exp(i\epsilon P_R), \quad (42)$$

where $f(r)$ is a smearing function and ϵ is a real dimensional constant. These satisfy the canonical Poisson bracket

$$\{R_f, U_\epsilon(P_R(r))\} = i\epsilon f(r) U_\lambda(P_R(r)). \quad (43)$$

(In defining these observables we have at our disposal a constant density that ensures the correct density weights in the integral for R_f and in the exponent of U_ϵ. This density is the phase space variable Λ which was set to unity when we performed the partial gauge fixing $\Lambda = 1$.)

We use similar definitions for the variables made from ϕ and P_ϕ, i.e.

$$\phi_f = \int_0^\infty dr f(r) \phi(r), \qquad V_\kappa(P_\phi) = \exp(i\kappa P_\phi).$$

The Poisson bracket of these matter variables mirrors that of the metric variables in (43).

The parameters ϵ and κ have the physical dimensions necessary to make the exponents in the corresponding U variables dimensionless. This scale will carry over to quantization. Since we are dealing with a quantization of gravity and matter, it is natural to suppose that both parameters are related to the Planck scale. In the following we will keep them separate.

The Poisson bracket of the metric variables is realized as an operator relation on a Hilbert space spanned by the basis states

$$|a_1, a_2, \cdots, a_n\rangle \quad (44)$$

where the real numbers a_i represent values of the configuration variable R at the radial points r_i. The points r_i provide a set where the phase space variables are sampled. The selection of space points r_i may be thought of as a lattice (or graph in the language used in loop quantum gravity). Since there is a basis state of this type for every countable set of points, the Hilbert space is nonseparable. In the following it will be convenient to work with a fixed and uniformly spaced set of points, although this is not necessary.

The inner product is

$$\langle a'_1, a'_2, \cdots, a'_n | a_1, a_2, \cdots, a_n\rangle = \delta_{a'_1,a_1} \cdots \delta_{a'_n,a_n} \quad (45)$$

if two states are associated with the same lattice points; if not, the inner product is zero. This inner product is background independent in the same way as, for example, the inner product for the Ising model; the difference is that for the latter there is a finite dimensional space of spins at each lattice point.

The configuration and translation operators are defined by the following expressions:

$$\hat{R}_f |a_1, a_2, \cdots a_n\rangle := \sum_i a_i f(r_i) |a_1, a_2, \cdots a_n\rangle, \quad (46)$$

$$\hat{U}_\epsilon(P_R(r_k)) |a_1, a_2, \cdots a_n\rangle := |a_1, a_2, \cdots, a_k - \epsilon, \cdots a_n\rangle. \quad (47)$$

It is readily verified that the commutator of these operators as defined provides a faithful realization of the corresponding Poisson bracket. Since the U operators are realized here as ladder operators for the field excitations, the parameter ϵ represents the discreteness scale in field configuration space.

This representation is one in which the momentum operator does not exist. There is however an alternative ϵ-dependent definition of momentum using the translation operators (47), given by

$$\hat{P}^\epsilon_R(r_k) := \frac{1}{2i\epsilon}(\hat{U}_\epsilon(P_R(r_k)) - \hat{U}^\dagger_\epsilon(P_R(r_k))), \quad (48)$$

which will be used in the definition of the Hamiltonian operator.

The representation for the matter variables is similar to that defined above for the metric variables. We write the basis states of the matter sector as

$$|b_1, b_2, \cdots, b_n\rangle.$$

With the inclusion of matter the kinematical Hilbert space is the tensor product of geometry and matter Hilbert spaces, with the basis

$$|\underbrace{a_1, \ldots, a_N}_{\text{gravity}}; \underbrace{b_1, \ldots, b_N}_{\text{matter}}\rangle. \quad (49)$$

