Initial conditions for $R+\epsilon R^2$ cosmology

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A pure gravity cosmology based on the $R+\epsilon R^2$ Lagrangian is known to exhibit inflation for a wide range of initial conditions. In this paper we use the wave function from quantum cosmology to describe this inflation as a chaotic inflationary phase immediately following the quantum creation of the Universe. We evaluate, compare, and discuss the distributions over initial conditions that are fixed by the two boundary-condition proposals of Hartle and Hawking ("no boundary") and Vilenkin ("tunneling from nothing"). We find that among all classical inflationary trajectories that begin on the classical-quantum boundary, those that lead to an inflation of at least 70 e-foldings make up a fraction of $\sim\exp(-10^{12})$ in the former case and $\sim 1-\exp(-8\times 10^{10})$ in the latter. Thus, in the simplest interpretation, the observable Universe would be the outcome of a rare event for the first boundary-condition proposal and a typical event for the second.

I. INTRODUCTION

Inflation has become standard in modern cosmology.[1] It can explain basic features of our present Universe and can occur rather generally in particle-physics models.[2]

The question that naturally follows the development of inflation is to ask what came before, a question that has been embedded in a broader context by the advent of chaotic inflation.[3,2] We shall understand by chaotic inflation that phase of the inflationary expansion during which some scalar field relaxes to the minimum of its potential, with the provision that (i) this relaxation need not be accompanied by any kind of phase transition; (ii) the scalar field potential can be of classical origin as well as due to quantum corrections; (iii) the preinflationary phase need not be a hot, radiation-dominated Robertson-Walker universe (as all models of old and new inflation have assumed, explicitly or implicitly); and (iv) the field's initial conditions have been assigned in some "random way."

As analysis has shown,[2] the typical initial conditions for chaotic inflation are Planck scale, so we might expect quantum gravity to come directly to play. In fact, as we argue hereafter, the idea of chaotic inflation can be joined with the older concept of quantum creation of the Universe.[4]

Two things are done in this paper: (i) we suggest a physical context, in which semiclassical wave functions (fixed by boundary conditions in quantum cosmology) can be used to compute the distribution of initial conditions for the classical inflationary expansion; and (ii) we apply this method to an inflationary model based on higher-derivative gravity where, in particular, we compare predictions resulting from different proposals for the boundary conditions.

The model we study is $R+\epsilon R^2$ gravity.[5–9] We provide the classical details necessary to our present work in Sec. II. One can think of this model as the relevant, dominant part of a renormalizable [and so far (perturbatively) nonunitary] higher-derivative gravity.[10] Perhaps a more promising context is that of an effective theory that describes the first short-distance corrections to general relativity, for example, the low-energy limit of superstrings.[11] Thus, we have an inflationary model without introducing an additional inflaton field especially for the purpose. This point lends the model some advantage over others.

The wave function for higher-derivative gravity with Hartle and Hawking's boundary condition has been studied analytically by Hawking and Luttrell and by Horowitz,[6] and numerically by Hawking and Wu.[7] They have shown that the wave function is oscillatory in a certain regime of superspace, corresponding to Lorentzian spacetime. We extend their discussion of the Hartle-Hawking boundary condition, compute the wave function in more detail, compare it to the wave function that satisfies Vilenkin's boundary condition,[12] and make contact with the scenario of chaotic inflation. We have earlier reported some preliminary results in the discussion following our own analysis of the classical model.[8]

If (in this model or in any other) we follow a classical trajectory backward in time to when the curvature approaches values $\sim l_{\rm Pl}^{-2}$, this trajectory will hit a highly quantum region. Classical equations of motion cannot be used any more. In fact, as we shall see, there remains a

substantial range of initial curvatures ($\epsilon^{-1} < R_i < l_{\rm Pl}^{-2}$) in this model for which quantum creation of the inflationary Universe may take place and classical inflationary trajectories may start. This range is large because ϵ is constrained to be large, $\epsilon \approx 10^{11} l_{\rm Pl}^2$, by a tiny observational bound on the anisotropy of the microwave background.

As shown in the literature,[5–9] the classical scenario of $R+\epsilon R^2$ cosmology is sensible and attractive within this parameter regime—it can give more inflation than minimally required and then lead smoothly to reheating of the Universe and initiation of a Friedmann phase. It is plausible (especially at the lower acceptable curvatures), though by no means necessary, that still higher-order correction terms to the Lagrangian would not change these results. In this paper we assume that whatever the true quantum theory of the world is, it should be well approximated in this regime by the quantum mechanics of the $R+\epsilon R^2$ model. Since we are interested in the phase when the Universe emerges as a classical object, the semiclassical limit of the quantum theory is sufficient. Hence, we do not worry about the (un)calculability of loop corrections. We do not consider initial curvatures below ϵ^{-1} because we confine ourselves to analysis of the inflationary phase which does not extend to such low curvatures. Moreover, for such low curvatures, the ϵR^2 term will not be important and the evolution of the Universe will be strongly affected by other terms (e.g., matter fields) in the Lagrangian, terms that we have not taken into account in our present calculation. We reject consideration of curvatures above $l_{\rm Pl}^{-2}$ because our quantum model is presumably not the fundamental theory. We take the Planck scale to be the scale above which a full theory must come into account. That is, we limit our attention and our analysis to the initial edge of the region of semiclassical inflationary trajectories.

Such an approach, as restricted as it is, still has the power to yield important information. It also might survive modifications that the development of a more fundamental theory would bring. There are, however, two obvious shortcomings of this work. First, in this truncated use of quantum cosmology we have dodged the problem of interpretation. In particular, we have not addressed the analog of the measurement problem from quantum mechanics. Second, a more technical weakness of our work is that, in order to carry out explicit calculation, we have resorted to calculating the wave function for Robertson-Walker models only. We reduce superspace to minisuperspace: all that is "chaotic" now in this inflation is the stochastic choice of the initial values of the scale factor, the homogeneous curvature, and their initial time derivatives. These four initial values for subsequent classical evolution will be determined by the wave function. We have ignored any distribution over inhomogeneity, anisotropy, etc. We hope that both of these weaknesses will be amended by further development.

In Sec. II we summarize the classical behavior of the $R+\epsilon R^2$ model and derive the Wheeler-DeWitt equation appropriate to the two homogeneous and isotropic variables of superspace. We spell out two competing boundary-condition proposals and explore their connection with quantum creation in Sec. III. In Sec. IV we then implement both proposals for the boundary conditions and fix their respective wave functions for our model. We finally explore consequences of these wave functions in their regime of validity and state our conclusions in Sec. V. An appendix is provided to support material in Sec. II.

II. ACTION AND THE WHEELER-DeWITT EQUATION

We study a model governed by the action

$$S=\frac{1}{16\pi G}\int d^4x\sqrt{-g}\,(R+\epsilon R^2) + \frac{1}{8\pi G}\int d^3x\sqrt{h}\,K(1+2\epsilon R) \tag{2.1}$$

that represents Einstein gravity with an additional quadratic gravitational correction term. Here R is the scalar curvature, g is the determinant of the spacetime four-metric, h is the determinant of the induced spatial three-metric on the boundary, and K is the trace of the extrinsic curvature. Our sign conventions are those of Ref. 13 and we choose units in which $\hbar=c=1$ and $G=l_{\rm Pl}^2$. The parameter ϵ will then have dimensions of l^2. The boundary term [displayed as the surface integral in Eq. (2.1)] is the expression needed to cancel out arbitrary variations of metric derivatives at the boundaries of the four-dimensional action integral. It is thus dependent on the form of the local Lagrangian density and in the Appendix we briefly provide details of its derivation.

For tractability we focus attention on a cosmological model described by the Robertson-Walker metric

$$ds^2=-dt^2+a^2(t)\left[\frac{dr^2}{1-kr^2}+r^2(d\theta^2+\sin^2\theta\,d\phi^2)\right], \tag{2.2}$$

where $a(t)$ is the scale factor, k is the sign of the spatial curvature, R is given by $R=12H^2+6\dot{H}+6k/a^2$ where H is the Hubble parameter $H=\dot{a}/a$, and the extrinsic curvature is $K=-3H$.

The present authors[8] and others[5,6,7,9] have analyzed the classical behavior of such a model and we summarize it here. The R^2 term drives inflation. Any initial matter content will be rapidly red-shifted and the evolution goes over to a pure gravity near–de Sitter expansion. The equation of motion can be written

$$\ddot{H}+3\dot{H}H+\frac{H}{12\epsilon}=\frac{\dot{H}^2}{2H}+\frac{kH}{a}\left[1-\frac{1}{12\epsilon H^2}-\frac{k}{2H^2a^2}\right]. \tag{2.3}$$

For a wide range of initial data, there will be a "linear" phase during which the terms on the right-hand side of Eq. (2.3) are neglectable and we have the solution

$$H(t)=H_i-\frac{t}{36\epsilon}. \tag{2.4}$$

This solution will be very nearly de Sitter if the linear decay is slow—which is the same requirement as for the

solution's validity. The linear decay of the Hubble parameter self-regulates its own inflationary epoch. The near–de Sitter behavior ends after $t_e \approx 36\epsilon H_i$ and the Universe then goes into an oscillation phase in which the scale factor increases on average as $\propto t^{2/3}$—as in a matter-dominated Friedmann expansion. This "scalaron" dominated phase is unstable to particle creation. The Universe will reheat to a temperature constrained below monopole production and above baryogenesis. The total number of expansion e-foldings, e, during the inflationary epoch is

$$e \approx 18\epsilon H_i^2 \ . \tag{2.5}$$

By analyzing perturbations (most importantly scalar perturbations), applying to our model their known observational limits, and requiring the inflationary period to be of sufficient duration, we have found the following parameter constraints:[8]

$$10^{11} l_{\rm Pl}^2 < \epsilon < 10^{15} l_{\rm Pl}^2 \ , \tag{2.6a}$$

$$H_i > 10^{-5} l_{\rm Pl}^{-1} \Longrightarrow R_i > R_h = 1.2\times 10^{-9} l_{\rm Pl}^{-2} \ . \tag{2.6b}$$

Here, R_h is the curvature at which the perturbation whose wavelength today is equal to the horizon size crossed the horizon during inflation.

