Homogeneous modes of cosmological instantons

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We discuss the $O(4)$ invariant perturbation modes of cosmological instantons. These modes are spatially homogeneous in Lorentzian spacetime and thus not relevant to density perturbations. But their properties are important in establishing the meaning of the Euclidean path integral. If negative modes are present, the Euclidean path integral is not well defined, but may nevertheless be useful in an approximate description of the decay of an unstable state. When gravitational dynamics is included, counting negative modes requires a careful treatment of the conformal factor problem. We demonstrate that for an appropriate choice of coordinate on phase space, the second order Euclidean action is bounded below for normalized perturbations and has a finite number of negative modes. We prove that there is a negative mode for many gravitational instantons of the Hawking-Moss or Coleman–De Luccia type, and discuss the associated spectral flow. We also investigate Hawking-Turok constrained instantons, which occur in a generic inflationary model. Implementing the regularization and constraint proposed by Kirklin, Turok and Wiseman, we find that those instantons leading to substantial inflation do not possess negative modes. Using an alternate regularization and constraint motivated by reduction from five dimensions, we find a negative mode is present. These investigations shed new light on the suitability of Euclidean quantum gravity as a potential description of our universe.

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I. INTRODUCTION

An important issue in the study of quantum gravity is the question of whether a consistent Euclidean formulation exists at all. There is of course the problem of renormalizability, but this may be considered a ''technical'' difficulty perhaps to be resolved by the inclusion of more degrees of freedom at high energies. Somewhat more fundamental is the apparent unboundedness of the Euclidean action itself, known as ''the conformal factor problem'' [1]. This problem has a deep physical origin in the fact that there is no canonical ensemble for gravitating systems. This is perhaps the major hazard to be faced by the use of non-perturbative Euclidean techniques.

In this paper we study the behavior of the action around a class of non-perturbative $O(4)$ invariant classical solutions of Euclideanized Einstein–scalar-field theory called cosmological instantons. These instantons have been used for some time in inflationary theory to describe the decay of an inflating false vacuum state [2]. In analogy with the instanton description of quantum tunneling [3,4], one expects such instantons to possess a single negative mode [5], leading to an imaginary contribution to the energy of the unstable state. For the tunneling interpretation to be valid, it is important to establish the presence of the negative mode. However, if such a mode exists, this equally establishes that the Euclidean path integral can only be regarded as an approximation since it is ill defined at a fundamental level.

Cosmological instantons are also used in another, more ambitious context. They provide a first approximation to the Euclidean no boundary path integral [6], and therefore are the possible foundation for a description of the initial conditions of the universe itself. One seeks solutions of the no boundary form, in which Lorentzian spacetime is analytically rounded off on a Euclidean region. Correlators of observables are then to be computed via a perturbation expansion in the Euclidean region. Since the Euclidean propagator is unique, in principle one should obtain unique Euclidean correlators which then, after analytic continuation to the Lorentzian region, fully define the theory [7].

The existence of negative modes should, we believe, be a major consideration in deciding whether or not instantons should be regarded as describing tunneling or whether they provide a fundamental description of the initial state for the universe. The complete set of fluctuation modes divides into those which are $O(4)$ invariant in the Euclidean region and those which are not. The latter describe inhomogeneous cosmological perturbations, and it is well known that they possess positive Euclidean action. Negative modes can however arise in the $O(4)$ invariant sector and in this paper we shall develop the technology necessary to describe them.

At first sight the conformal factor problem makes the problem of defining the number of negative modes intractable. If an inappropriate choice of variables is made, as in [8] for example, the Euclidean action is unbounded below with an infinity of negative modes appearing. Another approach has been proposed which involves Wick rotating infinite sub-classes of modes in the Euclidean region and arguing about the transformation properties of the measure [9,10]. This is related to the proposal of Gibbons, Hawking and Perry [1] of Wick rotating the conformal factor fluctuations to make the Euclidean path integral bounded. These methods seem rather arbitrary and contrived and do not seem to yield sensible results when applied to both Hawking-Moss as well as Coleman–De Luccia instantons.

Instead we shall attempt to continue to the Euclidean region in a well-defined manner following from a Hamiltonian formulation in the Lorentzian region. We integrate out gauge

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degrees of freedom in the Lorentzian region and analytically continue only physical degrees of freedom. It is important to note that the analytic continuation which generalizes the choice $t \rightarrow -i\tau$ in Minkowski spacetime is completely fixed by considering a hypothetical field only weakly coupled to gravity and demanding that its action be positive definite in the Euclidean region.

To quadratic order in the fluctuations, ''three-fourths'' of the conformal factor problem is solved by removing gauge degrees of freedom and taking the Einstein $G_{0\mu}$ constraint equations properly into account. The latter link the variation of the metric with the amplitude of the scalar field, so a quickly oscillating metric leads to a large scalar field fluctuation and large Euclidean action. This eliminates negative kinetic terms for $O(4)$ non-invariant modes (i.e. the spatially inhomogeneous modes in the Lorentzian universe), as discussed for example in Ref. [7].