With the quantization of the basic variables in hand, we now turn to defining the composite operators necessary to write the constraints and the Hamiltonian. For this we first need to define a localized field operator from R_f and ϕ_f. A localized field may be defined by taking, for example, $f(r)$ in Eq. (42) to be a Gaussian,

$$G(r, r_k, \sigma) = e^{-(r-r_k)^2/\sigma^2} \quad (50)$$

(or a smooth function of bounded support) which is sharply peaked at a radial point r_k. For illustration we will work with the Gaussian with the understanding that its width σ is such that the function is effectively zero at all lattice points except where it is peaked. This is easiest to see with a uniform lattice such that $\sigma \ll 1$ in Planck units. With this in mind we write

$$R_{G(r_k)} \equiv R_k, \tag{51}$$

with a similar expression for the scalar field ϕ. We also have the following action of the basic operators (where we have included explicitly the Planck length):

$$\hat{R}_k|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle = 2l_P^2 a_k|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle, \tag{52}$$

$$\hat{\phi}_k|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle = 2l_P^2 b_k|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle. \tag{53}$$

The field translation operators $\hat{U}_k(\epsilon) \equiv \hat{e}^{i\epsilon P_{R_k}}$ and $\hat{V}_k(\kappa) \equiv \hat{e}^{i\kappa P_{\phi_k}}$ act as

$$\hat{U}_k(\epsilon)|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle = |a_1,\ldots,a_k-\epsilon,\ldots a_N;b_1,\ldots,b_N\rangle \tag{54}$$

and

$$\hat{V}_k(\kappa)|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle = |a_1,\ldots a_N;b_1,\ldots,b_k-\kappa,\ldots,b_N\rangle. \tag{55}$$

Thus, with the choice of Gaussian smearing functions sharply peaked at the points r_k in the operators $\hat{R}_f$ and $\hat{\phi}_f$, the basic commutators are

$$[\hat{R}_k, \hat{U}_l(\epsilon)] = -2l_P^2\epsilon\delta_{kl}\hat{U}_l(\epsilon),\qquad [\hat{\phi}_k, \hat{V}_l(\kappa)] = -2l_P^2\kappa\delta_{kl}\hat{V}_l(\kappa). \tag{56}$$

Since $\hat{R}_k$ operators have zero in the spectrum (i.e. there are states such as $|a_1\cdots, a_k = 0, \cdots a_n\rangle$ that have zero eigenvalue), there is no inverse operator and an indirect definition is required. This is achieved by Poisson bracket identities such as

$$\{\sqrt{|R_k|}, U_l(\epsilon)\} = \frac{i}{2\sqrt{|R_k|}}\epsilon U_l(\epsilon)\delta_{kl}, \tag{57}$$

first noted by Thiemann. The operator

$$\hat{K}_k \equiv \frac{\hat{1}}{R_k} \equiv \left(\frac{2}{2l_P^2\epsilon^2}\hat{U}_k(-\epsilon)[\sqrt{|\hat{R}_k|}, \hat{U}_k(\epsilon)]\right)^2 \tag{58}$$

depends on the parameter ϵ through its dependence on the translation operators $\hat{U}_k\epsilon$. Its action on the basis states is

$$\frac{\hat{1}}{R_k}|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle = \frac{1}{2l_P^2\epsilon^2}(\sqrt{|a_k-\epsilon|}-\sqrt{|a_k|})^2|a_1,\ldots,a_N;b_1,\ldots,b_N\rangle. \tag{59}$$

A symmetric version of this operator is similarly defined.

Let us now turn to realizing operators corresponding to spatial derivatives of field variables such as ϕ' and R'. To do this in a controlled manner it is easier to first restrict the choices of points r_i so that they define a uniformly spaced lattice with spacing λ. This is the first place where we explicitly introduce a radial lattice. It also has the effect of selecting a subspace of the full Hilbert space we defined above, by working only with a fixed set of radial points. We can now follow what is done in numerical methods, i.e.

$$f'(r_k) \rightarrow \frac{f_{k+1}-f_k}{l_P\lambda} \tag{60}$$

and

$$f''(r_k) \rightarrow \frac{f_{k+1}-2f_k+f_{k-1}}{2l_P^2\lambda^2}, \tag{61}$$

for any function f_k. This first of these suggests the operator

$$\hat{R}'_k = \frac{\hat{\phi}_{k+1}-\hat{\phi}_k}{l_P\lambda}, \tag{62}$$

with similar expressions for other operators. Such choices are of course not canonical, and may be viewed as an additional freedom in realizing a quantum theory.