The inflation exhibited by this model is not substantially different than the inflation exhibited by any other chaotic inflationary model. The quadratic gravitational term lends to Einstein gravity an additional scalar degree of freedom. There is an explicit and very useful way to display the structure of this extra degree of freedom, due to Whitt,[14] which is to perform the conformal transformation

$$\begin{aligned} \tilde{g}_{\mu\nu} &= (1+2\epsilon R) g_{\mu\nu} \ , \\ d\tilde{s}^2 &= -d\tilde{t}^2 + \tilde{a}^2(\tilde{t}) \left[\frac{dr^2}{1-kr^2} + r^2 d\Omega^2 \right] \ . \end{aligned} \tag{2.7}$$

The action (2.1) can then be rewritten (with geometric quantities in conformal space denoted by a tilde) as

$$\begin{aligned} S = {} & \frac{1}{16\pi G} \int d^4x (-\tilde{g})^{1/2} \left[\tilde{R} - \frac{1}{4\epsilon} \right] + \frac{1}{8\pi G} \int d^3x (\tilde{h})^{1/2} \tilde{K} \\ & - \int d^4x (-\tilde{g})^{1/2} \left[\frac{3}{8\pi G} \phi_{,\mu} \phi_{,\nu} \tilde{g}^{\mu\nu} \right. \\ & \left. + \frac{e^{-2\phi}}{64\pi G \epsilon} (e^{-2\phi} - 2) \right] \ , \end{aligned} \tag{2.8}$$

with $\phi \equiv \frac{1}{2}\ln(1+2\epsilon R)$. An effective cosmological constant, $1/(8\epsilon)$, has been generated by the quadratic term. For $\epsilon R \gg 1$ the potential for ϕ is negligible and this effective cosmological constant dominates. As in the scalar inflaton case, if the kinetic term were to dominate initially it would decay away quickly as $\tilde{a}^{-6}$.

We study the distribution of possible initial conditions using the wave function. We specialize to the line element with $k=+1$. This is a tremendous winnowing of many possible variables down to the two homogeneous degrees of freedom, $a(t)$ and $R(t)$, or $\tilde{a}(\tilde{t})$ and $\phi(\tilde{t})$. We complete the spatial integrals in the action (2.8), $\int (-\tilde{g})^{1/2} d^4x = 2\pi \int \tilde{a}^3 d\tilde{t}$ and $\int (\tilde{h})^{1/2} d^3x = 2\pi^2 \tilde{a}^3$, to get the action in the simple form

$$\begin{aligned} S &= \int \mathcal{L} \left[\tilde{a}, \frac{d\tilde{a}}{d\tilde{t}}, \phi, \frac{d\phi}{d\tilde{t}} \right] d\tilde{t} \\ &= \frac{3\pi}{4G} \int d\tilde{t} \left[- \left[\frac{d\tilde{a}}{d\tilde{t}} \right]^2 \tilde{a} + \tilde{a}^3 \left[\frac{d\phi}{d\tilde{t}} \right]^2 \right. \\ & \left. + \tilde{a} \left[1 - \frac{\tilde{a}^2}{24\epsilon} (e^{-2\phi} - 1)^2 \right] \right] \ . \end{aligned} \tag{2.9}$$

From this action we can read off the Hamiltonian. First, however, we interpose one last change of variables to make dimensionless the scale factor and time: $\alpha \equiv \tilde{a}/(2G/3\pi)^{1/2}$ and $\tau \equiv \tilde{t}/(2G/3\pi)^{1/2}$ which give us

$$\pi_\alpha = \frac{\partial \mathcal{L}}{\partial \left[\frac{d\alpha}{d\tau} \right]} = -\alpha \frac{d\alpha}{d\tau} \ , \tag{2.10a}$$

$$\pi_\phi = \frac{\partial \mathcal{L}}{\partial \left[\frac{d\phi}{d\tau} \right]} = \alpha^3 \frac{d\phi}{d\tau} \ , \tag{2.10b}$$

$$\begin{aligned} S = {} & \frac{1}{2} \int d\tau \left[- \left[\frac{d\alpha}{d\tau} \right]^2 \alpha + \alpha^3 \left[\frac{d\phi}{d\tau} \right]^2 \right. \\ & \left. + \alpha \left[1 - \frac{G\alpha^2}{36\pi\epsilon} (e^{-2\phi} - 1)^2 \right] \right] \ , \end{aligned} \tag{2.10c}$$

and the classical Hamiltonian

$$\mathcal{H} = \frac{1}{2} \left[-\frac{\pi_\alpha^2}{\alpha} + \frac{\pi_\phi^2}{\alpha^3} - \alpha \left[1 - \frac{G}{36\pi\epsilon} \alpha^2 (e^{-2\phi} - 1)^2 \right] \right] \ . \tag{2.11}$$

To quantize we canonically substitute $\pi_\alpha \to \hat{\pi}_\alpha = -i\partial/\partial\alpha$ and $\pi_\phi \to \hat{\pi}_\phi = -i\partial/\partial\phi$. The Wheeler-DeWitt equation[15,16] in the minisuperspace governing the wave function Ψ over the two variables $\alpha = a(1+2\epsilon R)^{1/2} \times \sqrt{3\pi/2G}$ and $\phi = \frac{1}{2}\ln(1+2\epsilon R)$ is

$$\begin{aligned} & \left[\frac{\partial^2}{\partial\alpha^2} - \frac{1}{\alpha^2} \frac{\partial^2}{\partial\phi^2} \right. \\ & \left. - \alpha^2 \left[1 - \frac{G}{36\pi\epsilon} \alpha^2 (e^{-2\phi} - 1)^2 \right] \right] \Psi(\alpha,\phi) = 0 \ . \end{aligned} \tag{2.12}$$

Here we have chosen a simple factor ordering because our solution will be independent of factor ordering to the order of accuracy we demand. We display the restricted region of our analysis in minisuperspace in Fig. 1.

III. THE BOUNDARY CONDITIONS

The wave function of the Universe is a solution of the Wheeler-DeWitt equation for some specified boundary condition. We discuss here the motivation for two of the

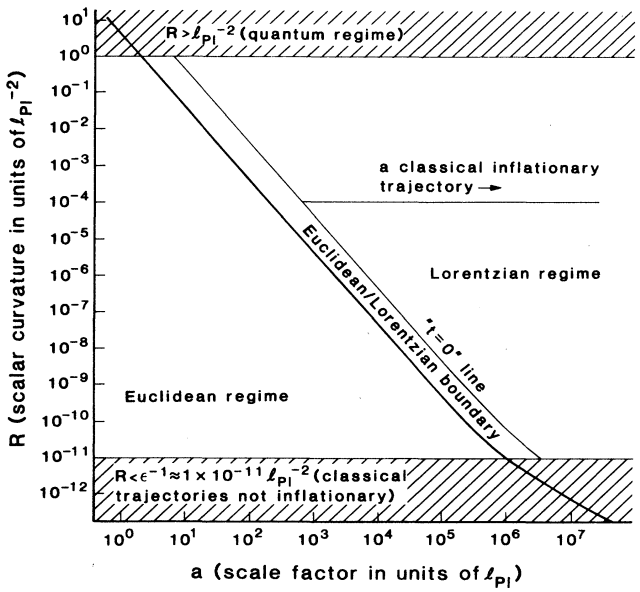

FIG. 1. Regions of minisuperspace. The thick line is the Euclidean-Lorentzian boundary, $a^2=24\epsilon(1+2\epsilon R)/(2\epsilon R)^2$ [cf. Eq. (3.6) with $\alpha=(3\pi/2G)^{1/2}(1+2\epsilon R)^{1/2}a$ and $\phi=\frac{1}{2}\ln(1+2\epsilon R)$]. Shaded regions of the figure are excluded from consideration, either because they are too far into the quantum domain for us to have any confidence in our model (region to the top of the figure with $R>l_{\rm Pl}^{-2}$) or because the classical solutions which do exist are not inflationary (region at the bottom of the figure with $R<\epsilon^{-1}$). Classical inflationary trajectories start at "$t=0$" (the thin line is the classical-quantum boundary) which is slightly away from the Euclidean-Lorentzian boundary.

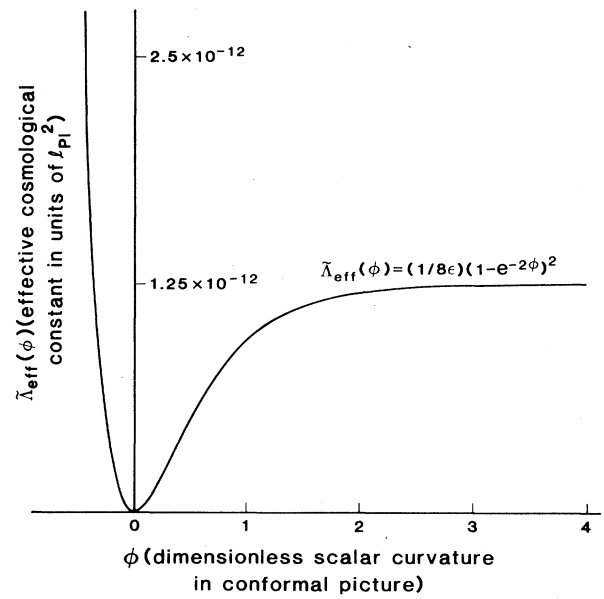

FIG. 2. Plot of the effective cosmological constant, $\tilde{\Lambda}_{\rm eff}(\phi)=(1/8\epsilon)(1-e^{-2\phi})^2$ [cf. Eq. (3.5)]. For ϕ large, this is a constant, $\approx 1/(8\epsilon)$, and we are in the regime of validity of the analysis of the early part of Sec. III.

most definite proposals for the boundary condition—the proposals of "no boundary" due to Hartle and Hawking[16,17] and "tunneling from nothing" due to Vilenkin.[12] We will then (in Sec. IV) examine the specific solutions of the Wheeler-DeWitt equation for our specific model—which will in turn help us to further our physical understanding of the boundary conditions.

