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# Consistent probabilities in loop quantum cosmology

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A fundamental issue for any quantum cosmological theory is to specify how probabilities can be assigned to various quantum events or sequences of events such as the occurrence of singularities or bounces. In previous work, we have demonstrated how this issue can be successfully addressed within the consistent histories approach to quantum theory for Wheeler-DeWitt-quantized cosmological models. In this work, we generalize that analysis to the exactly solvable loop quantization of a spatially flat, homogeneous and isotropic cosmology sourced with a massless, minimally coupled scalar field known as sLQC. We provide an explicit, rigorous and complete decoherent histories formulation for this model and compute the probabilities for the occurrence of a quantum bounce vs. a singularity. Using the scalar field as an emergent internal time, we show for generic states that the probability for a singularity to occur in this model is zero, and that of a bounce is unity, complementing earlier studies of the expectation values of the volume and matter density in this theory. We also show from the consistent histories point of view that all states in this model, whether quantum or classical, achieve arbitrarily large volume in the limit of infinite ‘past’ or ‘future’ scalar ‘time’, in the sense that the wave function evaluated at any arbitrary fixed value of the volume vanishes in that limit. Finally, we briefly discuss certain misconceptions concerning the utility of the consistent histories approach in these models.

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## I. INTRODUCTION

When do statements about the behavior of a physical system constitute a prediction, in the probabilistic sense, of the corresponding quantum theory? The answer, according to the consistent histories approach to quantum theory pioneered by Griffiths [1], Omnes [2, 3], Gell-Mann and Hartle [4], Halliwell [5] and others [6], is when – and only when – the quantum interference between the histories corresponding to those statements vanishes.

A framework of this kind is essential to the quantum theory of gravity applied to the universe as a whole because the universe is a closed quantum system. The usual formulation of quantum theory in which measurement by an external classical observer fixes whether a quantum amplitude determines a quantum probability is therefore not available [4]. Investigation of real measurement-type interactions [7–9] shows that a key feature of measurements is that they destroy the interference between alternative outcomes.<sup>1</sup> The consistent or decoherent histories approach to quantum theory formalizes this observation by supplying an objective, observer-independent measure of quantum interference between alternative histories called the *decoherence functional*. The decoherence functional, constructed from the system’s quantum state, both measures the interference between histories in a complete set of alternative possibilities, and, when that interference vanishes between all members of such a set, determines the probabilities of each such history. This framework reproduces the ordinary quantum mechanics of measured subsystems in situations to which it applies, but generalizes it to situations in which it does not, such as when applying quantum theory to a closed system such as the universe as a whole.

In previous work [10–12], we have developed the consistent histories framework for a model quantum gravitational system, a Wheeler-DeWitt quantization [13] of a spatially flat Friedmann-Robertson-Walker (FRW) cosmology sourced by a free, massless, minimally-coupled scalar field. In this paper, we give the consistent histories formulation of the corresponding model [13–15] in loop quantum cosmology (LQC). (See Ref. [16] for a review of LQC.) A key prediction of LQC is the existence of a bounce of the physical volume (or the scale factor) of the universe when the energy density of the matter content (in the present case, the scalar field  $\phi$ ) reaches a universal maximum  $\rho_{\max} = 0.41\rho_{\text{Planck}}$  in the isotropic models.<sup>2</sup> The existence of a bounce was first obtained for the model under consideration [13, 14, 18], and since then has been confirmed for a variety of matter models, using sophisticated numerical simulations.<sup>3</sup> These numerical simulations show that semi-classical states peaked at late times on classical expanding trajectories, bounce in the backward evolution (in ‘internal time’  $\phi$ ) to a classical contracting branch. Since the inner product, physical Hilbert space and a set of Dirac observables are completely known, the detailed physics can be extracted and reliable predictions can be made. Interestingly, the spatially flat isotropic model with a massless scalar field can be solved exactly in LQC [15]. This model, dubbed sLQC, serves as an important robustness check of various predictions in loop quantum cosmology. In particular, it has been shown that the bounce occurs for all the states in the physical Hilbert space, and the energy density is bounded above by the same universal maximum  $\rho_{\max}$  [15, 20].

All of these studies, though, address in practice only questions concerning *individual* quantum events, for example, the density or volume (of a fiducial spatial cell of the universe) at a given value of internal time. However, as discussed in detail in Refs. [10–12], conclusions drawn from such individual quantum events can be in certain situations badly misleading as a guide to probabilities for *sequences* of quantum occurrences – *histories* of the universe – precisely the kind of physical questions in which we are most interested in the context of the physics of cosmological history. The question is, when does the *amplitude* for a sequence of quantum events correspond to the *probability* for that particular history? The answer is, when, and only when, the interference between the alternative histories vanishes – just as in the two-slit experiment – as determined by the system’s decoherence functional.

In this paper we construct the decoherence functional for sLQC and employ it to study quantum histories of physical observables, concentrating on the physical volume of the fiducial cell. We examine both semiclassical and generic quantum states. We work within a complete predictive framework for the quantum mechanics of *history* to study the physics of the quantum bounce, showing that the corresponding quantum histories decohere, and that the probability of a cosmological bounce in these models is unity for generic quantum states (not just semiclassical ones). This stands in stark contrast to the predictions for the Wheeler-DeWitt quantization of the same model, which is shown in Refs. [12, 15] to be certain to be *singular* for generic quantum states.

We close this introduction with a note on the role played in quantum cosmology by larger issues in the interpretation of quantum mechanics. It is perhaps an understatement to observe that the philosophical challenges presented by the

<sup>1</sup> The archetypal classroom example of this is the two-slit experiment: when the experiment is configured in such a way as to gather information concerning which slit the particle passed through, the interference pattern is destroyed, and meaningful probabilities – in the sense that the usual probability sum rules are satisfied – may be assigned to the alternative histories  $\{(\text{upper slit}, y), (\text{lower slit}, y)\}$ , where  $y$  is the position of arrival of the electron on the screen. If information concerning the slit is not gathered, there is interference between the alternative histories, and no physically meaningful probability can be assigned to the slit through which the particle passed before arriving at position  $y$ . Quantum theory simply has no prediction concerning such histories. More pointedly, in quantum theory *there can be no logically consistent prediction* for these particular histories in this experimental configuration.

<sup>2</sup> The existence of a bounce in LQC has also been demonstrated for anisotropic models, however due to contributions from the anisotropic shear to the spacetime curvature, the bounce of the mean scale factor is not accompanied by a saturation of the energy density. The energy density and the shear scalar are however still bounded above. (See Ref. [17] for more discussion in different Bianchi models.)

<sup>3</sup> For a summary of results on the bounce in various models in LQC, see Ref. [16]. A review of numerical techniques, including the way comparisons with the classical theory are made, is available in Ref. [19].

effort to apply quantum theory to closed systems – particularly, the universe as a whole – do not end with questions of consistency of histories or decoherence. A fundamental challenge to the program is to offer a coherent account of the physical meaning of the probabilities at which one consistently arrives [4, 21, 22]. This profound question is not the subject of this paper. Indeed, there is little agreement on the “true” nature of probability even in classical physics, never mind quantum mechanics more broadly [23, 24] or the quantum theory of closed systems in particular. Here we adopt the pragmatic attitude fairly typical in physics. When multiple instantiations of the “same” physical system are available, probability is interpreted through “for all practical purposes” operational definitions based on relative frequencies of outcomes [25, 26]. For single systems (such as the whole universe), a frequentist interpretation is not so easily accessible.<sup>4</sup> Even though we do not shy away from writing down probabilities in this paper, we recognize the interpretational challenges and therefore concentrate particularly on a class of quantum predictions for which the interpretation of probabilities might be hoped to be less controversial: those which are *certain* i.e. have probabilities equal to 0 or 1 – or very close thereto [4, 21, 27].

The plan of the paper is as follows. In Sec. II we briefly summarize the framework of loop quantum cosmology and discuss the quantization of sLQC. Starting from the classical theory formulated in Ashtekar variables, we show the way inner product, physical Hilbert space and Dirac observables are constructed, and an evolution equation in the emergent ‘internal time’  $\phi$  is obtained. In Sec. III, we summarize generalized decoherent (or consistent) histories quantum theory in the context in sLQC, by rewriting the standard approach in proper time in terms of the internal time  $\phi$ . We describe the construction of the generalized quantum theory for sLQC, including definitions of its class operators (histories), branch wave functions, and decoherence functional. (More details of the classical theory of the model considered and the standard consistent histories approach can be found in our previous work [10–12].) In Sec. IV we apply these constructions to quantum predictions concerning histories of the cosmological volume by using some important properties of the eigenfunctions of the quantum Hamiltonian constraint derived recently [20]. We first introduce class operators for the volume observable, and discuss the way probabilities can be computed for histories involving single and multiple instants of internal time  $\phi$ . We evaluate the probability for occurrence of a quantum bounce for semi-classical states, as well as generic states. We show that the probability of occurrence of a bounce in sLQC turns out to be unity for *all* states in the theory. Sec. V closes with some discussion.

## II. LOOP QUANTIZATION OF FLAT, HOMOGENEOUS AND ISOTROPIC COSMOLOGY

In this section, we briefly outline the quantization of a spatially flat, homogeneous and isotropic spacetime in loop quantum cosmology.<sup>5</sup> A complete loop quantization of this model sourced with a massless, minimally coupled scalar field  $\phi$  was first provided in Refs. [13, 14, 18], and the model was demonstrated in Ref. [15] to be exactly solvable in the “harmonic gauge”  $N = a(t)^3$ , where  $a(t)$  denotes the scale factor of the universe described by the Friedmann-Lemaître-Robertson-Walker metric

$$g_{ab} = -N^2 dt_a dt_b + a^2(t) \hat{q}_{ab}. \quad (2.1)$$

Here  $\hat{q}_{ab}$  is a flat fiducial metric on the spatial slices  $\Sigma$ . In loop quantum cosmology the quantization procedure parallels that of loop quantum gravity (LQG). The gravitational phase space variables in loop quantum cosmology are the symmetric connection  $c$  and its conjugate triad  $p$ , obtained by a symmetry reduction of the gravitational phase space variables in LQG, the Ashtekar-Barbero  $SU(2)$  connection  $A_a^i$ , and the densitized triad  $E_i^a$ . These are related by

$$A_a^i = c V_o^{-1/3} \hat{\omega}_a^i, \quad E_i^a = p \sqrt{\hat{q}} V_o^{-2/3} \hat{e}_i^a. \quad (2.2)$$

Here  $V_o$  denotes the volume with respect to  $\hat{q}_{ab}$  of a fiducial cell introduced in order to define a symplectic structure on  $\Sigma$ ,<sup>6</sup> and  $\hat{e}_i^a$  and  $\hat{\omega}_a^i$  respectively denote a fiducial triad and co-triad compatible with the fiducial metric. (In these variables the physical volume of the fiducial cell is  $V = a^3 V_o = |p|^{3/2}$ .) For the massless scalar field model, the matter phase space variables are  $\phi$  and its conjugate momentum  $p_\phi$ . In terms of these phase space variables, the classical Hamiltonian constraint  $\mathcal{C}_{cl}$  can be written as

$$\mathcal{C}_{cl} = -3\pi G \hbar^2 b^2 \nu^2 + p_\phi^2, \quad (2.3)$$

<sup>4</sup> For some recent discussion, see Ref. [22].

<sup>5</sup> For various details, see Refs. [13–16].

<sup>6</sup> This choice is necessary if the topology of the manifold is non-compact (in the present case,  $\mathbb{R}^3$ ), as chosen in this analysis. The results obtained are independent of this choice, and are unaffected if we choose a compact topology (in the present case,  $\mathbb{T}^3$ ). See Ref. [16] for a brief discussion of this point.

where  $b$  and  $\nu$  are related to  $c$  and  $p$  by

$$b = \frac{c}{|p|^{1/2}}, \quad \nu = \frac{|p|^{3/2}}{2\pi\gamma l_p^2}. \quad (2.4)$$

Here  $l_p = \sqrt{G\hbar}$  is the Planck length. (We have set  $c = 1$ .) Note that  $\nu$ , though a measure of the physical volume of the fiducial cell, has dimensions of length. The modulus sign arises due to the two physically equivalent orientations of the triad. We will choose the orientation to be positive without any loss of generality.