Lastly the lattice local observable momentum operators are

$$\hat{P}_{Rk} \equiv \frac{l_P}{2i\epsilon}(\hat{U}_k(\epsilon)-\hat{U}_k^\dagger(\epsilon)),\qquad \hat{P}_{Rk}^2 \equiv \frac{l_P^2}{\epsilon^2}(2-\hat{U}_k(\epsilon)-\hat{U}_k^\dagger(\epsilon)), \tag{63}$$

$$\hat{P}_{\phi k} \equiv \frac{l_P}{2i\kappa}(\hat{V}_k(\kappa)-\hat{V}_k^\dagger(\kappa)),\qquad \hat{P}_{\phi k}^2 \equiv \frac{l_P^2}{\kappa^2}(2-\hat{V}_k(\kappa)-\hat{V}_k^\dagger(\kappa)), \tag{64}$$

with the action on basis states given by

$$\hat{P}_{\phi k}|a;b\rangle = \frac{l_P}{2i\kappa}(|a;b_1,\ldots,b_k-\kappa,\ldots,b_N\rangle - |a;b_1,\ldots,b_k+\kappa,\ldots,b_N\rangle) \tag{65}$$

and

$$\hat{P}_{\phi k}^2|a;b\rangle = \frac{l_P^2}{\kappa^2}(2|a;b\rangle - |a;b_1,\ldots,b_k-\kappa,\ldots,b_N\rangle - |a;b_1,\ldots,b_k-\kappa,\ldots,b_N\rangle). \tag{66}$$

In constructing more complicated operators the question of the operator ordering is important. One option is a symmetric ordering,

$$AB \rightarrow \widehat{AB} \equiv (\hat{A}\,\hat{B} + \hat{B}\,\hat{A})/2. \tag{67}$$

Another possibility is an order at which, e.g., $\hat{R}$ is to the right of $\hat{P}_R$. We will see in the following that it has an advantage of annihilating the state of zero gravitational excitations.

B. Constraint operator

Our goal in this section is to use the above definitions of basic operators to give a prescription for the reduced Hamiltonian (20). The main issue is the definition of the square root $\sqrt{Y}$ in this Hamiltonian, where

$$Y = (P_R R)^2 - \mathcal{R} - 16R^2 H_\phi, \quad \mathcal{R} = 16R^2(2RR'' - 1 + R'^2). \tag{68}$$

An operator representing this expression may be defined using a Dirac-like trick by suitably extending the kinematical Hilbert space [25]. However there is an alternative way to write the constraint (21) such that the square root problem is bypassed. Substituting for P'_Λ from Eq. (14) into the diffeomorphism constraint gives

$$C_r = -P'_R R - \frac{Y'}{2\sqrt{Y}} + P_\phi \phi' \simeq 0. \tag{69}$$

If supplemented with the requirement $Y > 0$ (which is the case for classical solutions), this is equivalent to

$$-\tfrac{1}{2}Y' + (P_\phi \phi' - P'_R R)\sqrt{Y} \simeq 0. \tag{70}$$

This implies the constraint

$$\mathcal{C} = Y'^2/4 - (P_\phi \phi' - P'_R R)^2 Y \simeq 0. \tag{71}$$

In this form it does not contain a square root, and it is now straightforward to construct the corresponding operator using the basic ones defined above. This path for constructing the constraint operator is one of the results of this paper, and provides an alternative to the Dirac-like method used earlier [25] where a square root operator is constructed.