Both proposals apply to a spatially closed Universe ($k=+1$) and are therefore intimately connected with the concept of quantum creation of the Universe. First, we illustrate the basic idea by considering the case of $\epsilon R \gg 1$ in Eq. (2.8), where the potential of the ϕ field is dominated by a cosmological constant $\tilde{\Lambda}_{\rm eff}=1/(8\epsilon)$. We display this effective cosmological constant as a function of the ϕ field in Fig. 2. For a spatially closed Robertson-Walker spacetime the classical equation of motion is

$$\tilde{H}^2=\frac{\tilde{\Lambda}_{\rm eff}}{3}-\frac{1}{\tilde{a}^2}\ . \tag{3.1}$$

There will be a classical Lorentzian trajectory for $\tilde{a}(\tilde{t})>(3/\tilde{\Lambda}_{\rm eff})^{1/2}$ only. We can think[4] of an initial configuration of finite size $\tilde{a}\sim(3/\tilde{\Lambda}_{\rm eff})^{1/2}$ being "spontaneously" born from the vacuum. If $\tilde{H}>0$ an expansion will follow. After quantization, Eq. (3.1) becomes a Wheeler-DeWitt equation

$$\left[-\frac{\hat{\pi}_{\tilde{a}}^2}{\tilde{a}}-\left[\frac{3\pi}{2G}\right]^2\tilde{a}\left[1-\tilde{a}^2\frac{\tilde{\Lambda}_{\rm eff}}{3}\right]\right]\Psi(\tilde{a})=0\ . \tag{3.2}$$

For $\tilde{a}>(3/\tilde{\Lambda}_{\rm eff})^{1/2}$, corresponding to the Lorentzian signature classical solution, the potential term is positive and the wave function will be oscillatory. For $\tilde{a}<(3/\tilde{\Lambda}_{\rm eff})^{1/2}$, we can introduce a classical solution with Euclidean signature, the potential term is negative, and the wave function will have exponential mode solutions. We observe that at both zero size for the Universe, $\tilde{a}\sim 0$, and at the Euclidean-Lorentzian boundary, $\tilde{a}\sim(3/\tilde{\Lambda}_{\rm eff})^{1/2}$, the potential term in the Wheeler-DeWitt equation vanishes. Therefore, the creation of a Lorentzian universe is not a process that can be described in classical terms, since the semiclassical approximation to the wave function breaks down in the boundary regions.

There is a semiclassical regime at large $\tilde{a}$ and, depending on the value of $\tilde{\Lambda}_{\rm eff}$, there might be another semiclassical regime for $l_{\rm Pl}\ll\tilde{a}\ll(3/\tilde{\Lambda}_{\rm eff})^{1/2}$, where a classical Euclidean solution might be introduced. The oscillatory-exponential character of the wave function is intimately tied to the Lorentzian-Euclidean character of the classical trajectory. It is the semiclassical regime on the Lorentzian side of the boundary (for large $\tilde{a}$) that provides initial conditions for the Lorentzian classical universe as we know it.

In the Lorentzian domain the two oscillatory modes can be chosen to correspond to expanding and contracting universes. Vilenkin's tunneling boundary condition proposal, in this one-dimensional example, is to fix the wave function by demanding that it describe the expanding Universe only. By the Wentzel-Kramers-Brillouin (WKB) matching conditions across the boundary, such a

solution would contain both exponentially growing and exponentially decaying modes in the Euclidean domain. Near $\tilde{a}=0$, of course, it is the exponentially growing mode which dominates. Thus we can think of this boundary condition as physically ascribing the origin of the Universe to the result of quantum tunneling within the Euclidean domain away from $\tilde{a}=0$. This is the main physical idea behind Vilenkin's proposal, and this wave function is said to describe tunneling from nothing.[12]

Next we turn to Hartle and Hawking's boundary condition. Their proposal[16,17] is that the wave function of the Universe is given by the Euclidean path integral over all compact four-geometries and regular matter fields that induce a given three-geometry and matter-field configuration on a given three-boundary. The physical motivation for the Hartle-Hawking proposal comes from the path-integral representation for a ground state. In a compact spacetime there is no preferred notion of energy and one can interpret their wave function as that for the state of minimal excitation. It is practically impossible, however, to compute this path integral in a closed form for any realistic model. In this paper, we determine the Hartle-Hawking wave function in the semiclassical regime by a semiclassical approximation to the path integral. This procedure fixes the solution that obeys the Hartle-Hawking boundary condition.

The structure of the minisuperspace with its Euclidean and Lorentzian domains is the same for both the "no boundary" and "tunneling" boundary conditions. The form of the wave function is different for the different boundary conditions, however, and the quantum mechanical probability for creation of a Universe of a certain size and certain matter configuration, etc., will also be different. It is a main goal of this work to compare the predictions which depend on the choice of boundary condition for the quantum cosmology of the $R+\epsilon R^2$ model.

Now we can state the boundary conditions for the wave function of the Universe in the $R+\epsilon R^2$ model. We will use the variables α and ϕ, with $\Psi=\Psi(\alpha,\phi)$ in Eq. (2.12). Following the usage of Ref. 12, we implement Vilenkin's boundary condition ("tunneling of the Universe from nothing") in our present model by choosing

(i) the outgoing mode in the Lorentzian regime, along the classical trajectory

and (3.3)

(ii) the wave function ϕ independent as $\alpha\to 0$, ϕ finite.

We implement Hartle and Hawking's boundary condition ("the Universe is without boundary") by fixing

$$\Psi^{\text{semiclass}}(\alpha,\phi)=\left[\int[\mathcal{D}\alpha][\mathcal{D}\phi]e^{-S_E[\alpha,\phi]}\right]_{\text{semiclass}} . \tag{3.4}$$

Here the path integral is to be evaluated over all compact four-geometries and regular field configurations that induce α and ϕ on the fixed three-surface and the subscript E means that the action is Euclidean.

When the full potential is kept in Eq. (2.8) we have

$$\tilde{\Lambda}_{\text{eff}}(\phi)=\frac{1}{8\epsilon}(1-e^{-2\phi})^2 . \tag{3.5}$$

The Wheeler-DeWitt equation (2.12) includes a kinetic term for the ϕ field as well. At the classical level the effect of such a term is well understood.[18–20] If the kinetic term were to dominate initially it would quickly decay away and leave the effective cosmological constant dominant. That is, the $\tilde{\Lambda}_{\text{eff}}(\phi)$-driven phase is an attractor[20] and the kinetic term becomes unimportant for classical inflationary evolution. We shall see that, for the quantum distribution over initial conditions as determined by the Hartle-Hawking or Vilenkin boundary conditions, the kinetic term is also unimportant. Then, the Euclidean-Lorentzian boundary in (α,ϕ) minisuperspace is still the curve on which the potential for the Wheeler-DeWitt equation vanishes:

$$1=\frac{G}{36\pi\epsilon}\alpha^2(1-e^{-2\phi})^2 . \tag{3.6}$$

We might say that a Universe of given scalar field strength becomes Lorentzian when its size exceeds the horizon size determined by that field strength.

The evolution of the Universe will follow classical equations of motion after the Universe crosses the classical-quantum boundary in the Lorentzian regime of superspace. Creation of the Universe then takes place on the Lorentzian side of the $V_{\text{WDW}}(\alpha,\phi)=0$ curve, but spaced away from it at the boundary of the semiclassical regime. The solution of the Wheeler-DeWitt equation, evaluated on this classical-quantum boundary (the "$t=0$" curve in Fig. 1), is the amplitude for creation of a classical Lorentzian universe with given (α,ϕ). The square modulus of this amplitude is the probability distribution over initial conditions for an inflationary universe. Since the values of α and ϕ are related to each other on the classical-quantum boundary (a curve near the Lorentzian-Euclidean curve, $V_{\text{WDW}}=0$), this distribution will depend on only one of the variables, and we shall take it to be ϕ. We thus interpret its value on the classical-quantum boundary, ϕ_i, as the initial "displacement" of this scalar field. In this sense we arrive at the chaotic inflationary picture.

IV. SOLUTIONS OF THE WHEELER-DeWITT EQUATION

We wish to find a distribution over initial conditions for the classical inflationary expansion described in Sec. II. This inflation takes place in the regime $\epsilon R \gg 1$ and we will limit ourselves to exploring semiclassical quantum cosmology during this early epoch.

In principle, the Schrödinger equation and the Feynman path integral are two equivalent ways of computing quantum amplitudes and, again in principle, we can use either of the two methods in quantum cosmology. However, for purposes of computation and comparison of differing boundary condition proposals we prefer to adopt the point of view of the Wheeler-DeWitt equation. We accordingly first solve for the (approximate) general solution of the Wheeler-DeWitt equation. We then imple-

ment Vilenkin's boundary condition by a straightforward imposition of (3.3). Finally, we evaluate the path integral (3.4) in the semiclassical approximation to determine Hartle and Hawking's wave function; but we shall think of this last procedure as fixing the specific Hartle-Hawking component of the general solution to the Wheeler-DeWitt equation.

In general, it is not possible to solve the partial differential Wheeler-DeWitt equation (2.12) in closed form—even to a WKB approximation. We shall study the general solution only for small α. For larger values of α, we treat the ϕ degree of freedom perturbatively by expanding in $\exp(-2\phi)\sim 1/(\epsilon R)$ on top of the semiclassical approximation.

A. The general solution for small α

For small α, it is possible to solve the Wheeler-DeWitt equation (2.12) to all orders in $1/(\epsilon R)$ (with our factor-ordering choice). For $\alpha^2 \ll \alpha_*^2 \equiv 36\pi\epsilon/G$, we can drop the α^4 term in Eq. (2.12):

$$\left[\frac{\partial^2}{\partial\alpha^2}-\frac{1}{\alpha^2}\frac{\partial^2}{\partial\phi^2}-\alpha^2\right]\Psi(\alpha,\phi)=0 \ . \tag{4.1}$$

We stress that this equation is in fact correct to arbitrary order in $1/(\epsilon R)$, since $(e^{-2\phi}-1)^2<1$ for the whole range of ϕ. Now, the equation separates. We write

$$\Psi(\alpha,\phi)=\mathcal{A}(\alpha)\Phi(\phi) \ . \tag{4.2}$$

The α part of the wave function, $\mathcal{A}(\alpha)$, satisfies

$$\left[\frac{d^2}{d\alpha^2}+\frac{\lambda^2}{\alpha^2}-\alpha^2\right]\mathcal{A}(\alpha)=0 \ , \tag{4.3}$$

where λ^2 is the separation constant. This has the general solution

$$\mathcal{A}(\alpha)=c_D\mathcal{A}_D(\alpha)+c_G\mathcal{A}_G(\alpha) \ , \tag{4.4}$$

where

$$\mathcal{A}_D\propto\alpha^{1/2}K_\nu(\alpha^2/2) \text{ and } \mathcal{A}_G(\alpha)\propto\alpha^{1/2}I_\nu(\alpha^2/2) \ . \tag{4.5}$$