Hamilton's equations for Eq. (2.3) yield the classical trajectories via the Poisson brackets  $\{b, \nu\} = 2\hbar^{-1}$  and  $\{\phi, p_\phi\} = 1$ . These yield  $p_\phi = V_o a^3 \dot{\phi}$  as a constant of motion, and relate  $\phi$  and  $\nu$  by

$$\phi = \pm \frac{1}{\sqrt{12\pi G}} \ln \left| \frac{\nu}{\nu_o} \right| + \phi_o, \quad (2.5)$$

where  $\nu_o$  and  $\phi_o$  are constants of integration. In the classical theory, for  $\nu \geq 0$  and regarding  $\phi$  as an emergent internal physical 'clock', there exist two disjoint solutions, one expanding and the other contracting, with a fixed value of  $p_\phi$ . In the limit  $\phi \rightarrow -\infty$  the expanding branch encounters a big bang singularity in the past evolution, whereas in the limit  $\phi \rightarrow \infty$  the contracting branch encounters a big crunch singularity in the future evolution. These singularities are reached in a finite proper time, and *all* the classical solutions are singular.

We now summarize the quantization procedure for this model in loop quantum cosmology in brief. As in LQG, the fundamental variables for quantization of the gravitational sector are the holonomies of the connection and the fluxes of the triads. Due to spatial homogeneity, the fluxes turn out to be proportional to the triads themselves [28], whereas the holonomies of the connection, along straight edges labelled by  $\mu$ , are given by

$$h_k^{(\mu)} = \cos\left(\frac{\mu c}{2}\right) \mathbb{I} - 2i \sin\left(\frac{\mu c}{2}\right) \frac{\sigma_k}{2}, \quad (2.6)$$

where the  $\sigma_k$  are the Pauli spin matrices. The matrix elements of the holonomies generate an algebra of almost periodic functions of the connection, the representation of which, found via the Gel'fand-Naimark-Segal construction, supplies the kinematical Hilbert space. It turns out that even at the kinematical level, the quantization of this model in LQC is strikingly different from that of the Wheeler-DeWitt theory. The gravitational sector of the kinematical Hilbert space in loop quantum cosmology is  $\mathcal{H}_{\text{grav}}^{(\text{kin})} = L^2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{Bohr}})$  where  $\mathbb{R}_{\text{Bohr}}$  is the Bohr compactification of the real line, and  $\mu_{\text{Bohr}}$  is the Haar measure on it. In contrast, the kinematical Hilbert space in the Wheeler-DeWitt theory is  $L^2(\mathbb{R}, dc)$ . Unlike the Wheeler-DeWitt theory, a generic state in the kinematical Hilbert space of LQC can be expressed as a countable sum of orthonormal eigenfunctions (matrix elements of holonomies).

The matrix elements of the holonomies act on states in the volume (or the triad) representation as translations. If  $|\nu\rangle$  denotes the eigenstates of the volume operator, which has the action  $\hat{V}|\nu\rangle = 2\pi\gamma l_p^2 |\nu| |\nu\rangle$ , then elements of the holonomies act as  $\widehat{\exp(i\lambda b)}|\nu\rangle = |\nu - 2\lambda\rangle$ . Here  $\lambda$  is a parameter determined by the underlying quantum geometry, and is given by  $\lambda^2 = 4\sqrt{3}\pi\gamma l_p^2$  [29]. A consequence is that the action of the Hamiltonian constraint operator, expressed in terms of the holonomies, on the states in the volume representation does not lead to a differential equation, but rather to a difference equation in which the discreteness scale is determined by the parameter  $\lambda$ . For the total Hamiltonian constraint  $\hat{C}_{\text{grav}} + 16\pi G \hat{C}_{\text{matt}} \approx 0$ , the resulting difference equation is given by

$$\Theta\Psi(\nu, \phi) := -\frac{3\pi G}{4\lambda^2} \left\{ \sqrt{|\nu(\nu + 4\lambda)|} |\nu + 2\lambda| \Psi(\nu + 4\lambda, \phi) - 2\nu^2 \Psi(\nu, \phi) \right. \\ \left. + \sqrt{|\nu(\nu - 4\lambda)|} |\nu - 2\lambda| \Psi(\nu - 4\lambda, \phi) \right\} \quad (2.7a)$$

$$= -\partial_\phi^2 \Psi(\nu, \phi), \quad (2.7b)$$

where the gravitational part of the constraint  $\Theta$  is a self-adjoint, positive definite operator.<sup>7</sup> The similarity of this equation to the Klein-Gordon equation is compelling. Since  $\phi$  is monotonic, it may be treated as an emergent internal time. Solutions of the constraint equation can then be divided into orthogonal, physically equivalent positive and negative frequency subspaces. As in the Klein-Gordon theory, it suffices to consider only one of these subspaces to extract physics. We consider states lying in the positive frequency subspace, satisfying

$$-i\partial_\phi \Psi(\nu, \phi) = \sqrt{\Theta} \Psi(\nu, \phi), \quad (2.8)$$

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<sup>7</sup> This expression is different from what is found in Refs. [14, 15] because we are using states that carry an additional factor of  $\sqrt{\lambda/|\nu|}$  relative to those states in order to simplify the form of the inner product, Eq. (2.9). Compare, for example, Refs. [30, 31].

which are normalized with respect to the inner product

$$\langle \Psi | \Phi \rangle = \sum_{\nu=4\lambda n} \Psi(\nu, \phi_o)^* \Phi(\nu, \phi_o) . \quad (2.9)$$

Note the inner product so defined is *independent* of the choice of  $\phi_o$ . Eq. (2.9) defines the Hilbert space of sLQC.

Physical states have a support on the lattices  $\nu = (4n \pm \epsilon)\lambda$ , with  $n \in \mathbb{Z}$  and  $\epsilon \in [0, 4)$ . Thus, there is super-selection among lattices with different  $\epsilon$ . In this manuscript, we will focus on the  $\epsilon = 0$  sector, which allows the states to have support on zero volume – the big bang singularity in the classical theory.

An additional requirement on the physical states  $\Psi(\nu, \phi)$  arises by noting that in the absence of fermions, physics should be independent of the orientation of the triad. We can thus choose physical states to be symmetric under this change, which therefore satisfy  $\Psi(\nu, \phi) = \Psi(-\nu, \phi)$ . Because of the symmetry of the physical states and observables under changes of orientation of the triad, we will as applicable treat  $\nu$  as positive in the sequel.

In order to extract physics, we introduce a set of Dirac observables. These are the volume of the fiducial cell at time  $\phi^*$ , and the conjugate momentum  $p_\phi$ , which have the following action (consistent with the inner product):

$$\hat{V}|_{\phi^*} \Psi(\nu, \phi) = 2\pi\gamma l_p^2 e^{i\sqrt{\Theta}(\phi-\phi^*)} |\nu| \Psi(\nu, \phi^*), \quad \hat{p}_\phi \Psi(\nu, \phi) = \hbar\sqrt{\Theta} \Psi(\nu, \phi) . \quad (2.10)$$

Using these observables, it is straightforward to also introduce an energy density observable, which turns out to have expectation values bounded above by a critical density  $\rho_{\max}$  for all the states in the physical Hilbert space [15, 20]. Analysis of these observables in sLQC, in confirmation with the earlier results in LQC obtained using numerical simulations [13, 14, 18], show that the expectation value of the volume observable has a minimum which is reached when the energy density reaches its maximum value. This is the quantum bounce in sLQC. Our goal is now to understand the occurrence of a bounce in sLQC using the consistent histories approach, which is addressed in the following.

### III. CONSISTENT HISTORIES FORMULATION OF SLQC

In this section we apply the ideas of the consistent histories approach to quantum mechanics (also known as ‘generalized quantum theory’ a la Hartle [4]) to the sLQC model discussed in Sec. II. The formalism will then be used in Sec. IV, to make quantum-mechanically consistent predictions concerning the behavior of the physical universe by employing the decoherence functional to measure the quantum interference between possible alternative histories.

Our definitions will naturally directly mirror those for the Wheeler-DeWitt quantization of the same model [10–12], facilitating easy comparison of the sometimes divergent predictions of the two models. Moreover, as noted, the construction of class operators, branch wave functions, and the decoherence functional for sLQC precisely mirrors that of the Wheeler-DeWitt theory. In this section, therefore, we restrict ourselves to a concise summary of the definitions and main formulæ, referring the reader to Ref. [12] for a more in depth discussion and commentary.

The three essential ingredients of a generalized quantum theory are: (i) The *fine-grained histories*, the most refined descriptions of a system it is possible to give. (These might be individual paths in a path integral formulation of the theory, for example.) (ii) The *coarse-grained histories*, a specification of the allowed partitions of the fine-grained histories into physically meaningful subsets. (Only diffeomorphism invariant partitions might be allowed in a covariant quantization of gravity, for example.) Since most all physical predictions concern highly coarse-grained descriptions of the universe, it is the coarse-grained histories which correspond to physically meaningful questions, and for which quantum theory must be able to determine probabilities – and indeed, if those probabilities are meaningful at all. (iii) The *decoherence functional* provides an objective, observer-independent measure of the quantum interference between alternative coarse-grained histories of a system. When that interference vanishes among all members of a coarse-grained family, that set is said to “decohere”, or to “be consistent”. In that case, and in that case only, does the decoherence functional assign logically consistent probabilities – in the sense that probability sum rules are satisfied – to the members of each consistent set of histories.

Any specific implementation of a generalized quantum theory must realize these elements in a coherent and mathematically consistent way. In formulations of quantum theory in Hilbert space, fine-grained histories can be specified by (for example) time-ordered products of Heisenberg projections onto eigenstates of physical observables, representing the history in which the system assumes those particular values of those particular observables at those particular times. Coarse-grained histories are represented by sums of such fine-grained histories. “Branch wave functions” corresponding to the state of a system that has followed a particular coarse-grained history are defined by the action of these history (or “class”) operators on the quantum state. The decoherence functional, which measures the interference between alternative histories, and also the probabilities of histories in consistent or decoherent families as

determined by the absence of such interference, can be defined by the physical inner product between branch wave functions.

In the consistent histories approach to ordinary non-relativistic quantum theory, histories are defined using coordinate time  $t$ . As discussed in the previous section, in sLQC, the role of time is naturally played by the massless scalar field  $\phi$ . Indeed, using Eq. (2.8) we see that the states  $|\Psi\rangle$  evolve unitarily in  $\phi$ ,

$$\Psi(\nu, \phi) = e^{i\sqrt{\Theta}(\phi - \phi_o)} \Psi(\nu, \phi_o) =: U(\phi - \phi_o) \Psi(\nu, \phi_o). \quad (3.1)$$

$U(\phi)$  is thus the propagator for evolution in ‘time’  $\phi$ . Using  $\phi$  as the internal time, we can define Heisenberg projections in analogy with non-relativistic quantum mechanics and obtain class operators, branch wave functions, and a decoherence functional.<sup>8</sup> In this set up, the class operators provide predictions concerning histories of values of the Dirac observables. Our strategy here directly parallels the one we followed for the quantization of the Wheeler-DeWitt model with a massless scalar field [12].

### A. Class operators

Class operators correspond to the physical questions that may be asked of a given system. All such questions come in exclusive, exhaustive sets – at the most coarse-grained level, simply “Does the universe have property  $\mathcal{P}$ , or not?” The sum of all the class operators in such an exclusive, exhaustive set must therefore be, in effect, the identity, up to an overall unitary factor. Homogeneous class operators describe possible sequences of (ranges of) values of observable quantities, with sums of them corresponding to coarse-grainings thereof. We will often refer to class operators simply as “histories”.

In quantum cosmology relevant physical questions include “What is the physical volume of the fiducial cell when the scalar field has value  $\phi^*$ ?” “Does the volume of the cell ever drop below a particular value, let us say  $\nu^*$ ?” “Is the momentum of the scalar field conserved during evolution?” Does the density exceed  $\rho^*$ ?” – and so forth. In the present model, which possesses a physical clock – the monotonic (unitary) internal time supplied by the scalar field  $\phi$  – class operators for questions of this kind may be constructed similarly to those of non-relativistic quantum theory, in which fine-grained class operators correspond to predictions concerning the values of physical observables at given moments of time. From a physical point of view, in quantum cosmology, class operators constructed in a similar manner correspond to physical questions concerning the *correlation* between values of various observable quantities and the value of the scalar field. It is no surprise, then, that class operators of this type naturally correspond to predictions concerning the values of relational observables, as noted in Sec. III D.<sup>9</sup> Stated in this way, it is clear that the interpretation of the scalar field  $\phi$  as a background physical clock is an inessential, if useful, feature of this particular model.