Before giving a construction of an operator analog of (71), we note, however, that this constraint may have quantum solutions, which are not solutions of the original constraint. There is, however, an obvious check using Eq. (19): after obtaining a solution, we must check that the expectation value of the operator analog of

$$-\frac{1}{2}Y' - (P_\phi \phi' - P_R R') \int_0^r (P_R R' + P_\phi \phi') dr' \tag{72}$$

in the proposed solution does not vanish. As we discuss below it is possible to construct the corresponding operator.

Let us first focus on the local operator $\hat{Y}_k$. Its ingredients include

$$\hat{R}_k^2 |a, b\rangle = 4 l_P^4 a_k^2 |a; b\rangle, \quad \hat{K}_k^2 |a; b\rangle = \frac{1}{4 l_P^4 \epsilon^4} (\sqrt{|a_k - \epsilon|} - \sqrt{|a_k|})^4 |a; b\rangle, \tag{73}$$

and

$$(\hat{\phi}'_k)^2 |a; b\rangle = \frac{4 l_P^2}{\lambda^2} (b_{k+1} - b_k)^2 |a; b\rangle, \tag{74}$$

and since all factors of the field Hamiltonian (density) commute,

$$\hat{H}_{\phi k} = \tfrac{1}{2} \hat{P}_{\phi k}^2 \hat{K}_k^2 + \tfrac{1}{2} \hat{R}_k^2 (\hat{\phi}'_k)^2. \tag{75}$$

To complete the construction of $\hat{Y}$ one needs also

$$(\hat{R}'_k)^2 |a; b\rangle = \frac{4 l_P^2}{\lambda^2} (a_{k+1} - a_k)^2 |a; b\rangle \tag{76}$$

and

$$\hat{R}''_k |a; b\rangle = \frac{1}{\lambda^2} (a_{k+1} - 2a_k + a_{k-1}) |a; b\rangle. \tag{77}$$

The last term is

$$P_R^2 R^2 \longrightarrow \tfrac{1}{2}(\hat{P}_R^2 \hat{R}^2 + \hat{R}^2 \hat{P}_R^2), \tag{78}$$

which acts as

$$\begin{aligned}(\widehat{P_R^2 R^2})_k |a; b\rangle = \frac{4 l_P^6}{\epsilon^2} (2a_k^2 |a; b\rangle - [(a_k - \epsilon)^2 + a_k^2] |a_1, \ldots, a_k \\ - \epsilon, \ldots, a_N; b\rangle - [(a_k + \epsilon)^2 + a_k^2] \\ \times |a_1, \ldots, a_k + \epsilon, \ldots, a_N; b\rangle).\end{aligned} \tag{79}$$

Putting these pieces together we get

$$\hat{Y}_k = (\widehat{P_R^2 R^2})_k - 16 \hat{R}_k^2 (2 \hat{R}_k \hat{R}''_k - 1 + \hat{R}'^2_k) - 16 \hat{R}_k^2 \hat{H}_{\phi k}. \tag{80}$$

To complete the constraint operator $\hat{C}_k$ one also needs the commuting operators $(\widehat{P_\phi \phi'})_k$, $(\widehat{P'_R R})_k$. Both are obtained by, e.g., applying the symmetric quantization condition Eq. (67) to the elementary operators of the previous section.

$$(\widehat{P_\phi \phi'})_k |a; b\rangle = \frac{l_P^2}{i \kappa \lambda} \left(\left(b_{k+1} - b_k + \frac{1}{2}\kappa \right) |a; \ldots, b_k - \kappa, \ldots\rangle - \left(b_{k+1} - b_k - \frac{1}{2}\kappa \right) |a; \ldots, b_k + \kappa, \ldots\rangle \right) \tag{81}$$

and

$$\begin{aligned}(\widehat{P'_R R})_k |a; b\rangle = \frac{l_P^2}{i \epsilon \lambda} \Big(a_k |\ldots, a_{k+1} - \epsilon, \ldots; b\rangle - \left(a_k - \frac{1}{2}\epsilon \right) |\ldots, a_k - \epsilon, \ldots; b\rangle - a_k |\ldots, a_{k+1} + \epsilon, \ldots; b\rangle \\ + \left(a_k + \frac{1}{2}\epsilon \right) |\ldots, a_k + \epsilon, \ldots; b\rangle \Big).\end{aligned} \tag{82}$$