Here, c_D and c_G are constants, D and G subscripts denote decaying and growing modes respectively, and K and I are modified Bessel functions with index, $\nu=\frac{1}{4}(1-4\lambda^2)^{1/2}$ (cf. Ref. 21). For $\alpha\ll 1$, we find

$$\mathcal{A}(\alpha)=\begin{cases} c_G\alpha^{(1+4|\nu|)/2}+c_D\alpha^{(1-4|\nu|)/2} & \text{for } 1-4\lambda^2>0 \ , \\ c_G\sqrt{\alpha}+c_D\sqrt{\alpha}\ln\alpha & \text{for } 1-4\lambda^2=0 \ , \\ c_G\sqrt{\alpha}\cos(s\ln\alpha)+c_D\sqrt{\alpha}\sin(s\ln\alpha) & \\ & \text{for } 1-4\lambda^2<0 \ , \end{cases} \tag{4.6}$$

where $s=\frac{1}{2}\sqrt{4\lambda^2-1}$ and the constants c_G and c_D are proportional to those of Eq. (4.4). For $1\ll\alpha\ll\alpha_*$, we have

$$\mathcal{A}(\alpha)=c_D\left[\frac{\pi}{\alpha}\right]^{1/2}e^{-\alpha^2/2}+c_G\left[\frac{1}{\pi\alpha}\right]^{1/2}e^{\alpha^2/2} \ , \tag{4.7}$$

independent of ν as long as $\nu\ll\alpha^2/2$. This form best displays the merit of designating the two modes decaying and growing. The corresponding solution for the ϕ wave function is

$$\Phi(\phi)=\begin{cases} c_1e^{i\lambda\phi}+c_2e^{-i\lambda\phi}, & \lambda\neq 0 \ , \\ c_1\phi+c_2, & \lambda=0 \ . \end{cases} \tag{4.8}$$

In this paper we choose to apply the Vilenkin boundary condition in the Lorentzian regime $\alpha>\alpha_*$, and this will necessitate WKB expansion combined with expanding to successive orders in $e^{-2\phi}\sim 1/(\epsilon R)$.

B. The zeroth-order equation

At zeroth order in $1/(\epsilon R)$ we can write Eq. (2.12) as

$$\left[\frac{\partial^2}{\partial\alpha^2}-\frac{1}{\alpha^2}\frac{\partial^2}{\partial\phi^2}-\alpha^2\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right]\right]\Psi_{(0)}(\alpha,\phi)=0 \ . \tag{4.9}$$

This equation also separates. We write, as before,

$$\Psi_{(0)}(\alpha,\phi)=\mathcal{A}(\alpha)\Phi(\phi) \tag{4.10a}$$

and obtain

$$\left[\frac{d^2}{d\alpha^2}+\frac{\lambda^2}{\alpha^2}-\alpha^2\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right]\right]\mathcal{A}(\alpha)=0 \tag{4.10b}$$

and

$$\left[\frac{d^2}{d\phi^2}+\lambda^2\right]\Phi(\phi)=0 \ , \tag{4.10c}$$

where λ^2 is the separation constant.

We focus attention on the equation for α dependence of the wave function (4.10b). This may be rewritten in the form of a Schrödinger equation:

$$-\mathcal{A}''(\alpha)+U(\alpha)\mathcal{A}(\alpha)=0 \ , \tag{4.11}$$

where

$$U(\alpha)=-\frac{\lambda^2}{\alpha^2}+\alpha^2\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right] \ .$$

Note that the sign of the potential in Eq. (4.11) differs from the one in the Wheeler-DeWitt equation [Eq. (2.12)], so that here the contribution of "matter" terms is negative while for "gravity" terms it is positive.

The qualitative features of the potential, $U(\alpha)$, especially near $\alpha=0$ will depend on the sign of the separation constant λ^2. The three possible cases are displayed in Fig. 3 and we discuss them as follows.

(i) $\lambda^2>0$. Here, there are two qualitatively different subcases, both depicted in Fig. 3(a). If $\lambda^2>\frac{1}{3}(24\pi\epsilon/G)^2$ then the Schrödinger potential $U(\alpha)$ remains negative for all α and the wave function $\mathcal{A}(\alpha)$ is oscillatory. For essentially the whole range of α, the semiclassical approx-

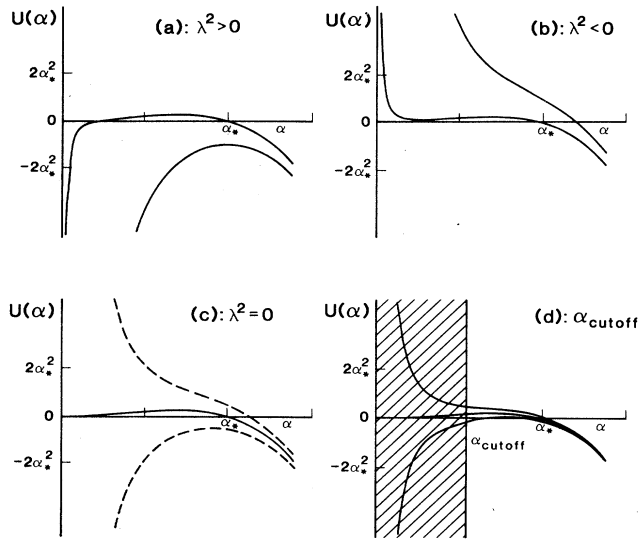

FIG. 3. The effective potential for the Schrödinger-type equation (4.11) for the expansion degree of freedom in the separation limit, $\phi \to \infty$ (cf. the qualitative analysis of Secs. IV B and IV C). The subfigures display the potential for different values of the separation constant λ^2 (where λ^2/α^3 corresponds to the kinetic energy in the ϕ field). (a) Typical potential curves for the separation constant positive [$\lambda^2>0$, case (i) of Sec. IV B]. (b) Typical potential curves for the separation constant negative [$\lambda^2<0$, case (ii) of Sec. IV B]. (c) The heavy line displays the potential curve for the separation constant equal to zero [$\lambda^2=0$, case (iii) of Sec. IV B]. Dashed curves display the potential curves for nonzero values of the separation parameter. Only $\lambda^2=0$ avoids the region of singular field energies at $\alpha=0$. (d) The near equivalence of potentials with different values of the separation constant where a short-distance region has been excluded from the theory (shaded region excluded for $\alpha<\alpha_{\text{cutoff}}$; cf. end of Sec. IV C).

imation is valid, and the corresponding classical solution describes (for small α) a Lorentzian universe expanding (*or* contracting) in a power-law manner ($\sim\tau^{1/3}$) out of the big-bang (or into the big-crunch) singularity. If, on the other hand, we have $0<\lambda^2<\frac{1}{3}(24\pi\epsilon/G)^2$, the potential is negative near $\alpha=0$, has a positive region between the two roots of the equation, $U(\alpha,\lambda^2>0)=0$, and then is negative again for large α. This corresponds to an oscillatory wave function near $\alpha=0$, exponential modes under the barrier, and oscillatory modes again outside. When $\lambda^2 \gg 1$ (recall $\epsilon/G \approx 10^{11}$), the semiclassical approximation will be valid even in the region near $\alpha=0$. This would represent expanding (or contracting) Lorentzian classical behavior near $\alpha=0$, Euclidean trajectories through the barrier, and a Lorentzian universe outside for large α. When $\lambda^2 \le 1$, the semiclassical approximation breaks down near $\alpha \approx 0$, and there will be a highly quantum-mechanical region in which the evolution cannot be described in classical terms. In any event, for $\lambda^2>0$, the potential diverges near $\alpha=0$. The field energies

$$-\frac{\hat{\pi}^2_\alpha}{\alpha}=\frac{1}{\alpha}\frac{d^2}{d\alpha^2}=\frac{U(\alpha)}{\alpha}=-\frac{\lambda^2}{\alpha^3}+\alpha\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right]$$

and (4.12)

$$\frac{\hat{\pi}^2_\phi}{\alpha^3}=-\frac{1}{\alpha^3}\frac{d^2}{d\phi^2}=\frac{\lambda^2}{\alpha^3}$$

both diverge at $\alpha \to 0$. We may think of this $\lambda^2>0$ case as describing expansion of a universe out of (or contraction of a universe into) a region of singular field energy (or a highly quantum-mechanical region) around $\alpha=0$ perhaps followed (or preceded) by a tunneling through a barrier at finite size into continued expansion (or from continued contraction).

(ii) $\lambda^2<0$. In this case [shown in Fig. 3(b)] $U(\alpha)$ is positive near $\alpha=0$ and crosses over to negative at the one real root of the equation, $U(\alpha,\lambda^2<0)=0$. The wave function is exponential under the barrier, switching to oscillatory for α outside the barrier. This corresponds to a tunneling trajectory near $\alpha=0$ for a universe to appear (or disappear) as Lorentzian at finite size. In parallel to case (i) above, if $-\lambda^2<\frac{1}{3}(24\pi\epsilon/G)^2$, there will be both a metastable minimum and a local maximum to the potential. Also, as in the $\lambda^2>0$ case, both energies (4.12) diverge at $\alpha=0$. Again, the semiclassical approximation is or is not valid near $\alpha \approx 0$ depending on whether or not $-\lambda^2 \gg 1$. Here, though, the singular region is hidden under the barrier.

(iii) $\lambda^2=0$. This special case avoids a divergence of the potential $U(\alpha)$ at $\alpha=0$ and it is displayed in Fig. 3(c). There are now two zeros of the potential, a root of $U(\alpha,\lambda^2=0)=0$ at the origin and another at $\alpha_*^2=(36\pi\epsilon/G)$. There are two extrema, at $\alpha=0$ and $\alpha^2=\alpha_*^2/2$. The first is a minimum and the second a maximum. This case allows exponential solutions under the barrier connecting to oscillatory modes outside (denoting Lorentzian expansion or contraction). It is rather remarkable that this case is the only one that avoids a singularity in the potential at $\alpha=0$. By itself, this divergence does not imply a singular wave function—just as the divergence of the effective potential for the radial equation in the elementary quantum mechanics central force problem [$l(l+1)$ plays the role of λ^2 here] does not imply a divergence of the wave function at the origin. However, in both the hydrogen atom and our model cosmology the case without this divergence is special: it corresponds to the ground state. We shall see that both the Vilenkin and Hartle-Hawking requirements pick the $\lambda^2=0$ case.