In sLQC, we have states  $|\Psi\rangle$  with a unitary evolution in  $\phi$  given by Eq. (3.1). As noted, among the physical questions of interest are the values of volume and scalar momentum at given values of  $\phi$ . To extract physical predictions concerning quantities of this kind, we proceed as in ordinary quantum theory. We consider a family of observables  $A^\alpha$ , labelled by index  $\alpha$ , with eigenvalues  $a_k^\alpha$  in the physical Hilbert space  $\mathcal{H}_{\text{phys}}$  of sLQC. We denote the ranges of eigenvalues as  $\Delta a_k^\alpha$ . Projections onto the corresponding eigensubspaces will be denoted  $P_{a_k^\alpha}^\alpha$  and  $P_{\Delta a_k^\alpha}^\alpha$ , respectively. For a given choice of observable  $A^{\alpha_i}$  at each time  $\phi_i$ , an exclusive, exhaustive set of fine-grained histories in sLQC may be regarded as the set of sequences of eigenvalues  $\{h\} = \{(a_{k_1}^{\alpha_1}, a_{k_2}^{\alpha_2}, \dots, a_{k_n}^{\alpha_n})\}$ , corresponding to the family of histories in which observable  $A^{\alpha_i}$  has value  $a_{k_i}^{\alpha_i}$  at time  $t_i$ . (Each  $k_i$  for fixed  $i$  therefore runs over the full range of the eigenvalues  $a_{k_i}^{\alpha_i}$ .) A different choice of observables  $(\alpha_1, \alpha_2, \dots, \alpha_n)$  leads to different exclusive, exhaustive families of histories  $\{h\}$ . Using the propagator

$$U(\phi_i - \phi_j) = e^{i\sqrt{\Theta}(\phi_i - \phi_j)} \quad (3.2)$$

we define “Heisenberg projections”

$$P_{\Delta a_k^\alpha}^\alpha(\phi) = U^\dagger(\phi - \phi_o) P_{\Delta a_k^\alpha}^\alpha U(\phi - \phi_o), \quad (3.3)$$

<sup>8</sup> For comparison, Ref. [6] constructed the decoherence functional, following earlier work [4], for a path integral quantization of closed type A minisuperspace models. The decoherence functional for spin foam models [32] and other quantum gravitational models without an internal time fits naturally into this more general framework.

<sup>9</sup> Relational questions of this form are certainly not the only physical questions in which one might be interested, or for which class operators may be constructed – either in ordinary quantum mechanics [4, 33] or in quantum cosmology [5, 6]. However, they are sufficient for the physical problems considered in this paper.

where  $\phi_o$  is a value of the scalar field at which the quantum state is defined.<sup>10</sup> The fine-grained history  $h$  may then be conveniently represented by the class operator<sup>11</sup>

$$C_h = P_{a_{k_1}}^{\alpha_1}(\phi_1)P_{a_{k_2}}^{\alpha_2}(\phi_2)\cdots P_{a_{k_n}}^{\alpha_n}(\phi_n) \quad (3.4a)$$

$$= U(\phi_o - \phi_1)P_{a_{k_1}}^{\alpha_1}U(\phi_1 - \phi_2)P_{a_{k_2}}^{\alpha_2}\cdots U(\phi_{n-1} - \phi_n)P_{a_{k_n}}^{\alpha_n}U(\phi_n - \phi_o). \quad (3.4b)$$

Since  $\sum_k P_{a_k}^\alpha = \mathbb{1}$  for each observable  $\alpha$ , the class operator  $C_h$  satisfies

$$\sum_h C_h = \sum_{k_1} \sum_{k_2} \cdots \sum_{k_n} P_{a_{k_1}}^{\alpha_1}(\phi_1)P_{a_{k_2}}^{\alpha_2}(\phi_2)\cdots P_{a_{k_n}}^{\alpha_n}(\phi_n) = \mathbb{1}, \quad (3.5)$$

corresponding to the fact that the set of fine-grained histories  $\{h\}$  represents a mutually exclusive, collectively exhaustive description of the possible fine-grained histories in sLQC.

The coarse-grained history

$$h = (\Delta a_{k_1}^{\alpha_1}, \Delta a_{k_2}^{\alpha_2}, \dots, \Delta a_{k_n}^{\alpha_n}), \quad (3.6)$$

in which the variable  $\alpha_1$  takes values in  $\Delta a_{k_1}^{\alpha_1}$  at  $\phi = \phi_1$ , variable  $\alpha_2$  takes values in  $\Delta a_{k_2}^{\alpha_2}$  at  $\phi = \phi_2$ , and so on, then has the class operator

$$C_h = P_{\Delta a_{k_1}}^{\alpha_1}(\phi_1)P_{\Delta a_{k_2}}^{\alpha_2}(\phi_2)\cdots P_{\Delta a_{k_n}}^{\alpha_n}(\phi_n), \quad (3.7)$$

where we suppress the superscripts on the eigenvalue ranges to minimize notational clutter. It is straightforward to see that the class operators for the coarse grained histories satisfy  $\sum_h C_h = \mathbb{1}$ , the identity on the physical Hilbert space  $\mathcal{H}_{\text{phys}}$ .

## B. Branch wave functions

Class operators capture the physical questions that may be asked of a system, as specified by an exclusive, exhaustive set of histories  $\{h\}$ . The amplitude for a quantum state  $|\Psi\rangle$  specified at  $\phi = \phi_o$  to “follow” one of the histories  $h$  – i.e. for the universe to have the properties described by  $h$  – is given by the branch wave function  $|\Psi_h\rangle$ .<sup>12</sup>

The branch wave function for a history  $h$  in the physical Hilbert space of sLQC is defined in a manner parallel to non-relativistic quantum mechanics. Defining

$$C_h(\phi) = C_h \cdot U^\dagger(\phi - \phi_o), \quad (3.8)$$

the branch wave function is given by

$$|\Psi_h(\phi)\rangle = U(\phi - \phi_o)C_h^\dagger|\Psi\rangle \quad (3.9a)$$

$$= U(\phi - \phi_n)P_{a_{k_n}}^{\alpha_n}U(\phi_n - \phi_{n-1})\cdots U(\phi_2 - \phi_1)P_{a_{k_1}}^{\alpha_1}U(\phi_1 - \phi_o)|\psi\rangle. \quad (3.9b)$$

This branch wave function is, by construction, a solution to the quantum constraint everywhere. The propagator  $U$  simply evolves the branch wave function to any convenient choice of  $\phi$ . All inner products will of course be independent of this choice. The projections implement, in the standard Copenhagen interpretation, “wave function collapse”. From the consistent histories point of view, however, the branch wave function is viewed merely as an amplitude from which one may ultimately construct the probabilities of individual histories – the likelihoods that the universe possesses these particular sequences of physical properties. In particular, the “collapse” is not to be regarded as a physical process in this framework.

<sup>10</sup> Because the evolution in  $\phi$  is unitary, this value is completely arbitrary and may be adjusted as necessary to remain outside the region of coarse-grainings of physical interest.

<sup>11</sup> Class operators constructed in this way are subject to the quantum Zeno effect if spaced too closely in “time” [5, 34, 35], and a more subtle definition may be required. We do not address this question in this paper, though we may return to it in a later work.

<sup>12</sup> Because of the unitary evolution of Eq. (3.1), the choice of  $\phi_o$  has no special physical significance. Indeed, from the point of view of the consistent histories framework, the quantum state of the system is most naturally viewed as a “timeless” property of the system, with the more familiar notion of the “state at a moment of time” being recovered, under appropriate circumstances, in the branch wave function [4].



### C. The decoherence functional

Given a complete exclusive, exhaustive set of histories  $\{h\}$  and a quantum state  $|\Psi\rangle$  in the physical Hilbert space, the decoherence functional measures the interference among the branch wave functions  $|\Psi_h\rangle$ , and, if that interference vanishes, determines also the probabilities of each of the  $|\Psi_h\rangle$  – in other words, the probability that a universe in the state  $|\Psi\rangle$  has the physical properties described by the history  $h$ . If the interference does not vanish, then quantum theory can make no predictions concerning the particular set of physical questions  $\{h\}$ , in just the same way the question of which slit a particle passed through cannot be coherently analyzed when it is not recorded.

The decoherence functional in non-relativistic quantum mechanics is defined by

$$d(h, h') = \langle \Psi_{h'} | \Psi_h \rangle, \quad (3.10)$$

and from Eq. (3.5) is normalized,  $\sum_{h, h'} d(h, h') = 1$ . In quantum cosmology the decoherence functional may be constructed from the branch wave functions in essentially the same manner [6].<sup>13</sup>

“Decoherent” or “consistent” sets of histories are by definition exclusive, exhaustive sets of histories  $\{h\}$  which satisfy

$$d(h, h') = p(h) \delta_{h'h} \quad (3.11)$$

among all members of the set. Here  $p(h)$  is the probability for the history  $h$ . The physical meaning of this expression is the following. When interference between all the members of an exclusive, exhaustive set of coarse-grained histories  $\{h\}$  vanishes,  $d(h, h') = 0$  for  $h \neq h'$ , that set of histories is said to decohere, or be consistent. In such sets, the probabilities of the individual histories are then simply the diagonal elements of the decoherence functional,  $p(h) = d(h, h)$ . It is easily verified that this is simply the standard Lüders-von Neumann formula for probabilities of sequences of outcomes in ordinary quantum theory, when such probabilities may be defined – typically in measurement situations or interactions with an external “environment” that leads to decoherence in the now-conventional sense [8]. In the framework of generalized (decoherent histories) quantum theory, however, no external notion of observers or measurement or environment is required. It is the objective, observer independent criterion of Eq. (3.11) that determines when probabilities may be defined, and which ensures these probabilities are meaningful in the sense that probability sum rules are obeyed when histories are coarse-grained:  $p(h_1 + h_2) = p(h_1) + p(h_2)$ , with  $\sum_h p(h) = 1$ . If histories do not decohere, then the diagonal elements of the decoherence functional do not sum to unity and cannot therefore be interpreted as probabilities. For such families of histories, quantum theory is silent: it simply has no logically consistent predictions at all.

Note that as constructed, the decoherence functional for sLQC involves an inner product of branch wave functions on a minusesuperspace slice of fixed  $\phi$ . The unitary evolution in  $\phi$ , and the fact that the branch wave functions  $|\Psi_h(\phi)\rangle$  are by construction everywhere solutions to the quantum constraint, makes the specific choice of  $\phi$  irrelevant in the definition of the branch wave functions and decoherence functional, and therefore may be chosen as is convenient.

### D. Relational observables

Class operators constructed according to Eq. (3.7) express questions concerning the correlation between the values of the quantities  $A^{\alpha_i}$  at the specified values  $\phi_i$  of the scalar field. Probabilities computed in this way therefore naturally correspond to predictions concerning the corresponding relational observables, such as for the volume Dirac observable  $\hat{\nu}|_\phi$  defined in terms of the propagator, Eq. (3.2), by

$$\hat{\nu}|_{\phi^*}(\phi) = U(\phi^* - \phi)^\dagger \hat{\nu} U(\phi^* - \phi). \quad (3.12)$$

(See, for example, Eq. (4.5).) In other words, as discussed in detail in Ref. [12], probabilities for histories of values of an observable  $\hat{A}$ , which does not commute with the constraint, are naturally expressed in terms of the corresponding relational Dirac observable  $\hat{A}|_{\phi^*}(\phi)$ , which does. In this sense the notion of relational observables arises naturally, indeed, almost inevitably, in the framework of consistent histories when predictions concerning correlations between values of observables are concerned.

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<sup>13</sup> The generalization of this definition to mixed states is also given in [6].

#### IV. APPLICATIONS

We now apply the generalized “consistent histories” quantum theory of loop-quantized cosmology we have constructed to a series of predictions concerning histories of physical quantities of interest. In each case the approach is the same. Within the decoherent histories framework for quantum prediction, for any physical question that is to be investigated the corresponding class operators and branch wave functions must be constructed. If the interference between these branch wave functions disappears – i.e. if the family of branch wave functions corresponding to the question decoheres – then quantum probabilities may be assigned to the alternatives according to the diagonal elements of the decoherence functional, the norms of the corresponding branch wave functions.