C. Hamiltonian operator

The asymptotic Hamiltonian is the surface term in (7) for which we need to define an operator for P_Λ. A direct quantization of the Hamiltonian density in Eq. (20) would require us to define the operator

$$\hat{H}_k^{\rm phys} = N_k^{r\prime}(\widehat{P_R R})_k + |\hat{Y}_k|^{1/2} + N_k^r((\widehat{P_R^\prime R})_k + (\widehat{P_\phi \phi^\prime})_k), \tag{83}$$

which has the square root term $|\hat{Y}_k|^{1/2}$, just as for the constraint. Since $\hat{Y}_k$ is not diagonal in the basis we are using, this operator is not easy to define unless we go to a different basis. However, from the constraint C_r we see that, classically, on the constraint surface we have

$$P_\Lambda(r) = \int_0^r dr^\prime (P_\phi \phi^\prime + P_R R^\prime). \tag{84}$$

This suggests that for physical states it is possible to compute the energy by finding an operator analog of the right-hand side of this equation. Since the quantization we are using utilizes a radial lattice, we can write the integral as a discrete sum over the lattice points r_k. It is therefore reasonable to suggest the definition

$$\hat{P}_{\Lambda k} = \lambda l_P \sum_{i=1}^k [(\widehat{P_\phi \phi^\prime})_i + (\widehat{P_R R^\prime}_i)]. \tag{85}$$

This operator is useful with the type of semiclassical states we define below in Sec. V. In such states a computation of the expectation value $\langle \psi | \hat{P}_{\Lambda k} | \psi \rangle$ is possible. The energy of the quantum spacetime would be this expression evaluated at the farthest lattice point; i.e. we would take the limit $k \to \infty$ after computing the expectation value. This would be a possible analog of the classical definition, where the energy

$$E = \lim_{r\to\infty} P_\Lambda(r) N^r(r). \tag{86}$$

We note that the asymptotic falloff of N^r is determined by the classical requirement of functional differentiability [8], and this behavior of N^r carries over to the quantum theory, since N^r is not a phase space variable.

IV. PHYSICAL STATES AND ENTANGLEMENT

Initial states of the gravity-matter system should satisfy the quantum constraint

$$\hat{\mathcal{C}} |\psi\rangle = 0, \tag{87}$$

which is supplemented by the requirement that $|\psi\rangle$ belong to the positive part of the spectrum of $|\hat{Y}|$. It remains to be seen whether any of the operator ordering choices allows for this to be satisfied on a sufficiently large set of states, or if another realization of the constraint is necessary to accomplish this. Nevertheless, it is already possible to make a few remarks. We give here two observations, on gravity-matter entanglement and on the information loss problem.

First, in the case of pure gravity ($\phi = P_\phi = 0$), the ordering that puts the $\hat{R}$ operator to the right results in an operator form of the constraint (71), which gives

$$\hat{\mathcal{C}}|0\rangle = (\hat{Y}^{\prime 2}/4 - \hat{P}_R^{\prime 2} \hat{R}^2 \hat{Y})|0\rangle = 0, \tag{88}$$

where $|0\rangle$ stands for the state with no excitations, i.e. all $a_i = b_i = 0$. This may be viewed as a ‘‘degenerate metric vacuum’’ because it is the eigenstate of the field operator $\hat{R}_k$ with zero eigenvalue at all points r_k.