The remaining negative kinetic terms are associated with the $O(4)$ invariant modes. As discussed above, the negativity is meaningful and we should not attempt to artificially remove it. Rather we seek to isolate it in a discrete number of clearly identified fluctuation modes. Changes of variable in the path integral can be very helpful for this purpose. Consider for example quantum mechanics in real time for a particle with a positive harmonic potential but a negative kinetic term. The real time path integral may be written

$$\int [dq]\exp\left[i\int dt\left(-\frac{A}{2}\dot{q}^2-\frac{B}{2}q^2\right)\right], \tag{1}$$

where both A and B are positive. If we perform the usual analytic continuation $t=-i\tau$, we obtain a Euclidean action with a negative kinetic term, analogous to the case of gravity. For normalized fluctuations in q the Euclidean action possesses an infinite number of negative modes. However, a functional Fourier transform sheds new light on the problem. We can reproduce the first term in the action with a functional integral over p, with the term $\int p\dot{q}+(1/2A)p^2$. We then integrate by parts in t and functionally integrate over q, obtaining, in place of Eq. (1),

$$\int [dp]\exp\left[i\int dt\left(\frac{1}{2B}\dot{p}^2+\frac{1}{2A}p^2\right)\right]. \tag{2}$$

We notice that the coefficients of the kinetic and potential terms have been interchanged, so that we now have a positive kinetic term and a negative potential term. Continuing as before via $t=-i\tau$, the Euclidean action now has a positive kinetic term. Of course the potential term is now negative, so we have merely replaced one ill-defined Euclidean path integral with another and one might think we had not gained much. But for the context below, where the Euclidean region is compact, the positivity of the kinetic term means that even if the potential term is negative, the action is bounded below for normalized perturbations and the number of negative modes is then finite.

The functional Fourier transform used above is of course just another way of introducing the full first order action on phase space (p,q) appropriate to a Hamiltonian treatment. The freedom we then exploit is the choice of the linear combination of p and q for the retained variable to be continued to the Euclidean region. If some particular linear combination yields a positive kinetic term throughout the Euclidean region, this is to be preferred since the number of negative modes is then countable. Note that just one linear combination of p and q is sufficient to completely define the theory in the Euclidean region, since correlators of the independent linear combination may be derived by differentiating with respect to time and using the Heisenberg equations of motion ($q=-\dot{p}/B$ in the example above).

Using the freedom to define the retained coordinate, and exploiting the fact that the number of negative modes of a Sturm-Liouville operator is independent of the measure chosen, we prove that large classes of regular gravitational instantons have negative modes. This puts tunneling interpretations of these instantons on a firmer footing. But as discussed above it raises doubts about using them to describe the beginning of the universe.

Indeed in theories with Hawking-Moss and Coleman–De Luccia instantons, there is usually a lower action instanton which does not possess negative modes. Consider theories where there is a global potential minimum, and it is positive. Then there is an instanton which is a round four-sphere. The radius of the sphere tends to infinity as the potential minimum decreases to zero. This instanton solution has no negative modes. Its analytic continuation is just empty de Sitter spacetime, or in the limit of zero potential minimum, Minkowski spacetime. It seems to us that this trivial vacuum state, defined by the lowest action instanton, is in fact the natural one implied by the Euclidean no boundary proposal for the sector of the theory with the simplest S^4 topology. Selecting another instanton with this topology (Hawking-Moss or Coleman–De Luccia) to describe the beginning of the universe seems unacceptable. Since those instantons possess negative modes, they may describe tunneling from one approximate, unstable state but to use them as the basis for a fundamental description is surely questionable.

The existence of singular, but finite action, constrained instanton solutions [11] in a generic inflationary model opens new possibilities in this regard. Such instantons may be made regular by a change of variables on superspace plus an appropriate regularization of the potential $V(\phi)$ at large values of the inflaton field ϕ [12]. In the regular description, the topology of the solutions is not S^4 but RP^4, and the scalar field is actually a twisted field living on that manifold. These instantons are classical solutions in a sector of the theory which is topologically distinct from the naive S^4 Euclidean vacuum discussed above. Implementing the regularization scheme of Kirklin, Turok and Wiseman [12], we show that the constraint removes negative modes for those instantons giving substantial inflation. There is therefore a stable valley in the configuration space of the Euclidean theory, and the Euclidean path integral for fluctuations about such solutions is well defined to quadratic order. It may therefore possess a well-defined perturbative expansion to higher orders.