C. Qualitative discussion of solutions

From Eq. (4.10c), we see that Vilenkin's boundary condition (3.3) picks out $\lambda^2=0$. We can also see that the words "tunneling from nothing" physically correspond to this case from Fig. 3. Only then do we avoid the region of separately singular field energies near $\alpha=0$ and we can associate the wave function with a tunneling amplitude from a classically stable minimum at the origin. Other choices for λ correspond to wave functions that describe an origin out of the region of separately singular field en-

ergies followed either by "tumbling" from some finite α, or a short-lived pass through the barrier. Occasionally,[12] regularity at the origin has been invoked as an explicit demand, but taken literally, the "tunneling from nothing" proposal (in the sense of tunneling from a state peaked at $\alpha \approx 0$) physically suggests $\lambda^2=0$. In our model, with our factor-ordering choice, this case (iii) corresponds to a nonsingular wave function at $\alpha=0$.

We shall see (in Sec. IV D) that $\lambda^2=0$ is a mathematical consequence of the path-integral formulation of the Hartle-Hawking proposal. By looking at the potential for the expansion degree of freedom this assumes a special physical significance: Recall first that the true potential has opposite sign from the one used for visual display in Fig. 3. The higher the maximum on Fig. 3(a), the lower the total potential energy is for the expansion degree of freedom, α (the total energy, summed over both the α and ϕ degrees of freedom, is always zero). That is, case (iii), with $\lambda^2 \to 0$, is the minimum limit of case (i) in the potential for the α degree of freedom. In case (ii), for λ^2 not too large, the minimum is even lower, but it is then only a local minimum. Therefore, the top of the potential on Fig. 3(c), corresponding to case (iii) above, is the lowest *global* minimum for all gravitational and matter field configurations. Now, the value of the potential in Fig. 3(c) at maximum is $U_{\max}=\alpha_*^2/4$. Thus, when we restore to α_* its ϕ dependence, a state of lower energy will correspond to larger α_* and we might expect the ground-state wave function to prefer a larger size for the start of the Lorentzian evolution, and consequently lower initial curvature.

As we shall see, the Hartle-Hawking wave function has this property. Understood in this way, Vilenkin's and Hartle and Hawking's boundary condition proposals are complementary: the former avoids the Euclidean connection between $\alpha \approx 0$ and the Lorentzian domain, while the latter is built around it (in the sense of being built from the path integral around trajectories in the Euclidean regime). This complementarity is reflected in the sign difference in the exponential of the square modulus of the wave function on the classical-quantum boundary, as we shall derive below [cf. Eqs. (5.8) and (5.9)].

One should also keep in mind that the model could be excluded from some small but nonzero length scale α_{cutoff} [pictured in Fig. 3(d)]. Then some nonzero λ^2's might be seen to be indistinguishable from $\lambda^2=0$. Other choices of λ might be used to mimic unknown physical effects from inside the cutoff region. Indeed, even without such a cutoff, there is no physical necessity, other than the physical motivations for the particular boundary condition proposals and their mathematical consequences, that the cases of nonzero λ^2 be excluded.

D. WKB solutions to zeroth order in $1/(\epsilon R)$

The preceding discussion has shown the general behavior of the solutions, how they differ in describing quantum creation, and where we might find the solutions that obey the two boundary condition proposals. We shall now work out the $\lambda^2=0$ case in detail and find the solutions explicitly.

Far under the barrier, for $\alpha^2 \ll 36\pi\epsilon/G$, Eq. (4.10b) becomes (with $\lambda^2=0$)

$$\left[\frac{d^2}{d\alpha^2}-\alpha^2\right]\mathcal{A}(\alpha)=0 \ . \tag{4.13}$$

The general solution for small α has been studied in Eqs. (4.4)–(4.7).

To take into account the other term in the potential of the Wheeler-DeWitt equation (4.9) we use the WKB method (still requiring $\epsilon R \gg 1$). The Wheeler-DeWitt potential, given by

$$V_{\text{WDW}}=-\alpha^2\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right] , \tag{4.14}$$

vanishes at $\alpha=0$ and $\alpha=\alpha_*=(36\pi\epsilon/G)^{1/2}$, so there are two WKB domains:

$$V_{\text{WDW}}(\alpha)<0, \quad 0<\alpha<\alpha_* \quad \text{and} \quad V_{\text{WDW}}(\alpha)>0, \quad \alpha>\alpha_* \ . \tag{4.15}$$

(Note that for ϵ large the semiclassical approximation is valid very near the barrier.) The zeroth-order WKB solution is obtained by

$$\mathcal{A}_{\text{WKB}\,(0)}(\alpha)=e^{-\mathcal{S}}, \quad \text{where} \quad \left[\frac{d\mathcal{S}}{d\alpha}\right]^2=\alpha^2\left[1-\frac{G}{36\pi\epsilon}\alpha^2\right]. \tag{4.16}$$

Its solutions are

$$\mathcal{A}_{\text{WKB}\,(0)}(\alpha)=\exp\left\{\pm\frac{\alpha_*^2}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2}\right]^{3/2}\right]\right\} \quad \text{for } 0<\alpha<\alpha_* \tag{4.17a}$$

and

$$\mathcal{A}_{\text{WKB}\,(0)}(\alpha)=\exp\left\{\pm\frac{\alpha_*^2}{3}\left[1+i\left[\frac{\alpha^2}{\alpha_*^2}-1\right]^{3/2}\right]\right\} \quad \text{for } \alpha>\alpha_* \ . \tag{4.17b}$$

The first-order WKB corrections are then obtained by

$$\mathcal{A}_{\text{WKB}\,(1)}(\alpha)=\mathcal{C}(\alpha)e^{-\mathcal{S}(\alpha)} , \quad \text{where} \quad \frac{d}{d\alpha}\left[\mathcal{C}^2(\alpha)\frac{d\mathcal{S}}{d\alpha}(\alpha)\right]=0 \ . \tag{4.18}$$

We solve to find

$$\mathcal{C}(\alpha)=\frac{C}{\left[\alpha^2\left[1-\frac{\alpha^2}{\alpha_*^2}\right]\right]^{1/4}} , \tag{4.19a}$$

where C is a constant. For first-order WKB accuracy we need keep only the leading part of this correction to find

$$\mathcal{C}(\alpha)=C\alpha^{-1/2} \quad \text{for } 0<\alpha<\alpha_* , \tag{4.19b}$$

$$\mathcal{C}(\alpha)=C\alpha_*^{1/2}\alpha^{-1}e^{\pm i\pi/4} \quad \text{for } \alpha>\alpha_* \ . \tag{4.19c}$$

We then summarize the behavior of the first-order WKB

solutions for the case $\lambda^2=0$ by writing

$$\Psi_{(0),\mathrm{WKB}\,(1)}(\alpha,\phi)=\mathcal{A}_{\mathrm{WKB}\,(1)}(\alpha)\Phi(\phi) \tag{4.20}$$

where we have the ϕ dependence from Eq. (4.10c),

$$\Phi(\phi)=a\phi+b\ , \tag{4.21}$$

and a and b are constants. For the α dependence we find

$$\mathcal{A}_{\mathrm{WKB}\,(1)}(\alpha)=c_D\mathcal{A}_{D,\mathrm{WKB}\,(1)}(\alpha)+c_G\mathcal{A}_{G,\mathrm{WKB}\,(1)}(\alpha) \quad \text{for } 0<\alpha<\alpha_* \tag{4.22a}$$

and

$$\mathcal{A}_{\mathrm{WKB}\,(1)}(\alpha)=c_L\mathcal{A}_{L,\mathrm{WKB}\,(1)}(\alpha)+c_R\mathcal{A}_{R,\mathrm{WKB}\,(1)}(\alpha) \quad \text{for } \alpha>\alpha_*\ . \tag{4.22b}$$

The modes themselves are (where constants have been fixed conveniently)

$$\mathcal{A}_{D,\mathrm{WKB}\,(1)}(\alpha)=\alpha^{-1/2}\exp\left\{-\frac{\alpha_*^2}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2}\right]^{3/2}\right]\right\} \tag{4.23a}$$

and

$$\mathcal{A}_{G,\mathrm{WKB}\,(1)}(\alpha)=\alpha^{-1/2}\exp\left\{+\frac{\alpha_*^2}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2}\right]^{3/2}\right]\right\}, \tag{4.23b}$$

both under the barrier, $0<\alpha<\alpha_*$. These forms (4.23a) and (4.23b) then agree with the forms (4.7) to within multiplicative constants for $\alpha\gg1$ and, again, D and G subscripts denote decaying and growing modes, respectively. Outside the barrier we find

$$\mathcal{A}_{R,\mathrm{WKB}\,(1)}(\alpha)=\frac{\alpha_*^{1/2}}{\alpha}\exp\left[-\frac{\alpha_*^2}{3}-i\frac{\alpha_*^2}{3}\left[\frac{\alpha^2}{\alpha_*^2}-1\right]^{3/2}+i\frac{\pi}{4}\right] \tag{4.23c}$$

and

$$\mathcal{A}_{L,\mathrm{WKB}\,(1)}(\alpha)=\frac{\alpha_*^{1/2}}{\alpha}\exp\left[+\frac{\alpha_*^2}{3}+i\frac{\alpha_*^2}{3}\left[\frac{\alpha^2}{\alpha_*^2}-1\right]^{3/2}-i\frac{\pi}{4}\right]. \tag{4.23d}$$

The R and L subscripts denote right- and left-moving modes (keeping in mind that the energy of the gravitational expansion is negative) and correspond, respectively, to expanding and contracting classical trajectories—as can be seen by applying the operator $\hat{\pi}_\alpha=-i\partial/\partial\alpha$ $[=-\alpha(d\alpha/d\tau)]$.

With the mode solutions in hand for the regime $\epsilon R\gg1$ we can proceed to implement the boundary condition proposals (3.3) and (3.4). Vilenkin's mode is just the one corresponding to the expanding classical trajectory. This is $\mathcal{A}_R$ in the oscillatory domain and connects to $i\mathcal{A}_D+\exp(-2\alpha_*^2/3)\mathcal{A}_G/2$ under the barrier.[22] Since the wave function is ϕ independent at $\alpha\to0$ we have $\Phi(\phi)=b$ (a constant) and we determine Vilenkin's wave function:

$$\Psi_{V,(0),\mathrm{WKB}\,(1)}(\alpha,\phi)\propto\begin{cases}\mathcal{A}_{R,\mathrm{WKB}\,(1)}(\alpha) & \text{for } \alpha>\alpha_*\ ,\\ i\mathcal{A}_{D,\mathrm{WKB}\,(1)}(\alpha)+\dfrac{e^{-2\alpha_*^2/3}}{2}\mathcal{A}_{G,\mathrm{WKB}\,(1)}(\alpha) & \text{for } 0<\alpha<\alpha_*\ .\end{cases} \tag{4.24}$$

We see that for α small the exponentially decaying mode dominates the other and hence justifies the tunneling interpretation of this solution.