Second, the presence of the matter-gravity terms in the constraint turns it into an entangling operator (see e.g. [23]). This can be seen by considering the constraint in the form of Eq. (71). It splits cleanly into a gravity part, and a separate gravity-matter interaction

$$\hat{\mathcal{C}} = \hat{\mathcal{C}}_G \otimes \mathbb{1}_M + \sum_\alpha \hat{\mathcal{C}}_\alpha^G \otimes \hat{\mathcal{C}}_\alpha^M. \tag{89}$$

The latter term contains monomials that involve gravity and matter operators. Consider their action on the basis states of the kinematical Hilbert space $\mathcal{H} = \mathcal{H}_G \otimes \mathcal{H}_M$. The term $\hat{P}_{\phi k} \hat{P}_{Rk}$ serves as an example:

$$\hat{P}_\phi^k \hat{P}_R^k |a\rangle \otimes |b\rangle \propto (|a_1 \cdots a_k - \epsilon \cdots a_N\rangle - |a_1 \cdots a_k\rangle - \epsilon \cdots a_N\rangle) \otimes (|b_1 \cdots b_k - \kappa \cdots b_M\rangle - |b_1 \cdots b_k + \kappa \cdots b_M\rangle), \tag{90}$$

which is a direct product of entangled gravity and matter modes. However, adding different terms in the constraint results in a superposition of such direct product states, and the constraint operator cannot be written as $\hat{\mathcal{C}} = \hat{\mathcal{C}}_G \otimes \hat{\mathcal{C}}_M$. Some states of the form $|\psi\rangle_G \otimes |\varphi\rangle_M$ may be transformed into a direct product form,

$$\hat{\mathcal{C}}(|\psi\rangle_G |\varphi\rangle_M) = |\psi^\prime\rangle_G |\varphi^\prime\rangle_M, \tag{91}$$

provided that they satisfy an additional constraint

$$\sum_\alpha \hat{\mathcal{C}}_\alpha^G \otimes \hat{\mathcal{C}}_\alpha^M (|\psi\rangle_G |\varphi\rangle_M) \propto |\psi^\prime\rangle_G |\varphi\rangle_M. \tag{92}$$

As a result, even if such states exist, they form a lower-dimensional set than the set of all physical states and, by themselves, do not form a vector space: their linear combinations are, by definition, entangled. Since we expect the semiclassical states to be suitably defined coherent states, we see that these configurations are geometry-matter entangled. This result of course holds regardless of whether a state corresponds to a classical black hole. The entanglement prevents the direct product gravity-matter decomposition of a generic physical state.

V. SEMICLASSICAL STATES

Semiclassical states that are peaked at given classical configurations may be defined for a field theory just as for a quantum mechanical system. For a constrained system such as the one we are considering, it is possible to obtain states that are peaked on classical constraint-free data. These may be viewed as approximate physical states in a precise sense.

For a constraint $\hat{C}$ in a field theory, the steps we propose are as follows: (i) begin with an explicit classical solution of the constraints, such as that given in Sec. II B, (ii) select sampling points r_i (or a lattice), and the corresponding solution values $R(r_i)$, $\phi(r_i)$, etc., (iii) construct a Gaussian state peaked at each field value $R(r_i)$ and $\phi(r_i)$, and finally (iv) take the product of the Gaussians, one at each point r_i, to give the field theory semiclassical state. This is what we describe in detail below.

Reasonable requirements for an approximate semiclassical state are that

$$\langle \hat{C}(r_k) \rangle = 0, \qquad \langle \hat{C}(r_k)^2 \rangle = 0, \tag{93}$$

for each sample point r_k. We give here a generalization of the semiclassical states for Friedmann-Robertson-Walker cosmology given in [27], and show how this can be utilized for the present model.