It should be noted that in general there are a number of distinct reasons decoherence might occur. Predictions concerning physical quantities at a single value of the scalar field (moment of ‘time’) *always* decohere, because the corresponding family of class operators are simply orthogonal projections. (Compare for example Eq. (4.4). This is essentially the reason the need for decoherence is not so evident in simple applications of quantum mechanics that do not concern predictions for *sequences* of quantum events.) More generally, decoherence might obtain because of symmetries or selection rules; because of individual properties of the histories in question; or because of properties of the particular quantum state. In the applications we consider, we encounter examples in which decoherence occurs for each of these reasons.

Predictions concerning histories of values of the scalar momentum  $p_\phi$  in sLQC – making precise the sense in which it is a conserved quantity in the quantum theory – follow precisely the same pattern as in the Wheeler-DeWitt theory, for which see Ref. [12]. Decoherence in this case is essentially a consequence of the fact that the scalar momentum commutes with the constraint.

Our primary goal in this paper, however, will be to demonstrate how probabilities for the quantum bounce of the volume observable can be computed. We begin with the construction of class operators for the volume of the fiducial cell of the universe at an instant of ‘time’  $\phi$ , and also a sequence of values of  $\phi$ . Predictions concerning *histories* of values of the volume are interesting because in this case decoherence is no longer trivial, and indeed will frequently not obtain. We will nonetheless exhibit several physical examples in which it does, and use these to study two important physical problems: quasiclassical behavior of the universe; and the quantum “bounce”.

##### A. Class operators for volume

We begin with the class operator for the history in which the volume  $\nu$  is in  $\Delta\nu$  when the scalar field has value  $\phi^*$ . It is simply given by

$$C_{\Delta\nu|\phi^*} = U^\dagger(\phi^* - \phi_o) P_{\Delta\nu}^\nu U(\phi^* - \phi_o), \quad (4.1)$$

where the projection  $P_{\Delta\nu}^\nu$  is

$$P_{\Delta\nu}^\nu = \sum_{\nu \in \Delta\nu} |\nu\rangle\langle\nu|. \quad (4.2)$$

Note that we employ here projections onto ranges of values of the volume operator  $\hat{\nu}$ , not the Dirac observable  $\hat{\nu}|_{\phi^*}$ . These ranges form a collection of disjoint sets that cover the full range of discrete volume eigenvalues,  $0 \leq |\nu| = 4\lambda n < \infty$ , such that  $\sum_i C_{\Delta\nu_i|\phi^*} = \mathbf{1}$ .

If  $|\Psi\rangle$  denotes a quantum state of the universe at  $\phi = \phi_o$ , the branch wave functions for these histories are

$$|\Psi_{\Delta\nu|\phi^*}(\phi)\rangle = U(\phi - \phi_o) C_{\Delta\nu|\phi^*}^\dagger |\Psi\rangle. \quad (4.3)$$

Because in this instance the class operators are simply projections, the branch wave functions for these histories are orthogonal,

$$\langle\Psi_{\Delta\nu_i|\phi^*} | \Psi_{\Delta\nu_j|\phi^*}\rangle = \langle C_{\Delta\nu_i|\phi^*}^\dagger \Psi | C_{\Delta\nu_j|\phi^*}^\dagger \Psi\rangle \quad (4.4a)$$

$$= \langle\Psi_{\Delta\nu_i|\phi^*} | \Psi_{\Delta\nu_i|\phi^*}\rangle \cdot \delta_{ij}. \quad (4.4b)$$

This implies that for this family of histories decoherence is automatic. One can thus meaningfully compute the quantum probabilities. Using Eqs. (4.1) and (4.2), the probability that the universe has volume in the range  $\Delta\nu$  when

$\phi = \phi^*$  is then given by

$$p_{\Delta\nu}(\phi^*) = \langle \Psi_{\Delta\nu|\phi^*} | \Psi_{\Delta\nu|\phi^*} \rangle \quad (4.5a)$$

$$= \langle \Psi | C_{\Delta\nu|\phi^*}^\dagger | \Psi \rangle \quad (4.5b)$$

$$= \langle \Psi(\phi^*) | P_{\Delta\nu}^\nu | \Psi(\phi^*) \rangle \quad (4.5c)$$

$$= \sum_{\nu \in \Delta\nu} |\Psi(\nu, \phi^*)|^2. \quad (4.5d)$$

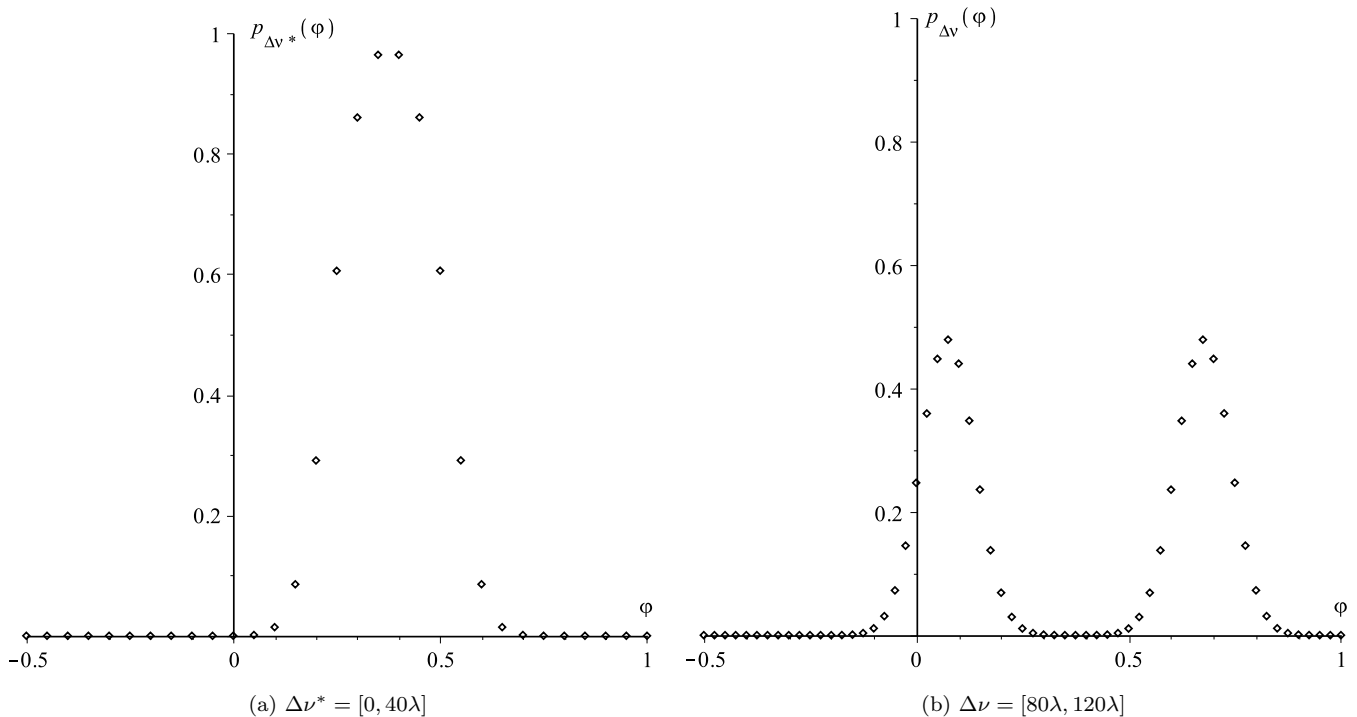


FIG. 1. Plots of the probability  $p_{\Delta\nu}(\phi)$  that the volume of (a fiducial cell of) a quantum universe specified by a state which is semiclassical at large  $|\phi|$  is in the range  $\Delta\nu$  when the scalar field has value  $\phi$  for two choices of range  $\Delta\nu$ . The bounce connecting the semiclassical phases is clearly visible in both plots. The first plot shows the probability that the volume of the universe is less than  $\nu^* = 40\lambda$  as a function of  $\phi$ . For this particular state the volume at which the universe “bounces” is smaller than  $\nu^*$ , and the probability the volume of the universe is less than  $\nu^*$  at the bounce is therefore close to unity, becoming zero as  $|\phi|$  becomes large. The second plot shows the probability that the volume of the fiducial cell is in the range  $\Delta\nu = [80\lambda, 120\lambda]$ , a range the state passes through on both sides of the bounce. The state shown has  $\tilde{\Psi}_{sc}(k) = 1/\sqrt{2\sigma\sqrt{\pi}} \exp(-(k-\bar{k})^2/2\sigma^2) \exp(-ik \ln|\bar{\nu}/\lambda|) + (k \leftrightarrow -k)$  in Eq. (4.15), with  $\phi_o = 0$ ,  $\bar{\nu} = 10\lambda$ ,  $\bar{k} = 15$ , and  $\sigma = 2$ . This state is peaked on a solution to the “effective” cosmological equations of LQC [16, 36, 37] that approaches classical expanding/collapsing solutions at large volume, joined by a bounce at small volume in between – as depicted, for example, in Figs. 2-3. (In those figures, however, the effective trajectory shown happens to be symmetric about  $\phi = 0$ , which is not the generic case.) For the given parameters this state “bounces” at  $(\nu_B, \phi_B) = (30\lambda, 0.375)$  in units in which  $G = 1$ . (For details of the correspondence between the trajectories of semiclassical states in LQC and solutions to the effective equations see Ref. [38].)

By way of example, Fig. 1 shows probabilities calculated from Eq. (4.5) that a state which is quasiclassical at large volume<sup>14</sup> takes on volumes in the range  $\Delta\nu$  for two choices of that range. For example, Fig. 1a shows the probability that the universe takes on small volume. Specifically, the plot shows the probability as a function of the scalar field  $\phi$  that the volume of the fiducial spatial cell has volume less than or equal to  $\nu^*$  i.e. that  $|\nu| \in \Delta\nu^*$ , where  $\Delta\nu^* = [0, \nu^*]$ :

$$p_{\Delta\nu^*}(\phi) = \sum_{|\nu| \in \Delta\nu^*} |\Psi(\nu, \phi)|^2. \quad (4.6)$$

<sup>14</sup> That is, a state for which  $\tilde{\Psi}(k)$  in Eq. (4.15) is a symmetric superposition of Gaussians in  $k$  – one each corresponding to the collapsing and expanding Wheeler-DeWitt branches of the bouncing solution at large volume; see Ref. [38] for details.

The quantum bounce is clearly visible in the plot, the probability the universe has small volume becoming zero as  $|\phi|$  becomes large.

We now consider the more interesting case when a sequence of ‘time’ instants is involved. In contrast to the class operator representing the volume of the universe at an instant  $\phi = \phi^*$  (Eq.(4.1)), the class operator for the volume to take particular values in ranges  $\Delta\nu_i$  at a sequence of different instances of internal time  $\{\phi_1, \dots, \phi_n\}$  is not a simple projection. It is given by

$$C_{\Delta\nu_1|\phi_1;\Delta\nu_2|\phi_2;\dots;\Delta\nu_n|\phi_n} = P_{\Delta\nu_1}^\nu(\phi_1)P_{\Delta\nu_2}^\nu(\phi_2)\cdots P_{\Delta\nu_n}^\nu(\phi_n), \quad (4.7)$$

where the sets of ranges  $(\{\Delta\nu_1\}, \{\Delta\nu_2\}, \dots, \{\Delta\nu_n\})$  partition the allowed range of volumes. As remarked earlier, in general it is neither obvious nor trivial that the corresponding branch wave functions (Eq. (3.9)) decohere. Nevertheless, in the following we will exhibit several important (and typical) examples for which they do, and extract the corresponding quantum probabilities.