From our qualitative discussion we have some notion of the solution that obeys the Hartle-Hawking boundary condition, but to find it explicitly we have to evaluate the path integral. In the semiclassical approximation we may write it (employing the conformal rotation procedure of Ref. 16 and Ref. 23) as

$$\Psi^{\mathrm{semiclass}}(\alpha,\phi)=\sum e^{-S_E}\ , \tag{4.25}$$

where the sum goes over all classical solutions that satisfy the imposed boundary condition on the path integral. The Euclidean action [with $\tau_E=i\tau$ denoting Euclidean time in Eq. (2.10c)] is

$$S_E=\tfrac{1}{2}\int d\tau_E\left\{-\left[\frac{d\alpha}{d\tau_E}\right]^2\alpha+\alpha^3\left[\frac{d\phi}{d\tau_E}\right]^2-\alpha\left[1-\left[\frac{\alpha}{\alpha_*}\right]^2\right]\right\}. \tag{4.26a}$$

This action in turn determines the Euclidean classical path

$$\frac{d^2\phi}{d\tau_E^2}+\frac{3}{\alpha}\frac{d\alpha}{d\tau_E}\frac{d\phi}{d\tau_E}=0 \tag{4.26b}$$

and

$$2\alpha\frac{d^2\alpha}{d\tau_E^2}+\left[\frac{d\alpha}{d\tau_E}\right]^2+3\alpha^2\left[\frac{d\phi}{d\tau_E}\right]^2-1+3\frac{\alpha^2}{\alpha_*^2}=0\ . \tag{4.26c}$$

We choose $\tau_E=0$ at $\alpha=0$ and consider paths that link $\alpha=0$ to the boundary α_0,ϕ_0 at $\tau_E>0$. The path that has finite ϕ and $d\alpha/d\tau_E$ at $\alpha=0$ is simply $\phi=\phi_0$, $\alpha=\alpha_*\sin(\tau_E/\alpha_*)$. (This is an expanding and contracting 3-sphere.) Inserting this into the action (4.26a), we find

$$S_E(\alpha,\phi)=-\frac{\alpha_*^2}{3}\left[1-\frac{\alpha^2}{\alpha_*^2}\right]^{3/2}, \tag{4.27}$$

and, hence,

$$\Psi^{\text{semiclass}} \propto \exp\left[-\frac{\alpha_*^2}{3}\left[1-\frac{\alpha^2}{\alpha_*^2}\right]^{3/2}\right] . \tag{4.28}$$

We see that the Hartle-Hawking boundary condition has automatically picked out the $\lambda^2=0$ case (due to the regularity of $d\phi/d\tau_E$ at $\alpha=0$).

We can now compare this expression with the semiclassical approximation to the general solution of the WDW equation, Eq. (4.23), to find

$$\Psi_{\text{HH}}(\alpha,\phi) \propto \mathcal{A}_{G,\text{WKB}\,(1)}(\alpha) . \tag{4.29}$$

A calculation of the Hartle-Hawking wave function without resorting to the semiclassical approximation is pursued in Ref. 24 for small α [Eq. (4.5)], where the same result is obtained. Thus, the growing mode, $\mathcal{A}_G$, is indeed the Hartle-Hawking wave function in the Euclidean regime and we can connect this outside the barrier to $\exp(2\alpha_*^2/3)\mathcal{A}_R+\mathcal{A}_L$. We determine the wave function

$$\Psi_{\text{HH},(0),\text{WKB}\,(1)}(\alpha,\phi) \propto \begin{cases} e^{2\alpha_*^2/3}\mathcal{A}_{R,\text{WKB}\,(1)}(\alpha)+\mathcal{A}_{L,\text{WKB}\,(1)}(\alpha) & \text{for } \alpha>\alpha_* , \\ \mathcal{A}_{G,\text{WKB}\,(1)}(\alpha) & \text{for } 0<\alpha<\alpha_* . \end{cases} \tag{4.30}$$

As explained in the literature[16,25,26] one can as well compute the path integral directly in the Lorentzian regime to find that left- and right-moving components should contribute with equal weight. Our answer [keeping in mind our normalization of the modes, Eqs. (4.23)] confirms both this and our earlier qualitative guesses.

At this zeroth order of approximation in $1/(\epsilon R)$ the amplitude of either solution is just a constant (apart from the power-law factor). Thus we can discern the process of creation of an inflationary Lorentzian universe, but we have not yet determined the ϕ- or α-dependent amplitude for its generation. To obtain this, we have to go to the next approximation in $1/(\epsilon R)$.

E. Solutions to first order in $1/(\epsilon R)$

When terms of order $e^{-2\phi}$ are left in the potential, $V(\alpha,\phi)$, the Wheeler-DeWitt equation (2.12) is no longer separable and we are confronted with a two-dimensional WKB problem. Instead of working out the general two-dimensional WKB solution, we would like to restrict ourselves to its subclass that contains both the WKB approximation to Ψ_V and the WKB approximation to Ψ_{HH}. We observe that both Ψ_V (4.24) and Ψ_{HH} (4.30) are ϕ independent and yield a zero kinetic term for the ϕ field in Eq. (2.12). When terms of order $e^{-2\phi}$ are kept, this kinetic term will no longer be zero, but we expect that, for the Vilenkin and Hartle-Hawking wave functions, it will be of order $\alpha^{-2}e^{-2\phi}$. Hence, in the region of superspace where $\alpha \gg 1$ and $e^{-2\phi}$ is negligible, we can restrict ourselves to the subclass of wave functions that satisfy

$$\left[\frac{\partial^2}{\partial\alpha^2}-\alpha^2\left[1-\frac{\alpha^2}{\alpha_*^2(\phi)}\right]\right]\Psi(\alpha,\phi)=0 , \tag{4.31}$$

where

$$\alpha_*^2(\phi)\equiv\alpha_*^2(1+2e^{-2\phi}) . \tag{4.32}$$

As in Eq. (4.18), we write the WKB wave function

$$\Psi_{(1),\text{WKB}\,(1)}(\alpha,\phi)=\mathcal{C}(\alpha,\phi)e^{-\mathcal{S}(\alpha,\phi)} . \tag{4.33}$$

The WKB equation for $\mathcal{S}(\alpha,\phi)$ is

$$\left[\frac{\partial\mathcal{S}}{\partial\alpha}\right]^2-\alpha^2\left[1-\frac{G\alpha^2}{36\pi\epsilon}(1-2e^{-2\phi})\right]=0 . \tag{4.34}$$

This equation for $\mathcal{S}$ is valid to first order in $e^{-2\phi}$ in the region of superspace where $1\ll\alpha<\alpha_*(\phi)$ and $\alpha^4\alpha_*^{-2}e^{-2\phi}\gg 1$. In this region, the terms dropped from the equation are negligible compared to the terms included. Indeed, it is straightforward to evaluate the path integral with the Hartle-Hawking boundary condition in the semiclassical approximation in this region of superspace to see that it satisfies Eq. (4.34).

We solve (4.34) under the barrier to find

$$\mathcal{S}(\alpha,\phi)=\pm\frac{\alpha_*^2(\phi)}{3}\left[1-\frac{\alpha^2}{\alpha_*^2(\phi)}\right]^{3/2}\pm f(\phi) .$$

The integration constant $f(\phi)$ is determined by matching this to the general solution of Eq. (2.12) in the limit $\alpha^2\ll\alpha_*^2(\phi)$ [cf. Eq. (4.7)]. We see that requiring $\partial^2/\partial\phi^2\sim e^{-2\phi}$ has restricted us to the case $\lambda^2=0$. From this we obtain

$$\mathcal{S}(\alpha,\phi)=\pm\frac{\alpha_*^2(\phi)}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2(\phi)}\right]^{3/2}\right] . \tag{4.35}$$

In hindsight, we have merely performed the rather trivial substitution of the function $\alpha_*(\phi)$ for the constant α_* in the zeroth-order solutions. The prefactor $\mathcal{C}$ in Eq. (4.32) can be obtained from this $\mathcal{S}$ and Eq. (4.31). We summarize the semiclassical wave functions to first order in $1/(\epsilon R)$: Inside the barrier [for $1\ll\alpha<\alpha_*(\phi)$] we have

$$\Psi_{D,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) = \alpha^{-1/2}\exp\left\{-\frac{\alpha_*^2(\phi)}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2(\phi)}\right]^{3/2}\right]\right\} \tag{4.36a}$$

and

$$\Psi_{G,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) = \alpha^{-1/2}\exp\left\{+\frac{\alpha_*^2(\phi)}{3}\left[1-\left[1-\frac{\alpha^2}{\alpha_*^2(\phi)}\right]^{3/2}\right]\right\}. \tag{4.36b}$$

Outside the barrier [for $\alpha > \alpha_*(\phi)$], we have, by analytic continuation,

$$\Psi_{R,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) = \frac{\alpha_*^{-1/2}}{\alpha}\exp\left\{-\frac{\alpha_*^2(\phi)}{3}\left[1+i\left[\frac{\alpha^2}{\alpha_*^2(\phi)}-1\right]^{3/2}\right] + i\frac{\pi}{4}\right\} \tag{4.36c}$$

and

$$\Psi_{L,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) = \frac{\alpha_*^{-1/2}}{\alpha}\exp\left\{+\frac{\alpha_*^2(\phi)}{3}\left[1+i\left[\frac{\alpha^2}{\alpha_*^2(\phi)}-1\right]^{3/2}\right] - i\frac{\pi}{4}\right\}. \tag{4.36d}$$

The wave function that obeys Vilenkin's boundary condition ("tunneling from nothing") is

$$\Psi_{V,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) \propto \begin{cases} i\Psi_{D,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) + \dfrac{e^{-2\alpha_*^2(\phi)/3}}{2}\Psi_{G,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) & \text{for } 1 \ll \alpha < \alpha_*(\phi)\,, \\ \Psi_{R,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) & \text{for } \alpha > \alpha_*(\phi)\,. \end{cases} \tag{4.37}$$