Let us consider first a single lattice point r_k and the basis states at this point defined by $|a_k\rangle \equiv |m\epsilon\rangle_k$, where m is an integer. Let us consider the state at r_k defined by the linear combination

$$|P_R^0, R^0\rangle_{r_k}^{t,\epsilon} = \frac{1}{C} \sum_{m=-\infty}^{\infty} e^{-(t/2)(\epsilon m)^2} e^{m\epsilon R^0} e^{im\epsilon P_R^0} |m\epsilon\rangle_{r_k}. \tag{94}$$

This is a Gaussian state of width t (measured in Planck units), where the (real) parameters P_R^0 and R^0 are the field values corresponding to a classical configuration at the point r_k. The width t is a measure of how strongly peaked the state is on a given classical configuration; i.e. $t \ll 1$ means that fluctuations around P^0, R^0 are small. We shall see in the following that this state has a number of desirable properties, and because of this, it allows a construction of approximate physical states of the theory we are considering. (There may be other non-Gaussian states with such properties but our purpose here is to point out that this one is useful.)

The normalization condition for the state gives an expression for the constant C. It is the convergent sum

$$C^2 = \sum_{m=-\infty}^{\infty} e^{-t\epsilon^2 m^2} e^{2R^0 \lambda m}. \tag{95}$$

Calculation with this state gives the expectation value [27]

$$\langle \hat{U}_\epsilon \rangle = e^{i\epsilon P_R^0(r_k)} e^{-t\epsilon^2/4} K(\epsilon, t, R^0), \tag{96}$$

where

$$K(\epsilon, t, R^0) = \left(\frac{1 + 2\sum_{m\neq 0} \cos[\frac{2\pi m R^0}{\epsilon t}(1 + \frac{t\epsilon}{2R^0})] e^{-\pi^2 m^2/t\epsilon^2}}{1 + 2\sum_{m\neq 0} \cos[\frac{2\pi m R^0}{\epsilon t}] e^{-\pi^2 m^2/t\epsilon^2}} \right). \tag{97}$$

Equation (96) together with the definition (48) gives the expectation value

$$\langle \hat{P}_R^\epsilon \rangle = \frac{\sin[P_R^0(x_k)\epsilon]}{\epsilon} e^{-t\epsilon^2/4} K(\epsilon, t, R^0). \tag{98}$$

This formula has the limits

$$\lim_{t\to 0} \langle \hat{P}_R^\epsilon \rangle = \sin(P_R^0(r_k)\epsilon)/\epsilon, \tag{99}$$

$$\lim_{\epsilon\to 0} \langle \hat{P}_R^\epsilon \rangle = P_R^0(r_k). \tag{100}$$

The first shows that the semiclassical state in field space is peaked at the corresponding phase space value. The second shows that the field continuum limit of the momentum expectation value has the appropriate peaked value in this state, even though only field translation operators exist in the representation we are using.

These semiclassical states defined at each point r_i can now be used to give a state for the entire radial lattice given any classical field configuration $R(r)$, $P_R(r)$ by taking a product of the point states over the lattice $\{r_k\}_{k=1}^N$, i.e.

$$|R(r), P(r)\rangle^{t,\epsilon} := \prod_{k=1}^{N} |R(r_k), P_R(r_k)\rangle_{r_k}^{t,\epsilon}. \tag{101}$$

The simplest semiclassical state for both sets of fields is the product

$$|\chi\rangle \equiv |R(r), P(r)\rangle^{t,\epsilon} |\phi(r), P_\phi(r)\rangle^{t,\delta}. \tag{102}$$

It is not difficult to configure entangled products of semiclassical states, given two distinct classical solutions of the constraints.

Given that the expectation values in these states give the classical peaking values, it follows that the states peaked on classical constraint-free data, such as those constructed in Sec. II, satisfy the expectation value

$$\langle \chi | \hat{C} | \chi \rangle = 0 + \mathcal{O}(t^\sigma), \tag{103}$$

where $\sigma > 1$. We note also that the construction we have given is quite specific, and there is control on the fluctuation $\langle \hat{C}^2 \rangle$, which is itself a function of the width t of the point Gaussian states. Its value can be tuned to reduce the fluctuations. It is in this sense that these states are approximately physical for sharply peaked states $t \ll 1$. One can now compute quantities such as the expectation value of the energy in such states, which is tedious put possible.