## B. Decoherence for semiclassical states

We first apply this framework to states which are semi-classical at late times in this loop quantized model. Analysis of such states in loop quantum cosmology using sophisticated numerical simulations was first performed in Refs. [13, 14, 18] for the spatially flat homogeneous and isotropic model sourced with a massless scalar field.<sup>15</sup> The states are chosen such that they are initially peaked on classical trajectories in a macroscopic universe, and evolved using the quantum gravitational Hamiltonian constraint (see Eq. (2.7)). Numerical simulations show that such states remain peaked on classical trajectories until the spacetime curvature reaches almost a percent of its value at the Planck scale. As the Planck scale is approached, significant departures arise between the classical trajectory, Eq. (2.5), and the trajectory obtained from the expectation value of the volume observable. Instead of reaching the classical big bang singularity, such states bounce when the energy density of the universe reaches a maximum value  $\rho_{\max} \approx 0.41\rho_{\text{Planck}}$ . After the bounce, states are found to be peaked on an expanding classical solution (disjoint in the classical theory from the one where the initial state was peaked) [13, 14]. This result, initially obtained using numerical simulations for a class of semiclassical states, can be generalized to all the states in the physical Hilbert space. It turns out that in sLQC the expectation value of the volume observable has a minimum irrespective of the choice of state [15]. Further, *all* states in the physical Hilbert space reach arbitrarily large volume in the infinite past and future ( $\phi \rightarrow \pm\infty$ ). The minimum of the expectation value of volume translates to an upper bound on the expectation values of the energy density observable [15]. Recently, this result has also been understood from an analytical study of the properties of the eigenfunctions of the gravitational constraint, Eq. (2.7) [20]. An important result of various numerical investigations in loop quantum cosmology is that states which are semi-classical at late times follow an effective trajectory throughout their evolution [16]. The effective trajectory is derived using an effective Hamiltonian constraint obtained via geometrical methods of quantum mechanics [36, 37]. As with the expectation value of the volume observable, significant departures exist between the effective and the classical trajectories at the Planck scale, whereas at spacetime curvatures much smaller than the Planck value, the effective and classical trajectories coincide.

How is the question of whether or not a given state follows a classical or an effective trajectory posed within the framework of generalized quantum theory? A state ‘‘follows a trajectory’’ in minisuperspace when it exhibits a correlation between  $\phi$  and  $\nu$  given by that trajectory with a high probability. The fidelity of this correlation may be specified with varying degrees of precision. To accomplish this, we consider a coarse-graining of minisuperspace on a set of slices  $\{\phi_1, \phi_2, \dots, \phi_n\}$  by positive ranges of volume  $\{\Delta\nu_{i_k}, k = 1 \dots n\}$  on each slice  $\phi_k$ , so that  $\cup_{i_k} \Delta\nu_{i_k} = [0, \infty)$  on each slice  $k$ . To track a particular minisuperspace trajectory  $\gamma$ , choose the partitions  $\{\Delta\nu_{i_k}\}$  such that one range  $\Delta\nu_{\gamma_k}$  from each partition encloses  $\gamma$  at each  $\phi_k$ . To the degree of precision specified by this coarse-graining, a state  $|\Psi\rangle$  may be said to ‘‘follow’’  $\gamma$  with near certainty if the only branch wave function that is not essentially zero is

$$|\Psi_\gamma\rangle = U(\phi - \phi_o)P_{\Delta\nu_{\gamma_n}}^\nu(\phi_n)\cdots P_{\Delta\nu_{\gamma_2}}^\nu(\phi_2)P_{\Delta\nu_{\gamma_1}}^\nu(\phi_1)|\Psi\rangle \quad (4.8a)$$

$$\equiv U(\phi - \phi_o)C_\gamma|\Psi\rangle. \quad (4.8b)$$

If indeed the branch wave function for the complementary history  $\bar{\gamma}$  (‘‘does not follow  $\gamma$ ’’) vanishes,

$$|\Psi_{\bar{\gamma}}\rangle \equiv U(\phi - \phi_o)(\mathbb{1} - C_\gamma)|\Psi\rangle \approx 0, \quad (4.9)$$

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<sup>15</sup> Subsequently, these studies have been extended to different models in loop quantum cosmology. For a review of numerical studies of these models, see Ref. [19].

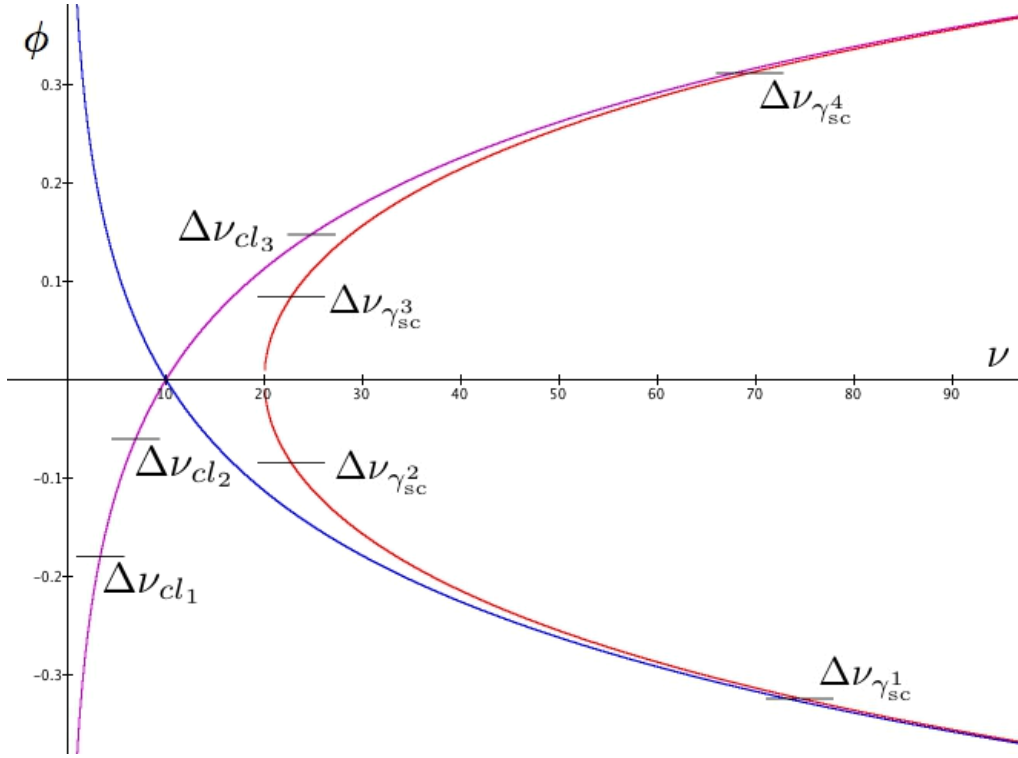


FIG. 2. This plot depicts coarse-graining by ranges of values of the volume at different values of the scalar field for two histories. The first is a coarse-grained history ( $\Delta\nu_{cl_1}, \Delta\nu_{cl_2}, \Delta\nu_{cl_3}$ ) describing an expanding universe peaked on an expanding classical trajectory. The second history ( $\Delta\nu_{\gamma_{sc}^1}, \Delta\nu_{\gamma_{sc}^2}, \dots$ ) describes a trajectory in loop quantum cosmology, characterized by a symmetric bounce, which is peaked on symmetrically related expanding and collapsing classical trajectories at large  $|\phi|$ . Such bouncing trajectories for states which are semiclassical at large  $|\phi|$  can be obtained from the effective Hamiltonian approach in LQC [16], which leads to modified versions of the standard Friedmann and Raychaudhuri equations.

then the partition  $(\gamma, \bar{\gamma})$  – i.e. (“follows  $\gamma$ ”, “does not follow  $\gamma$ ”) – decoheres, and  $|\Psi\rangle$  may be said to follow the trajectory  $\gamma$  with probability 1. Put another way, the state  $|\Psi\rangle$  may be said to exhibit the pattern of correlation between volume and scalar field specified by the trajectory  $\gamma$  with a high probability.

Even for a state *centered* on  $\gamma$ , whether or not  $|\Psi_{\bar{\gamma}}\rangle \approx 0$  will depend on the width of the intervals  $\Delta\nu_{\gamma_k}$  relative to the width of the state  $\Psi(\nu, \phi_k)$  at each  $\phi_k$ . Trying to specify the path too narrowly will lead to a partition which fails to decohere and must be further coarse-grained (by combining some of the intervals surrounding the  $\Delta\nu_{\gamma_k}$ ) to regain decoherence, and therefore the means to define probabilities consistently. Thus, as is usual in quantum theory, attempting to specify a path *too* precisely leads to a loss of predictability. For further discussion, see Ref. [12].

In loop quantum cosmology, as noted above, numerical simulations show that states  $|\Psi_{sc}\rangle$  which are semi-classical<sup>16</sup> at early times on a contracting branch are peaked on classical solutions at large volume and connect to the expanding branch smoothly through a “bounce” in the Planck regime. Such states are peaked on a trajectory which is a solution to the modified Friedmann and Raychaudhuri equations of LQC noted above for the entire evolution. If  $\gamma_{sc}$  is chosen to be such an effective trajectory in Fig. 2, and the widths  $\Delta\nu_{\gamma_k}$  chosen to be wider than the width of  $\Psi_{sc}(\nu, \phi_k)$  at each  $\phi_k$ ,<sup>17</sup> then essentially the only non-zero branch wave function will be the state  $|\Psi_{\gamma_{sc}}\rangle$  of Eq. (4.8), and  $|\Psi_{sc}\rangle$  follows the trajectory  $\gamma_{sc}$  with probability 1.

The origin of this behavior can also be analytically understood via the dynamical eigenstates  $e_k^{(s)}(\nu)$  [20]. *All* states in sLQC – whether semiclassical or not – approach a particular symmetric superposition of expanding and contracting Wheeler-DeWitt universes at large volume. If the state is chosen in such a way that it is peaked on a collapsing classical trajectory at large volume as  $\phi \rightarrow -\infty$  (say), then this state will be peaked on a corresponding expanding classical trajectory as  $\phi \rightarrow +\infty$ . (See Ref. [38] for further details.) The asymptotic behavior of the eigenfunctions dictates the

<sup>16</sup> There are various ways to define such states. A simple way is to consider a Gaussian state at large volume constructed using the eigenfunctions of the gravitational constraint operator  $\hat{\Theta}^{WdW}$  in the Wheeler-DeWitt theory analogous to Eq. (2.7). Another way is to compute the eigenfunctions of the  $\hat{\Theta}$  operator either numerically (as done eg. in Refs. [13, 14]) or analytically [20, 38], and use them to construct a semi-classical state.

<sup>17</sup> The dispersions of states in sLQC are discussed in detail in Refs. [39–41].

symmetric nature of the bounce.

### C. Singularity avoidance in loop quantum cosmology

We have already discussed the manner in which semi-classical states which are peaked on classical trajectories in a large macroscopic universe at early times bounce at a finite volume in LQC, connecting collapsing and expanding classical solutions. In this way, such states avoid the classical singularity at zero volume. As first shown analytically in Ref. [15], this behavior is generic: the expectation value of the volume is bounded below for *all* states (in the domain of the physical operators) in sLQC.

In this subsection we discuss the quantum bounce for generic states from the perspective of consistent histories. In Ref. [12], the problem of the singularity in a Wheeler-DeWitt quantized flat scalar Friedmann-Lemaître-Robertson-Walker cosmology was addressed through a study of the volume observable. There it was shown that for *any* choice of fixed volume  $V^*$  of the fiducial cell, the volume of the quantum universe would invariably fall below it with unit probability. The Wheeler-DeWitt universes are therefore inevitably singular in the sense that they assume arbitrarily small volume at some point in their history.<sup>18</sup>

In this analysis, the role of a proper understanding of quantum *history* proved crucial. As noted, the loop quantization of this model yields states which are a symmetric superpositions of expanding and contracting cosmologies at large volume. Ref. [12] therefore analyzed a superposition of expanding and contracting Wheeler-DeWitt universes with an eye toward the question of whether this superposition itself could in some sense be the *reason* for the bounce. Calculation of the probability that the universe is found at small volume for such a superposition reveals that at **any** given value  $\phi$  of the scalar field, the probability that the universe has volume less than  $V^*|\phi$  is in general between 0 and 1. The probability that the universe is *not* at arbitrarily small volume at  $\phi = -\infty$  or  $\phi = +\infty$  is therefore in general not 0. Naively this suggests the possibility that a superposition of expanding and contracting Wheeler-DeWitt universes has a non-zero probability of being at non-zero volume at *both*  $\phi = -\infty$  and  $\phi = +\infty$  i.e. that there is a non-zero probability of a quantum bounce.