The wave function that obeys Hartle and Hawking's boundary condition ("no boundary") is

$$\Psi_{\mathrm{HH},(1),\mathrm{WKB}\,(1)}(\alpha,\phi) \propto \begin{cases} \Psi_{G,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) & \text{for } 1 \ll \alpha < \alpha_*(\phi)\,, \\ e^{2\alpha_*^2(\phi)/3}\Psi_{R,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) + \Psi_{L,(1),\mathrm{WKB}\,(1)}(\alpha,\phi) & \text{for } \alpha > \alpha_*(\phi)\,. \end{cases} \tag{4.38}$$

V. CONCLUSION

We are now in a position to find the distribution over the initial conditions for chaotic inflation. The classical evolution of the Universe begins when the phase of the wave function is rapidly oscillating, i.e., $\mathcal{S}(\alpha,\phi) \gg 1$. The classical-quantum boundary, $\alpha = \alpha_c$, is very close to the Euclidean-Lorentzian boundary $\alpha = \alpha_*(\phi)$ in our present model due to the large parameter, $\epsilon/G \approx 10^{11}$. The evolution is classical when α is slightly larger than $\alpha_*(\phi)$:

$$\frac{\alpha}{\alpha_*(\phi)} > 1 + \frac{G}{36\pi\epsilon}(1-e^{-2\phi})\,. \tag{5.1}$$

It is straightforward to determine how the initial conditions of a classical trajectory (α, ϕ, $d\alpha/d\tau$, and $d\phi/d\tau$) are correlated. The rapidly oscillating phase, $\mathcal{S}(\alpha,\phi)$, of the wave function in the classical region is given by

$$\mathcal{S}_\pm(\alpha,\phi) = \mp\frac{\alpha_*^2(\phi)}{3}\left[\frac{\alpha^2}{\alpha_*^2(\phi)}-1\right]^{3/2}, \tag{5.2}$$

where the upper sign ($\mathcal{S}_+$) corresponds to Ψ_R and the lower sign ($\mathcal{S}_-$) corresponds to Ψ_L.

The initial "velocities" of a classical trajectory are correlated to α and ϕ as

$$\alpha^3\frac{d\phi}{d\tau} = \left[\frac{\partial\mathcal{S}_\pm}{\partial\phi}\right]_{\alpha=\alpha_c} \approx \pm\left[\frac{\alpha^3}{6\alpha_*^3}\frac{\partial}{\partial\phi}(\alpha_*^2)\right]_{\alpha=\alpha_c} \tag{5.3}$$

and

$$-\alpha\frac{d\alpha}{d\tau} = \left[\frac{\partial\mathcal{S}_\pm}{\partial\alpha}\right]_{\alpha=\alpha_c} \approx \pm\left[\frac{\alpha}{\alpha_*}\right]_{\alpha=\alpha_c}, \tag{5.4}$$

where the right-hand sides are to be evaluated on the classical-quantum boundary $\alpha = \alpha_c \approx \alpha_*(\phi)$. These relations can be transformed back to the physical variables a, R, da/dt, and dR/dt: On the classical-quantum boundary,

$$a \approx \left[\frac{12}{R}\right]^{1/2}, \tag{5.5}$$

$$\frac{dR}{dt} \approx \mp\frac{2}{3\epsilon}\left[\frac{R}{12}\right]^{1/2}, \tag{5.6}$$

and

$$H = \frac{1}{a}\frac{da}{dt} \approx \pm\left[\frac{R}{12}\right]^{1/2}, \tag{5.7}$$

where the upper (lower) sign corresponds to Ψ_R (Ψ_L). We see that the Ψ_L component in the Hartle-Hawking wave function (4.38) corresponds to a collapsing universe and is irrelevant to our cosmological observations.[26] The correlation (5.7) is particularly important: It indicates that the Ψ_R component corresponds to a universe that

begins its classical evolution with $R_i \approx 12H_i^2$, i.e., right at the beginning of the linear phase described by Eq. (2.4) (cf. Ref. 8 for detailed analysis of the classical evolution). If H and R were not so correlated on the classical-quantum boundary, there would be some complicated dynamical evolution before the universe would follow an inflationary trajectory.

With the correlations, Eqs. (5.5)–(5.7), the distributions over initial conditions are determined by the distributions over R_i (or equivalently, ϕ_i), and we need just the square modulus of the wave function in the Lorentzian regime near the classical-quantum boundary. Unlike the correlations (5.5)–(5.7), which take the same form for both Ψ_V and $\Psi_{\rm HH}$ (or the Ψ_R component of $\Psi_{\rm HH}$), the distributions over R_i differ for the two wave functions. For Vilenkin's boundary condition it is

$$|\Psi_V(\alpha,\phi)|^2 \propto \frac{\alpha_*}{\alpha^2} e^{-2\alpha_*^2(\phi)/3} . \tag{5.8}$$

For Hartle and Hawking's boundary condition it is (with the irrelevant component Ψ_L dropped)

$$|\Psi_{\rm HH}(\alpha,\phi)|^2 \propto \frac{\alpha_*}{\alpha^2} e^{+2\alpha_*^2(\phi)/3} . \tag{5.9}$$

We express this probability distribution near the Lorentzian boundary as a function of (initial) curvature, R_i. We have

$$dP(R_i) \propto d\mu(R_i)|\Psi(\alpha(R_i),R_i)|^2 . \tag{5.10}$$

The measure, $d\mu(R_i)$ is just the line element along the classical-quantum boundary, given through the natural metric on minisuperspace,[27] which can be read off the kinetic terms in the Wheeler-DeWitt Hamiltonian (2.11). It is

$$\delta\sigma^2 = -\alpha\delta\alpha^2 + \alpha^3\delta\phi^2 . \tag{5.11}$$

For $\epsilon R_i \gg 1$, the classical-quantum boundary is simply $\alpha = \text{const}$, and we have

$$d\mu(R_i) \propto d\phi = \frac{dR_i}{R_i} . \tag{5.12}$$

We finally obtain the probability distributions (using $\alpha_*^2(\phi) \approx (36\pi\epsilon/G)[1+1/(\epsilon R_i)]$)

$$dP_V \propto \frac{dR_i}{R_i} e^{-24\pi/GR_i} \tag{5.13a}$$

and

$$dP_{\rm HH} \propto \frac{dR_i}{R_i} e^{+24\pi/GR_i} . \tag{5.13b}$$

We sketch the distributions in Fig. 4. Remarkably, they are complementary. This is not something that we have been able to expect from the formulation of the boundary conditions [Eqs. (3.3) and (3.4)], but we hope to have gleaned some qualitative understanding through the discussion of Secs. III and IV.

We should note that distribution (5.13a) has been proposed on its own merit by Linde.[28] Namely, this distribution gives a preference for Planck-scale creation, which is what one might expect from quantum cosmology. Here, high values of the curvature are favored and the Universe is more likely to be small after tunneling. The power-law factor that bends the distribution, thereby creating a maximum, could be modified with, say, a different factor ordering. However, the maximum will remain very roughly on the Planck scale. The value of this maximum is in fact somewhat above the Planck scale, $R_{i,\max} = 24\pi l_{\rm Pl}^{-2}$.

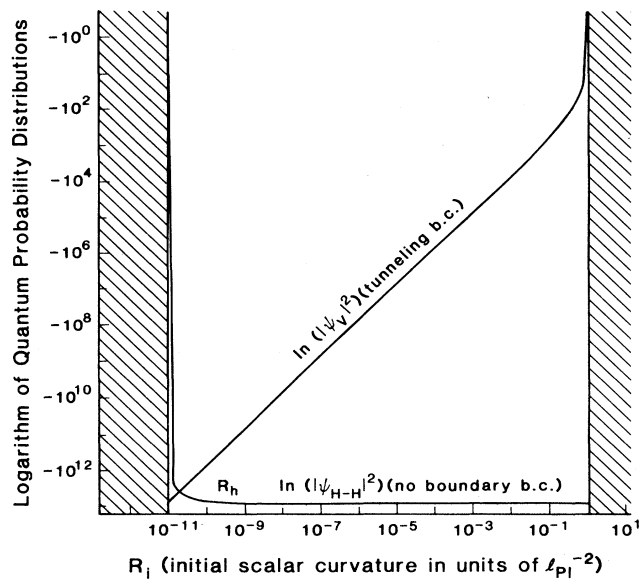

FIG. 4. The distributions over initial curvature R_i for classical inflationary trajectories are plotted, as determined by the boundary condition proposals of quantum cosmology. The distribution derived from the wave function obeying Vilenkin's boundary condition is peaked to the right, preferring large values of the initial curvature [cf. Eq. (5.7a)]. The distribution derived from the wave function obeying Hartle and Hawking's boundary condition is peaked to the left, preferring low values of the initial curvature [cf. Eq. (5.7b)]. We have restricted our analysis to $\epsilon^{-1} \approx 10^{-11} l_{\rm Pl}^{-2} < R_i < l_{\rm Pl}^{-2}$ for reasons elaborated in the Introduction. An inflation sufficient that is consistent with observations has to start at $R_i > R_h \approx 10^{-9} l_{\rm Pl}^{-2}$.

The Hartle-Hawking distribution prefers the Universe to start out at low curvature. The Universe starts out in the linear phase and R can only decrease in the subsequent classical evolution. In light of our earlier qualitative discussion of their boundary condition (Sec. IV C) this is not surprising—we expect the typical Hartle-Hawking universe to be born large and spend not too many e-foldings in the inflationary phase.

In numbers, the difference between the two proposals is dramatic. We normalize both distributions in our target range (see Sec. I), $\epsilon^{-1} < R_i \ll l_{\rm Pl}^{-2}$, and find that the likelihood of an inflationary phase which would at least be sufficient for the current horizon volume (in one trial "universe") is

$$P_V(R_i \geq R_h) = 1 - e^{-8\times 10^{10}} \tag{5.14a}$$

or

$$P_{\rm HH}(R_i \geq R_h) = e^{-10^{12}} , \tag{5.14b}$$

where $R_h \sim 10^{-9} l_{\rm Pl}^{-2}$ is the value of the curvature at which the perturbation whose wavelength today is equal to the horizon size crossed the horizon during inflation [cf. Eq. (2.6b)].