Effective equations

One approach for obtaining quantum gravity corrections is to use semiclassical states to derive "effective constraints." These can then be used to obtain modified equations of motion in the usual way. This approach is qualitatively related to the ideas underlying Ehrenfest's theorem in quantum mechanics. One computes expectation values of the constraints in states peaked on classical configurations that are not solutions of the initial value constraints to obtain

$$\begin{aligned} &\langle \phi, P_\phi, R, P_R | \hat{C} | \phi, P_\phi, R, P_R \rangle \\ &\quad = C^{\mathrm{classical}}(\phi, P_\phi, R, P_R) + \mathcal{O}(t^\sigma). \end{aligned} \tag{104}$$

It is understood here that the classical term on the right-hand side is a function of the phase space configuration on which the states are peaked. The corrections are functions of the state's width t in Planck units.

This approach has been used for homogeneous isotropic cosmology [28], but requires careful scrutiny in the field theory case here. One has to check that the Poisson algebra of the effective constraints closes with the state width corrections included, since these corrections are also functions of the phase space peaking values of the semiclassical state. One of the goals of the program presented here is to obtain consistent effective equations of motion starting from semiclassical states.

VI. SUMMARY AND DISCUSSION

The paper contains a number of developments beyond earlier works on the spherically symmetric gravity-scalar model. One such development is the construction of semiclassical states for the quantum theory of gravity coupled to a minimally coupled massless scalar field. These states may be utilized for constructing semiclassical effective constraints, which may then be used for classical numerical evolution. If used in conjunction with constraint-free data, such as those given in Sec. II B, this construction gives the first known examples of *physical* semiclassical states. A second development is an alternative construction of the Hamiltonian operator in a fixed time gauge which can serve as a starting point for Monte Carlo simulations of the quantum theory. Since this model is a two-dimensional system that is effectively written as a lattice theory, this method has the potential to reveal interesting nonperturbative quantum phenomena such as phase transitions. This is presently being studied.

The form of the Hamiltonian also reveals that matter-gravity entanglement is an inherent feature of evolution in quantum gravity; the action of the Hamiltonian on a product state gives an entangled state after a single evolution step. In the full quantum problem the constraint operator forces a bipartite entanglement (with the two subsystems being the kinematical Hilbert spaces of matter and gravity degrees of freedom, respectively) already on the initial physical states. It is tempting to summarize this observation by modifying Wheeler's one line description of general relativity [29]: quantum gravity tells geometry and matter how to entangle.

The degree of entanglement may be computed in the usual way by tracing a density matrix over either matter or geometry degrees of freedom. If a state describes a black hole, there is a second entropy that may be calculated, namely, that obtained by tracing the (pure) density matrix over both geometry and matter degrees of freedom inside a trapped region. This of course would be different from the usual entanglement entropy where the trace in the interior applies only to the matter degrees of freedom.

It will be apparent to the reader that the extraction of physical results from this formalism requires further work. This could proceed along two distinct avenues. The first is the derivation of semiclassical effective equations where one would compute expectation values of the constraint operators in suitable states to obtain "effective" constraints. These would then be used as the basis of a quantum gravity corrected classical dynamics which could be integrated using numerical methods. Among other things it would be useful to see what becomes of the critical scaling observed at the onset of black hole formation, especially the critical solution. Initial results using this approach [30,31] indicate that black holes form with a mass gap, but so far there are no results on the critical solution itself; with expected singularity avoidance, it is likely that this is replaced by a critical and unstable bound state—a finely tuned boson star.

The second approach to studying dynamics could utilize Monte Carlo methods. The quantum model as formulated here is like a statistical mechanical system, with the difference that it is still a constrained theory. One can imagine sampling from phase space such that the samples are solutions of the constraints up to some threshold, along with the usual Monte Carlo selection criteria. Such an approach would have the potential to yield fundamental information concerning phase transitions.

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