A more careful consistent histories analysis showed that this naive possibility is not realized. The physical statement that the universe “bounces” is the statement that the volume of the universe is large at *both*  $\phi = -\infty$  and  $\phi = +\infty$ . A proper characterization of the bounce is therefore a statement about the volume of the universe at a *sequence* of values of  $\phi$  – a history. Ref. [12] shows that for generic initial states the histories corresponding to the alternatives {bounce, singular} decohere in the limit  $|\phi| \rightarrow \infty$  so that probabilities may be consistently assigned to them, and that the probability for the bouncing history  $p_{\text{bounce}} = 0$ : even superpositions of expanding and contracting Wheeler-DeWitt universe cannot bounce for any choice of state.<sup>19</sup>

We now show in detail that, in sharp contrast to the case of the Wheeler-DeWitt quantization, the probability that *generic* quantum states in sLQC are at small volume as  $\phi \rightarrow \pm\infty$  is zero. In fact, for any choice of volume  $V^*$ , we show in a sense to be made precise below that the probability the volume of the universe is larger than  $V^*$  is unity as  $|\phi| \rightarrow \infty$ : *all* states in this model achieve arbitrarily large volume in both limits. In this sense every state retains some flavor of the striking “bounce” of the narrowly peaked quasi-classical ones.

Next, we address histories of the volume with evolution in  $\phi$ . We show that for arbitrary quantum states the family of coarse-grained alternative histories {bounce, singular} decoheres, as in the Wheeler-DeWitt case. However, in contrast to the Wheeler-DeWitt case, the probability that the universe is singular in the scalar past or future is zero, and the probability that the universe bounces, unity. *All* states in sLQC bounce from arbitrarily large volume in the “past” ( $\phi \rightarrow -\infty$ ) to arbitrarily large volume in the “future” ( $\phi \rightarrow +\infty$ ).

As in the Wheeler-DeWitt theory, it is worth emphasizing the role of the limit  $\phi \rightarrow \pm\infty$ . One may expect that for wide classes of states such as localized states with certain peakedness properties decoherence obtains to a high degree of approximation at finite  $\phi$ . Nonetheless, it is only in the limit  $\phi \rightarrow \pm\infty$  that we are guaranteed decoherence, and hence a bounce with probability 1, for *all* states, and therefore – in that limit – that a bounce is a universal prediction of the theory.

**REMARK:** In Refs. [43] it is argued that the consistent histories approach to quantum theory is insufficient to address questions such as whether a quantum bounce takes place because histories involving ‘genuine’ quantum states are inconsistent when more than two moments of (scalar) time are involved, or in other words, that in this case only histories for semiclassical states decohere. We do not agree.

<sup>18</sup> Ref. [15] showed previously that the expectation value of the volume observable vanishes when  $\phi \rightarrow -\infty$  in an expanding branch, and the matter density always diverges in these Wheeler-DeWitt quantized models.

<sup>19</sup> See also Ref. [42] for early work related to this question.

The basis for this argument is a nice calculation (in the Wheeler-DeWitt quantization) along the lines of the one we perform in Ref. [12] and below of the interference between histories characterized by the alternatives {bounce, singular} in both the infinite scalar past and future, but with a third projection onto these alternatives at an arbitrary intermediate  $\phi$ . The authors calculate a representative off-diagonal (interference) matrix element of the decoherence functional and argue that it is zero if and only if the corresponding state is semiclassical in the sense that it is sharply peaked on a classical trajectory. Unfortunately, it is easy to generate a wide range of counter-examples to the claim that the calculated matrix element is zero only for semiclassical states. Therefore, it is simply not the case that it is only for semiclassical states that families of histories that study the bounce at more than two values of scalar time decohere. We do, however, expect the calculation the authors of Refs. [43] give of the decoherence functional itself for such three ‘time’ histories to be useful.

Moreover, it is probably worth a certain emphasis that there are many instances in which one would *not* expect decoherence of a family of histories, and indeed, would be suspicious of a quantum theory that purports to do so. Far from being a defect of the theory, it is a necessary requirement of a theory that reproduces the predictions (or absence thereof) of quantum theory without the introduction of e.g. non-local hidden variables. (For the purposes of this remark we include the de Broglie-Bohm formulation in this class of theories.) The two-slit experiment is the classic example: any theory which assigns observationally verifiable probabilities to the individual paths the electron follows when the physical setup is not such that which-path information is gathered is not quantum mechanics, and indeed will have a difficult time reproducing the predictions of quantum mechanics absent such non-local modifications. However, when there are additional degrees of freedom (such as a gas of air molecules in the two-slit apparatus) which might carry a record of which-path information, decoherence is to be expected and probabilities for individual paths may be assigned. In a similar way, in cosmological models with realistic inhomogeneous matter degrees of freedom (for example), one would expect decoherence of histories for bulk variables like the volume for most quantum states.

### 1. Probability for zero volume in sLQC

Following Ref. [12], one way to approach the question of whether a quantum universe is in some sense singular is to ask whether it achieves zero volume at any point in its evolution.<sup>20</sup> In Sec. IV A we showed how to calculate the probability that the volume falls in a range specified by  $\Delta\nu = [\nu_1, \nu_2]$ . To ask whether the volume of the universe is ever small we choose a reference volume  $\nu^*$  and partition the volume into the range  $\Delta\nu^* = [0, \nu^*]$  and its complement,  $\overline{\Delta\nu^*} = (\nu^*, \infty)$ . The universe then has small volume at scalar time  $\phi^*$  if  $|\nu| \in \Delta\nu^*$  at  $\phi^*$  and not if  $|\nu| \in \overline{\Delta\nu^*}$ . (See Fig. 3.) The class operators for these alternatives are simply the (Heisenberg) projections given by Eq. (4.1) with  $\Delta\nu = \Delta\nu^*, \overline{\Delta\nu^*}$  and corresponding branch wave functions, Eq. (4.3). The probabilities are given by Eq. (4.5). Thus

$$|\Psi_{\Delta\nu^*|\phi^*}(\phi)\rangle = U(\phi - \phi^*)P_{\Delta\nu^*}^\nu|\Psi(\phi^*)\rangle \quad (4.10a)$$

$$= U(\phi - \phi^*) \sum_{|\nu| \in \Delta\nu^*} |\nu\rangle \Psi(\nu, \phi^*) \quad (4.10b)$$

and

$$p_{\Delta\nu^*}(\phi) = \sum_{|\nu| \in \Delta\nu^*} |\Psi(\nu, \phi)|^2, \quad (4.11)$$

where since  $\phi^*$  is arbitrary we have set  $\phi^* = \phi$  in the expression for the probability.

In order to compute this probability, we will use some key properties of the symmetric eigenfunctions of the gravitational constraint operator  $\hat{\Theta}$  of Eq. (2.7), labelled by  $k \in (-\infty, \infty)$ :

$$\hat{\Theta}e_k^{(s)}(\nu) = \omega_k^2 e_k^{(s)}(\nu), \quad (4.12)$$

where  $\omega_k$  is related to  $p_\phi$  and  $k$  by  $p_\phi = \pm\hbar\omega_k$  and  $\omega_k = \sqrt{12\pi G}|k|$ , respectively. The symmetric eigenfunctions are real and satisfy  $e_{-k}^{(s)}(\nu) = e_k^{(s)}(\nu)$  and  $e_k^{(s)}(-\nu) = e_k^{(s)}(\nu)$  [14, 20]. A notable property of these eigenfunctions is that they decay exponentially to zero for volumes smaller than a cutoff value proportional to the value of  $\omega_k$ . This result was first obtained in numerical simulations [14], and subsequently derived analytically in Ref. [20], in which it was shown that the cutoff occurs along the lines  $|k| = |\nu|/2\lambda$ . Thus, one can consider  $|k| = |\nu|/2\lambda$  as an ultra-violet

<sup>20</sup> Since the matter density is, classically, the ratio of the (square of the) scalar momentum – a constant of the motion – and the (square of the) volume, one expects that zero volume corresponds to a diverging matter density in the quantum theory. This expectation is born out by the structure of the proofs of Refs. [15, 20] that the matter density is bounded above in sLQC.

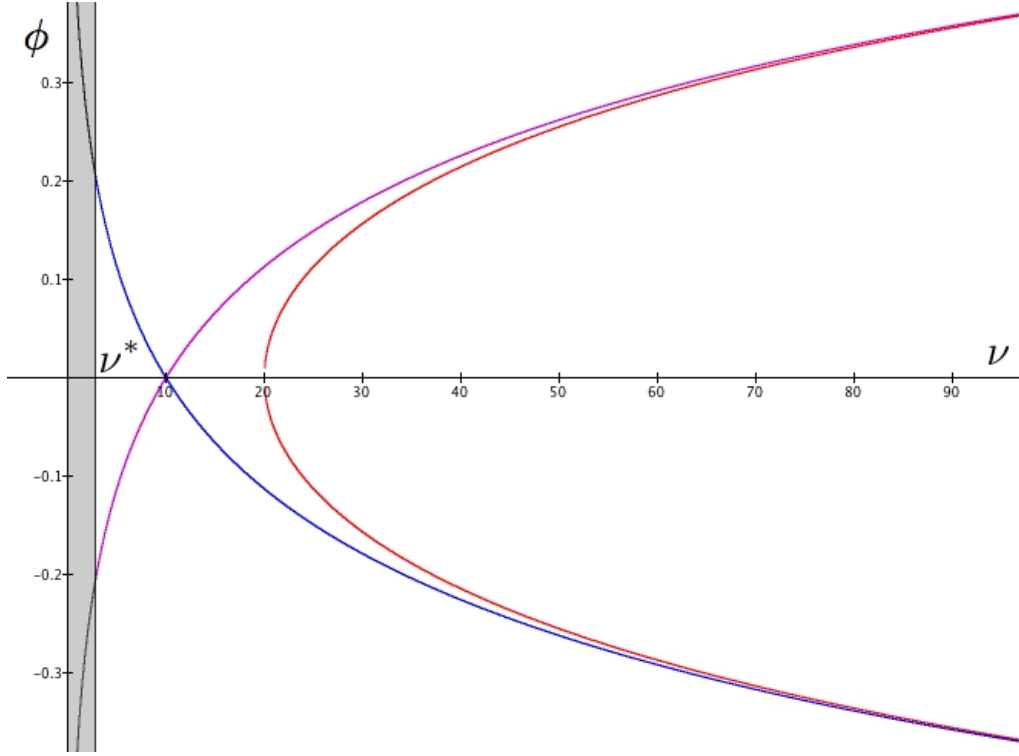


FIG. 3. Coarse-graining of minisuperspace suitable for studying the probability that the universe assumes large or small volume. Partition the volume  $\nu$  into the range  $\Delta\nu^* = [0, \nu^*]$  (the shaded region in the figure) and its complement  $\overline{\Delta\nu^*} = (\nu^*, \infty)$ . The quantum universe may be said to attain small volume if the probability for the branch wave function  $|\Psi_{\Delta\nu^*}(\phi)\rangle$  is near unity while that for  $|\Psi_{\overline{\Delta\nu^*}}(\phi)\rangle$  is near zero for arbitrary choices of  $\nu^*$ . Conversely, the universe may be said to attain arbitrarily large volume over some range of  $\phi$  if the probability for  $|\Psi_{\overline{\Delta\nu^*}}(\phi)\rangle$  is near unity for arbitrary choice of  $\nu^*$  over that range of  $\phi$ . Note that in sLQC, unlike in the Wheeler-DeWitt quantization of the same model, volume is discrete.

momentum space cutoff in sLQC. The exponential decay of the eigenfunctions coincides with the volume at which the energy density attains a maximum value and the universe bounces; the linear scaling of the cutoff with volume is what leads to a universal maximum matter density that is independent of the quantum state.