The simplest interpretation of this result follows: Like every quantum probability, this distribution represents a set of classical outcomes. In this case the set is the ensemble of "all possible universes" that could be created on the restricted classical-quantum boundary. Our Universe is one such outcome, a particular result of a single process of quantum creation. As we understand it, our Universe apparently attained its long age, remarkable flatness, homogeneity, and isotropy due to an initial inflationary phase of at least ~ 70 e-foldings. Thus, within this interpretation, and within the adopted restrictions of the model, we can only say that if the boundary condition is the one proposed by Vilenkin, our Universe is a highly typical product of quantum creation. If the boundary condition is the one proposed by Hartle and Hawking our Universe is an atypical event.

Of course, we have dealt with a severely limited model, and a better statement will have to await more realistic analysis (treating other degrees of freedom, both in the gravitational and matter sectors). However, we do not expect the basic picture to become very different. Studies so far in this[20] and other models (at the classical[29,30] and quantum[31] levels) have shown that the effects of a large initial kinetic term, a large initial anisotropy, and a small initial inhomogeneity all become rapidly unimportant. Thus, apart from the unexplored case of a large initial inhomogeneity, the dominant input from quantum dynamics is in the distribution over initial curvature (or size), which was the subject of this work. In another approach to this model,[32] the probability of $R+\epsilon R^2$ inflation is studied using the canonical measure of Ref. 33. It is shown that this canonical measure leaves open the question of the predominance of inflationary over noninflationary trajectories.

As for the interpretation of (5.5)–(5.7), (5.13a), and (5.13b) advocated here, we confront what may be expected to become a general feature of quantum cosmology: Two (or more) competing hypotheses lead to predictions (probability statements) that include our Universe as an outcome (where "our Universe" means a classical model that agrees with observation as far as it goes). We are left with two possible criteria to judge such hypotheses. First, we might prefer the hypothesis that is more readily extendible to more and more realistic models. Only further refinement of quantum cosmology can explore this possibility. Second, we might prefer the hypothesis that shows that our Universe is the more probable outcome. This arguably more observationally based criterion can be weakened when we allow the interjection of some form of an anthropic principle, which can exclude from our consideration cosmological outcomes that are not likely to be like our Universe (not likely to evolve observers to observe them). We simply state the horns of this dilemma because our rather unrefined model makes any choice premature.

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APPENDIX: THE BOUNDARY TERM FOR $R+\epsilon R^2$ GRAVITY

The action (2.1), just as is well known for Einstein gravity (i.e., $\epsilon=0$), does not lead to a well-posed variational problem without a boundary term. That is, we wish to extremize the classical action under arbitrary variations of the metric which vanish on the boundary. In general, however, the varied action can depend on variations of *derivatives* of the metric on the boundary which, indeed, need not vanish. The boundary term is required in order to cancel just these surface variations of metric derivatives. Further, as a quantitative piece of the action, the boundary term plays a necessary role in evaluation of the path integral for the Hartle-Hawking approach to the wave function. Therefore, we sketch here its derivation for $R+\epsilon R^2$ gravity.

There are two methods of derivation we consider. The first is straightforward: If we stay within the full fourth-order theory we have only to rework carefully a usual ($\epsilon=0$) derivation of the boundary term. We start from the "bare" gravitational action (2.1)—the action without boundary term and without matter content ($L_m=0$) or cosmological constant ($\Lambda=0$). This bare action we write as

$$S' = \frac{1}{16\pi G}\int d^4x(-g)^{1/2}(R+\epsilon R^2) . \tag{A1}$$

A head-on algebraic assault will find

$$\begin{aligned}\delta S' = {}& \frac{1}{16\pi G}\int(-g)^{1/2}\{R_{\mu\nu}-\tfrac{1}{2}g_{\mu\nu}R+2\epsilon[R(R_{\mu\nu}-\tfrac{1}{4}g_{\mu\nu}R)+R_{;\alpha\beta}(g^{\alpha\beta}g_{\mu\nu}-\delta^{\alpha}{}_{\mu}\delta^{\beta}{}_{\nu})]\}\delta g^{\mu\nu} \\ & -\frac{1}{16\pi G}\int d^4x(-g)^{1/2}[(1+2\epsilon R)_{;\delta}(g^{\delta\lambda}g_{\sigma\tau}-\delta^{\delta}{}_{\sigma}\delta^{\lambda}{}_{\tau})\delta g^{\sigma\tau}]_{;\lambda} \\ & +\frac{1}{16\pi G}\int d^4x(-g)^{1/2}[(1+2\epsilon R)g^{\alpha\lambda}g^{\gamma\delta}(\delta g_{\alpha\gamma;\delta}-\delta g_{\gamma\delta;\alpha})]_{;\lambda} .\end{aligned} \tag{A2}$$

Here we see three distinct terms emerge. The first term merely displays the $R+\epsilon R^2$ field equations, the second term yields a surface integral which will give only vanishing contributions on the boundary (because variations of the metric itself vanish on the boundary), and the last term gives also a surface integral which, however, need not vanish. We can, though, follow almost directly the argument of Wald[34] (given there for the $\epsilon=0$ case) to rewrite the third term as

$$\frac{1}{16\pi G}\int d^4x(-g)^{1/2}[(1+2\epsilon R)g^{\alpha\lambda}g^{\gamma\delta}(\delta g_{\alpha\gamma;\delta}-\delta g_{\gamma\delta;\alpha})]_{;\lambda}$$
$$=-\frac{1}{8\pi G}\int d^3x\sqrt{h}\,(1+2\epsilon R)\delta K+\text{ vanishing surface pieces.} \quad \text{(A3)}$$

Now ignoring the contributions which vanish by reason of vanishing metric variations on the boundary, we obtain the form

$$\delta S'=\frac{1}{16\pi G}\int d^4x(-g)^{1/2}(\text{field equations})\delta g^{\mu\nu}$$
$$-\frac{1}{8\pi G}\int d^3x\sqrt{h}\,(1+2\epsilon R)\delta K\ . \quad \text{(A4)}$$

One final twist not present in the $\epsilon=0$ case is readily verified:

$$-\frac{1}{8\pi G}\int d^3x\sqrt{h}\,(1+2\epsilon R)\delta K$$
$$=-\frac{1}{8\pi G}\delta\int d^3x\sqrt{h}\,(1+2\epsilon R)K\ . \quad \text{(A5)}$$

We thus derive the boundary term for the action (2.1):

$$S=S'+\frac{1}{8\pi G}\int d^3x\sqrt{h}\,(1+2\epsilon R)K\ . \quad \text{(A6)}$$

The conformal picture inspires another derivation. Whitt[14] originally transformed the equations of motion for the fourth-order theory into the Einstein equations and then read off an action for the scalar degree of freedom. Here, we shall transform directly the action (A1) and find the boundary term on the way. We are motivated in this approach because we know from the analysis at linearized level[10] that the theory (2.1) has in its spectrum a scalar degree of freedom with mass, $m^2=1/(6\epsilon)$ (with ϵ/G large). We also know that the scalar curvature itself obeys an equation of motion

$$R_{;\alpha\beta}g^{\alpha\beta}-\frac{R}{6\epsilon}=0\ . \quad \text{(A7)}$$

We can thus take the scalar curvature to be an interpolating field for that same scalar degree of freedom. With our conventions, a mass term will appear in the action with a $(-)$ sign. Therefore, we begin with the action in the physical picture,

$$S=\frac{1}{16\pi G}\int d^4x(-g)^{1/2}(R+\epsilon R^2)+\text{b.t.}\ , \quad \text{(A8)}$$

where b.t. stands for the unknown boundary term. We then split the quadratic term according to

$$R+\epsilon R^2=R(1+p\epsilon R)-(p-1)\epsilon R^2 \quad \text{(A9)}$$

to simulate a mass term (here p is some real number). The expression that multiplies the scalar curvature in the first term can be removed by a conformal transformation to leave a pure Einstein action. We need

$$\tilde{g}_{\alpha\beta}=\Omega g_{\alpha\beta}\ ,\quad (-\tilde{g})^{1/2}=\Omega^2(-g)^{1/2}\ ,$$

and (A10)

$$R=\Omega\tilde{R}+3\tilde{\Box}\Omega-\tfrac{9}{2}(\Omega)^{-1}\Omega_{,\rho}\Omega_{,\sigma}\tilde{g}^{\rho\sigma}\ .$$

The special choice, $\Omega=1+p\epsilon R$, does the trick. After one integration by parts of the second term we obtain a kinetic term for the R field and a surface term is generated:

$$S=\frac{1}{16\pi G}\int d^4x(-\tilde{g})^{1/2}$$
$$\times\left[\tilde{R}-\frac{3}{2}\frac{p^2\epsilon^2}{(1+p\epsilon R)^2}\right.$$
$$\left.\times\left[R_{,\beta}R_{,\delta}\tilde{g}^{\beta\delta}+\frac{2}{3}\frac{p-1}{p^2\epsilon}R^2\right]\right]$$
$$+\text{b.t.}-\frac{1}{8\pi G}\int d^3x(h)^{1/2}\tfrac{3}{2}(1+p\epsilon R)_{,t}\ . \quad \text{(A11)}$$

We are led uniquely to the choice $p=2$ to secure the correct mass term at linear order. The kinetic term for the scalar degree of freedom can be brought into canonical form by the substitution $\phi=\frac{1}{2}\ln(1+2\epsilon R)$ [cf. Eq. (2.8)]. Since we manifestly have just a scalar field plus Einstein gravity, the original boundary term and the surface term in Eq.(A11) should combine to give the standard boundary term for Einstein gravity.

In the $3+1$ split of spacetime in which the boundary is a $t=$const slice, we make use of the identity

$$\tilde{K}(\tilde{h})^{1/2}=\Omega K\sqrt{h}-\tfrac{3}{2}\sqrt{h}\,\Omega_{,t} \quad \text{(A12)}$$

and find

$$\text{b.t.}=\frac{1}{16\pi G}\int d^3x\sqrt{h}\,2K(1+2\epsilon R)\ , \quad \text{(A13)}$$

as we found in Eq. (A6).

One remaining question is just what fields are to be held fixed on the boundary. In the conformal picture, the answer is straightforward: As the theory is only Einstein gravity plus a scalar field, we need only fix the field ϕ and the conformal three-metric on the boundary to obtain a well-posed variational problem.[34] From the conformal transformation (A10), with $\Omega=1+2\epsilon R$, we see that this corresponds to fixing the physical three-metric and scalar curvature on the boundary.

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