The symmetric eigenfunctions  $e_k^{(s)}(\nu)$  satisfy

$$\sum_{\nu=4\lambda n} e_k^{(s)}(\nu) e_{k'}^{(s)}(\nu) = \delta^{(s)}(k, k') \quad (4.13)$$

and

$$\int_{-\infty}^{+\infty} dk e_k^{(s)}(\nu) e_k^{(s)}(\nu') = \delta_{\nu, \nu'} . \quad (4.14)$$

Physical states  $\Psi$  in sLQC can be constructed using the eigenfunctions  $e_k^{(s)}(\nu)$ ,

$$\Psi(\nu, \phi) = \int_{-\infty}^{\infty} dk \tilde{\Psi}(k) e_k^{(s)}(\nu) e^{i\omega_k \phi}, \quad (4.15)$$

where we have set  $\phi_o = 0$  for convenience. As a consequence of the ultra-violet cutoff on the eigenfunctions,

$$\Psi(\nu, \phi) \cong \int_{-\nu/2\lambda}^{\nu/2\lambda} dk \quad (4.16)$$

Note in Eq. (4.10) that  $\nu$  is bounded by  $\nu^*$ . Further, the  $e_k^{(s)}(\nu)$  are well-behaved functions of  $k$  for all values of  $\nu$ . For any fixed value of  $\nu$ , their rate of oscillation in  $k$  is fixed by  $\nu$ .<sup>21</sup>

<sup>21</sup> In fact, this rate is approximately constant in  $\nu$ , as can be seen by observing that the  $e_k^{(s)}(\nu = 4\lambda n)$  have  $2n - 1$  nodes in the full



Thus, for large  $|\phi|$  – meaning at a minimum  $\omega_k|\phi| \gg 1$  – rapid oscillation of the factor  $\exp(i\omega_k\phi)$  will according to the Riemann-Lebesgue lemma eventually suppress the integral, and we find

$$\lim_{\substack{|\phi| \rightarrow \infty \\ \nu \text{ fixed}}} \Psi(\nu, \phi) = 0 \quad (4.17)$$

for any fixed value of  $\nu \leq \nu^*$ . In other words, for any fixed  $\nu$ ,  $|\phi|$  eventually becomes large enough to suppress the state, driving the state to larger volume as  $|\phi|$  increases. Thus  $\Psi(\nu, \phi)$  for  $\nu < \nu^*$  will always be suppressed for large enough  $|\phi|$  for arbitrary states in the theory.

On the other hand, for the complementary branch wave function  $|\Psi_{\overline{\Delta\nu^*}}(\phi)\rangle$  corresponding to large volume universes,  $\nu$  can be arbitrarily large. As  $\nu$  becomes larger a wider range of  $k$ 's can contribute nontrivially to the integral in Eq. (4.16). For  $\nu \gg 2\lambda|k|$  the rate of oscillation of the  $e_k^{(s)}(\nu)$  with  $k$  is fixed by the asymptotic limit of the symmetric eigenfunctions, increasing in proportion with  $\ln|\nu|$  [20]. Again, for any fixed  $\nu$  the state is suppressed as  $|\phi| \rightarrow \infty$ , so that the region of support of this branch wave function in the  $(\nu, \phi)$  plane must have  $\ln|\nu|$  increasing in proportion with  $|\phi|$  – just the behavior of Wheeler-DeWitt quantized states.

We find, therefore, that since  $\Psi(\nu, \phi)$  at any fixed  $\nu$  vanishes in the limit  $|\phi| \rightarrow \infty$ ,

$$\lim_{\phi^* \rightarrow -\infty} |\Psi_{\Delta\nu^*}(\phi)\rangle = 0 \quad \text{and} \quad \lim_{\phi^* \rightarrow +\infty} |\Psi_{\Delta\nu^*}(\phi)\rangle = 0. \quad (4.18)$$

As the intervals  $\Delta\nu^*$  and  $\overline{\Delta\nu^*}$  are complementary, this implies

$$\lim_{\phi^* \rightarrow -\infty} |\Psi_{\overline{\Delta\nu^*}}(\phi)\rangle = |\Psi(\phi)\rangle \quad \text{and} \quad \lim_{\phi^* \rightarrow +\infty} |\Psi_{\overline{\Delta\nu^*}}(\phi)\rangle = |\Psi(\phi)\rangle. \quad (4.19)$$

As a consequence, one finds for the probabilities

$$\lim_{\phi \rightarrow -\infty} p_{\Delta\nu^*}(\phi) = 0 \quad \lim_{\phi \rightarrow +\infty} p_{\Delta\nu^*}(\phi) = 0 \quad (4.20a)$$

$$\lim_{\phi \rightarrow -\infty} p_{\overline{\Delta\nu^*}}(\phi) = 1 \quad \lim_{\phi \rightarrow +\infty} p_{\overline{\Delta\nu^*}}(\phi) = 1. \quad (4.20b)$$

We can see already from this that loop quantum states invariably bounce: the probability the universe is found at small volume as  $|\phi| \rightarrow \infty$  is zero, regardless of the state.

Eqs. (4.20) say that *all* states in sLQC achieve arbitrarily large volume in each of the limits  $\phi \rightarrow -\infty$ ,  $\phi \rightarrow +\infty$ . States in sLQC don't merely refrain from becoming singular. They inevitably grow to large volume, no matter how non-classical the state. (This result complements that of Ref. [15] that the expectation value of the volume becomes infinite in those limits for all states.) In the next section we will use this to show that the family of histories describing a quantum bounce decoheres, and that indeed all states in the theory bounce *from* arbitrarily large volume to arbitrarily large volume.

Finally, we observe that as the state  $|\Psi\rangle$  was arbitrary and

$$P_{\Delta\nu^*}^\nu(\phi) + P_{\overline{\Delta\nu^*}}^\nu(\phi) = \mathbb{1}, \quad (4.21)$$

Eqs. (4.18-4.19) may be conveniently expressed in terms of volume projections as

$$\lim_{\phi \rightarrow -\infty} P_{\Delta\nu^*}^\nu(\phi) = 0 \quad \lim_{\phi \rightarrow +\infty} P_{\Delta\nu^*}^\nu(\phi) = 0 \quad (4.22a)$$

$$\lim_{\phi \rightarrow -\infty} P_{\overline{\Delta\nu^*}}^\nu(\phi) = \mathbb{1} \quad \lim_{\phi \rightarrow +\infty} P_{\overline{\Delta\nu^*}}^\nu(\phi) = \mathbb{1} \quad (4.22b)$$

on all states in the theory.<sup>22</sup>

Note we have not so far addressed the question of whether the universe *ever* assumes volumes in  $\Delta\nu^*$  with non-zero probability. In fact, examination of Eq. (4.11) should be sufficient to show that so long as  $\nu^* > 0$ , there always exist states for which it will. (See, for example, Fig. 1.) However, this is *not* sufficient to show that the universe might become singular in sLQC. Recall that the eigenfunctions  $e_k^{(s)}(\nu)$  decay exponentially for volumes smaller than

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range of oscillation  $|k| \lesssim 2n$  [20]. These functions therefore exhibit precisely  $n$  full oscillations over that range, giving a mean oscillation frequency  $n/\Delta k \cong n/4n = 1/4$ , independent of the volume  $n$ , and in particular exhibit only a finite number of oscillations in any fixed range of  $k$ . The oscillations in  $k$  for any given  $n$  do tend to become more rapid for smaller  $|k|$ , and in the regime  $|\nu| \gg \lambda|k|$  the angular frequency of oscillation in  $|k|$  grows as  $\ln|\nu/\lambda|$  i.e. grows slowly with  $\nu$ .

<sup>22</sup> Indeed, one may carry out the argument made above in terms of  $\Psi(\nu, \phi)$  directly at the level of the Heisenberg projections by expanding the propagators in the projections in symmetric eigenkets  $|k^{(s)}\rangle$  and using  $e_k^{(s)}(\nu) = \langle \nu|k^{(s)}\rangle$ . One arrives in just the same way at Eqs. (4.22), but the formulæ getting there are somewhat messier simply because one is dealing with operators rather than states.

$|\nu| = 2\lambda|k|$  and vanish at  $\nu = 0$ , and thus, from Eq. (4.11) the probability that *any* state in sLQC assumes precisely zero volume is **zero**,

$$p_{\nu=0}(\phi) = 0. \quad (4.23)$$

This result stands in sharp contrast with the situation in Wheeler-DeWitt theory, where the rapid oscillations in the eigenfunctions as  $\nu \rightarrow 0$  inevitably ‘draw in’ Wheeler-DeWitt states to zero volume and infinite density, and the probability for a singularity turns out to be non-vanishing – and indeed, is unity for all states in the limits  $|\phi| \rightarrow \infty$  [12].

## 2. Quantum bounce

It is tempting to conclude that Eqs. (4.20) are sufficient to demonstrate that all states in sLQC “bounce” *from* large volume as  $\phi \rightarrow -\infty$  *to* large volume as  $\phi \rightarrow +\infty$ . However, as emphasized in Refs. [10–12], statements concerning a quantum bounce are inherently assertions concerning the volume at a *sequence* of values of  $\phi$ , and, as in the two-slit experiment, it is in precisely such situations that decoherence becomes critical in order to arrive at consistent quantum predictions. Indeed, in Ref. [12] it is shown that consideration of the single- $\phi$  volume probability  $p_{\Delta\nu^*}(\phi)$  alone for Wheeler-DeWitt states which are superpositions of expanding and contracting universes may lead one to the incorrect conclusion that a bounce is possible in that model. However, a proper analysis of the histories describing a quantum bounce shows that this naive conclusion based on single- $\phi$  probabilities is misleading, and that indeed the probability for a bounce is zero.

How, then, is a “bounce” characterized within quantum theory? The assertion that a universe bounces is the statement that the universe assumes large volume at both “early” ( $\phi \rightarrow -\infty$ ) and “late” ( $\phi \rightarrow +\infty$ ) values of  $\phi$ . A (highly coarse-grained) description of a bounce may therefore be obtained by making a choice of  $\phi$ -slices  $\phi_1$  and  $\phi_2$  and volume partitions  $(\Delta\nu_1^*, \overline{\Delta\nu_1^*})$  and  $(\Delta\nu_2^*, \overline{\Delta\nu_2^*})$  on them. The class operator for the history in which the universe “bounces” between  $\phi_1$  and  $\phi_2$  – i.e. is at large volume at both  $\phi_1$  and  $\phi_2$  – is then

$$C_{\text{bounce}}(\phi_1, \phi_2) = C_{\overline{\Delta\nu_1^*}; \overline{\Delta\nu_2^*}} = P_{\overline{\Delta\nu_1^*}}^\nu(\phi_1) P_{\overline{\Delta\nu_2^*}}^\nu(\phi_2). \quad (4.24)$$

On the other hand, the class operator for the alternative history that the universe is found at small volume at either or both of  $\phi_1, \phi_2$  is

$$C_{\text{sing}}(\phi_1, \phi_2) = \mathbb{1} - C_{\text{bounce}}(\phi_1, \phi_2) \quad (4.25a)$$

$$= C_{\Delta\nu_1^*; \Delta\nu_2^*} + C_{\Delta\nu_1^*; \overline{\Delta\nu_2^*}} + C_{\overline{\Delta\nu_1^*}; \Delta\nu_2^*}. \quad (4.25b)$$

It is clear from Eq. (4.25b) that  $C_{\text{sing}}(\phi_1, \phi_2)$  encodes the various ways the universe can be at small volume at  $\phi_1$  and/or  $\phi_2$ .

We now demonstrate that the only branch wave function which is non-vanishing in the limits  $\phi_1 \rightarrow -\infty$  and  $\phi_2 \rightarrow \infty$  is the one corresponding to the bounce.

Using Eqs. (4.22), one finds,

$$\begin{aligned} \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} P_{\overline{\Delta\nu_2^*}}^\nu(\phi_2) P_{\overline{\Delta\nu_1^*}}^\nu(\phi_1) |\Psi\rangle &= \lim_{\phi_2 \rightarrow +\infty} P_{\overline{\Delta\nu_2^*}}^\nu(\phi_2) \cdot 0 \\ &= 0; \end{aligned} \quad (4.26a)$$

$$\begin{aligned} \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} P_{\overline{\Delta\nu_2^*}}^\nu(\phi_2) P_{\Delta\nu_1^*}^\nu(\phi_1) |\Psi\rangle &= \lim_{\phi_2 \rightarrow +\infty} P_{\overline{\Delta\nu_2^*}}^\nu(\phi_2) \cdot 0 \\ &= 0; \end{aligned} \quad (4.26b)$$

$$\begin{aligned} \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} P_{\Delta\nu_2^*}^\nu(\phi_2) P_{\overline{\Delta\nu_1^*}}^\nu(\phi_1) |\Psi\rangle &= \lim_{\phi_2 \rightarrow +\infty} P_{\Delta\nu_2^*}^\nu(\phi_2) |\Psi\rangle \\ &= 0; \end{aligned} \quad (4.26c)$$

$$\begin{aligned} \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} P_{\Delta\nu_2^*}^\nu(\phi_2) P_{\Delta\nu_1^*}^\nu(\phi_1) |\Psi\rangle &= \lim_{\phi_2 \rightarrow +\infty} P_{\Delta\nu_2^*}^\nu(\phi_2) |\Psi\rangle \\ &= |\Psi\rangle. \end{aligned} \quad (4.26d)$$

Using Eqs. (4.25) and (4.26), we find that the branch wave function for an sLQC quantum universe to encounter the singularity vanishes,

$$|\Psi_{\text{sing}}(\phi)\rangle = U(\phi - \phi_o) \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} C_{\text{sing}}^\dagger(\phi_1, \phi_2) |\Psi\rangle = 0. \quad (4.27)$$

On the other hand, the branch wave function for the history corresponding to a bounce in sLQC is

$$|\Psi_{\text{bounce}}(\phi)\rangle = U(\phi - \phi_o) \lim_{\substack{\phi_1 \rightarrow -\infty \\ \phi_2 \rightarrow +\infty}} C_{\text{bounce}}^\dagger(\phi_1, \phi_2) |\Psi\rangle = |\Psi(\phi)\rangle. \quad (4.28)$$

Thus, the family of histories (bounce, singular) in sLQC decoheres,

$$d(\text{bounce}, \text{sing}) = \langle \Psi_{\text{sing}} | \Psi_{\text{bounce}} \rangle = 0, \quad (4.29)$$

and a bounce is predicted with probability 1,

$$d(\text{bounce}, \text{bounce}) = \langle \Psi_{\text{bounce}} | \Psi_{\text{bounce}} \rangle \quad (4.30a)$$

$$= \langle \Psi | \Psi \rangle \quad (4.30b)$$

$$= 1. \quad (4.30c)$$

Note that in this analysis, no assumption has been made on the the choice of state  $|\Psi\rangle$ , and thus this result holds for all states in the theory. Thus, we have shown in the consistent histories approach that the bounce is a universal feature of all states in sLQC.

We finally note that the existence of bounce at a non-zero volume is tied to the existence of an upper bound on the expectation values of the energy density operator of the scalar field:  $\langle \hat{\rho} | \phi \rangle = \langle p_\phi \rangle^2 / 2 \langle V | \phi \rangle^2$ . For more discussion, see Refs. [15, 20]. Unlike the Wheeler-DeWitt theory, in sLQC the spacetime curvature thus never diverges during the evolution.

## V. DISCUSSION

The essence of quantum superposition is that independent reality cannot be assigned to the elements of that superposition unless interference among them vanishes. In the language of consistent or decoherent histories “generalized” quantum mechanics, physical probabilities cannot be inferred from the transition amplitudes unless the corresponding family of histories is consistent, as emphasized in [10, 11]. For a closed quantum system, therefore, it is essential to have available an internally consistent measure of quantum interference in order to be able to arrive at meaningful quantum predictions.

In a closed system such as the universe as a whole, an objective measure of quantum interference is provided by the system’s decoherence functional. Construction of the decoherence functional is therefore an essential component of any quantum theory of gravity in which one intends to apply the theory to the whole universe, as in quantum cosmology.

The point of view of the decoherent or consistent histories framework as applied here<sup>23</sup> may be sufficiently unfamiliar to some that it is important to emphasize that, in almost every respect, it is simply “quantum mechanics as usual”. The single – but crucial – new concept is the addition of the decoherence functional to the technical and interpretational apparatus of quantum theory. The decoherence functional is essentially an extension of the concept of quantum state<sup>24</sup> to provide an objective, internally consistent measure of quantum interference, thus replacing the vague criterion of measurement by external classical observers with a rigorously formulated measure that reproduces the results of classical measurement theory when it is applicable, but extends it to situations when it is manifestly, and profoundly, **not** applicable – crucially, to closed systems for which the notion of external measurements is clearly meaningless. Simple examples of the necessity for such an extension are easy to come by in quantum gravity. For example, how is one to assign probabilities to the quantum density fluctuations that putatively lead to the large scale cosmological structure we observe today when no classical systems existed to “observe” them?

<sup>23</sup> It is to be noted that the broad framework of generalized quantum theory [4, 44], quantum measure theory [21] and related generalizations does indeed allow for significant generalizations beyond the standard quantum formalism, and indeed, allowing this freedom – while retaining characteristic features of quantum theory such as superposition and interference – was one of the theory’s originating motivations. Agreement with standard quantum theory in familiar regimes does however constrain that freedom considerably.

<sup>24</sup> Especially as viewed from the point of view of the algebraic formulation of quantum theory [45].

The focus on “histories” may also give the framework an unfamiliar feel. However, it is precisely for making predictions concerning *sequences* of quantum outcomes that ordinary measurement-based formulations of quantum mechanics have no answers, no predictions, for closed quantum systems. Yet, patterns of correlations between observable quantities – paths, or “histories” of those observables – are precisely the kind of quantities in which one is principally interested in cosmology. The decoherent histories framework provides a consistent and rigorous foundation for calculating quantum probabilities, whether for single quantum events, or sequences thereof, in terms of quantum amplitudes given by the system’s state and physical inner product. In a properly formulated generalized quantum theory of cosmology, the physical meaning of the “wave function of the universe” is unambiguous; there is no need to rely on heuristic arguments [46] to extract physical predictions [4, 6, 12]. The methodology for quantum prediction is precise and clear.

We noted in the introduction that the interpretation of the meaning of probability in quantum theory quite generally – not only in the quantum mechanics of closed systems – remains controversial. Notwithstanding, we are not reluctant to write down expressions for quantum probabilities such as those found in Sec. IV with the expectation that their interpretation is as clear in context as it ever is in quantum mechanics.<sup>25</sup> In recognition nonetheless of the special status of closed systems, we focus particular attention on quantum predictions which are certain, those for which the probabilities are 1 or 0 – or close to it. For such predictions, the meaning of the probabilities is unambiguous: the universe either will (or will not) exhibit the property (or history) in question. If observation contradicts this prediction, the theory is simply incorrect. (Hartle [4, 27] and Sorkin [21] in particular have emphasized the special role played by such certain predictions in the quantum theory of closed systems.)

In an exactly solvable model of loop quantum cosmology (sLQC) [15], for example, we have shown in a quantum mechanically consistent way that *all* states in the theory – whether peaked on classical trajectories at large volume or not – “bounce” in the sense that the universe must have a large volume in the limit of large  $|\phi|$ . In stark contrast to the corresponding classical model, and also to its older Wheeler-DeWitt-type quantization, these quantum universes are not drawn into an infinite density singularity, and indeed, cannot be.

The role of the large- $|\phi|$  limit in our predictions is worth comment. As noted in passing in Sec. IV C, for a given state  $|\Psi\rangle$  it is certainly possible that the histories described by  $C_{\text{bounce}}(\phi_1, \phi_2)$  and  $C_{\text{sing}}(\phi_1, \phi_2)$  will decohere to a high degree of approximation at finite  $\phi_{1,2}$ . Indeed, wide classes of states such as states which are semi-classical at late times, i.e. peaked on classical trajectories at large volume, will do so. However, it is only in the limit that  $|\phi|$  becomes large that *all* states, no matter how “quantum” (with no peakedness properties), are guaranteed to decohere and exhibit a quantum bounce. This is the role of the limit: it is in this limit we arrive at a *universal*, and certain, prediction of sLQC – including both decoherence and unit probability – valid for all states. The bounce is a robust, universal prediction of sLQC.<sup>26</sup>

It is of course the case that it was rigorously shown in Ref. [15, 20] that the matter density remains bounded above for all states in the theory (in the domain of the relevant physical operators.) Here, we complement this result and add a little more. First, as emphasized in Refs. [10, 11], the physical question of whether a quantum universe exhibits a “bounce” is fundamentally a prediction about the correlation of the volume with (at least) two different values of the scalar field – at two different emergent ‘times’. It is precisely for such predictions that the question of the decoherence of the corresponding histories becomes critical. Here we have shown that the coarse-grained histories describing a bounce do indeed decohere and predict a bounce with probability 1.

This actually goes further than the assertion that the matter density remains bounded above. In fact, we showed that for arbitrary choice of volume  $\nu^*$ , the branch wave function  $|\Psi_{\Delta\nu^*}\rangle$  describing a universe with volume  $|\nu|$  in  $\Delta\nu^* = [0, \nu^*]$  becomes 0 as  $|\phi| \rightarrow \infty$ , complementing the result of Ref. [15] that the expectation value of the volume becomes infinite in those limits for all states. The fact that  $\nu^*$  is completely arbitrary implies that *all* quantum states in sLQC will eventually end up at large volume, and therefore, be described by a superposition of Wheeler-DeWitt quantum states in that regime [20, 38]. (Of course, that does not mean all states behave quasiclassically if the state is highly quantum. It only means that sLQC passes over to the Wheeler-DeWitt quantum theory at large volume, and that that limit obtains for every loop quantum state for some range of large  $|\phi|$ . For a detailed analysis of the precise sense in which sLQC approximates the Wheeler-DeWitt theory, see Ref. [15].) This rules out, for example, the possibility of a highly quantum state that lingers indefinitely near the “big bang” (i.e. at large matter density).

Consistent with the prediction that all states “bounce”, as noted all states in sLQC look like a particular symmetric superposition of expanding and collapsing Wheeler-DeWitt universes at large volume [20]. While this is certainly a *necessary* condition for a theory in which a bounce is a generic feature, one may be led to inquire whether the presence of this superposition is in some sense the *reason* for the bounce. The answer is definitely “NO”. In fact, it was shown in Ref. [10–12] that a superposition of expanding and contracting universes in the Wheeler-DeWitt quantization of

<sup>25</sup> We write down and use probabilities for predictive purposes all the time in physics even when there is no realistic expectation of access to more than one copy of a system. In spite of the foundational challenges – which we fully recognize – we trust this simple observation is not controversial.

<sup>26</sup> The arguments of Refs. [43] notwithstanding; see our remarks in Sec. IV C above.

this same physical model does not, and indeed *cannot* bounce: all states are sucked in to the singularity at large  $|\phi|$ . If a physical reason for the bounce is to be sought, it is in the “quantum repulsion” generated at small volume in loop quantum gravity,<sup>27</sup> and manifested in this model in the ultraviolet cutoff in the dynamical eigenfunctions [20], not in the superposition of large expanding and contracting classical universes.

We have so far exhibited the construction of a generalized decoherent-histories quantum theory in two mathematically complete quantizations of cosmological models, sLQC in this analysis, and the corresponding Wheeler-DeWitt model in an earlier work [10–12], demonstrating how these theories may be used to arrive at quantum mechanically consistent physical predictions. In both of these models, the presence of an internal time, a monotonic physical clock provided by the scalar field in the canonical quantization of the models, simplified the construction of the generalized quantum theories through the structural analogy with ordinary quantum particle mechanics. Is this feature essential to the construction of a generalized quantum theory? The answer is no. A path integral formulation for a closed Bianchi model was studied in detail in Ref. [6] and references cited therein, and upon which much of the present work is based. More rigorously, we have now constructed along the same lines the generalized quantum theory for a path-integral (spin foam) quantization [30, 31, 48] of the same physical model (flat scalar FRW) as studied here [32]. This will again be employed to study the same physical questions examined here, in particular, the quantum behavior near the classical singularity. This example shows that the presence of an internal time in the model, while convenient, is not essential to the formulation of its class operators, branch wave functions, and decoherence functional.<sup>28</sup> Taken together, these examples lay the foundation for the construction and application of generalized quantum theories – the quantum theory of closed physical systems – in quantum cosmology and quantum gravity more broadly.

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<sup>27</sup> One way to understand this quantum gravitational repulsion is via the effective dynamics derived from the effective Hamiltonian constraint. Modifications to the Friedmann and Raychaudhuri equations in effective LQC are such that they correspond to a repulsive gravity effect at small volumes, causing the Hubble rate and the spacetime curvature to be bounded [47].

<sup>28</sup> The most significant difference between canonical and path integral formulations of generalized quantum theories concerns the manner in which quantum alternatives are specified. In canonical constructions one is largely limited to histories that can be specified by superpositions of chains of projections onto ranges of physical observables. In theories defined by a sum-over-histories, alternatives can be specified by partitioning the paths that contribute to the sum according to whether the paths exhibit some particular property, and branch wave functions by restricting to integrals (sums) over the appropriate class of paths. This can lead to interesting differences between canonical and path integral formulations, even in ordinary non-relativistic quantum mechanics.

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