The outline of the paper is as follows. We review negative modes of Hawking-Moss instantons, before discussing regular Coleman–De Luccia instantons and then generic singular

Hawking-Turok instantons. Motivated by the construction of Ref. [12] we regularize the latter by matching the scalar potential $V(\phi)$ at large ϕ to a certain class of exponentially decaying potentials. We discuss an alternate regularization and constraint motivated by Garriga'a construction of singular instantons as dimensionally reduced five dimensional regular solutions [13]. In the latter construction, a negative mode is always present for a generic slow-roll potential. Finally implications of this work for Euclidean quantum gravity are commented upon.

Our study yields a simple picture of Euclidean configuration space for a generic inflationary theory, into which the known classical solutions fit. The valley we have identified for Hawking-Turok instantons is potentially of much interest since it may provide a well-defined perturbative basis for Euclidean approaches to inflationary cosmology.

We would like to draw to the attention of the reader the recent work of Khvedelidze, Lavrelashvili and Tanaka [14,15], which also addresses the issue of negative modes about Coleman–De Luccia instantons.

II. SECOND ORDER ACTION

Our starting point is the second order action for scalar perturbations in the Lorentzian universe, as discussed in Sec. 4 of [7]. We consider a scalar field ϕ with potential $V(\phi)$ minimally coupled to gravity. The background field equations are

$$\phi''+2\mathcal{H}\phi'=-a^2V_{,\phi}(\phi),$$

$$\mathcal{H}^2=\frac{\kappa}{3}\left(\frac{1}{2}\phi'^2+V(\phi)a^2\right)-\mathcal{K}, \tag{3}$$

where $\kappa=8\pi G$, $\mathcal{H}=a'/a$, primes denote derivatives with respect to conformal time and $\mathcal{K}=0,\pm1$ for flat, closed and open Friedmann-Robertson-Walker (FRW) universes. With the perturbed line element

$$ds^2=a^2\{-(1+2A)d\tau^2+2B_{|i}dx^id\tau+[(1-2\psi)\gamma_{ij}+2E_{|ij}]dx^idx^j\}, \tag{4}$$

and the scalar field represented as $\phi+\delta\phi$, with ϕ the background solution, the second order action for fluctuations is given by Eq. (18) of [7], reproduced here:

$$S_2=\frac{1}{2\kappa}\int d\tau d^3xa^2\sqrt{\gamma}\Big\{-6\psi'^2-12\mathcal{H}A\psi'+2\Delta\psi(2A-\psi)-2(\mathcal{H}'+2\mathcal{H}^2)A^2+\kappa(\delta\phi'^2+\delta\phi\Delta\delta\phi-a^2V_{,\phi\phi}\delta\phi^2)$$
$$+2\kappa(3\phi'\psi'\delta\phi-\phi'\delta\phi'A-a^2V_{,\phi}A\delta\phi)+\mathcal{K}[-6\psi^2+2A^2+12\psi A+2(B-E')\Delta(B-E')]$$
$$+4\Delta(B-E')\left(\frac{\kappa}{2}\phi'\delta\phi-\psi'-\mathcal{H}A\right)\Big\}. \tag{5}$$

This is well defined for all values of ϕ' and the three-space Laplacian Δ. In an open universe Δ takes the value zero for the spatially homogenous mode and $-p^2-1$ with $p^2>0$ for the continuum of square integrable modes. In a closed universe Δ is given by $-n^2+1$ with $n\in\mathcal{N}$.

The momenta canonically conjugate to ψ, E, and $\delta\phi$ are

$$\Pi_\psi=\frac{2a^2\sqrt{\gamma}}{\kappa}\left(-3\psi'+3\frac{\kappa}{2}\phi'\delta\phi-3\mathcal{H}A-\Delta(B-E')\right),$$

$$\Pi_E=\frac{2a^2\sqrt{\gamma}\Delta}{\kappa}\left(\psi'-\frac{\kappa}{2}\phi'\delta\phi+\mathcal{H}A-\mathcal{K}(B-E')\right),$$

$$\Pi_{\delta\phi}=a^2\sqrt{\gamma}(\delta\phi'-\phi'A). \tag{6}$$

Under an infinitesimal scalar coordinate transformation $x^\mu\to x^\mu+\lambda^\mu$, where $\lambda^\mu=(\lambda^0,\lambda^{|i})$, the perturbation fields and momenta transform as

$$\psi\to\psi-\mathcal{H}\lambda^0,\quad B\to B+\lambda'-\lambda^0,\quad A\to A+\lambda^{0\prime}+\mathcal{H}\lambda^0,$$

$$E\to E+\lambda,\quad \delta\phi\to\delta\phi+\phi'\lambda^0,$$

$$\Pi_\psi\to\Pi_\psi+\frac{2a^2\sqrt{\gamma}}{\kappa}(\Delta+3\mathcal{K})\lambda^0,\quad \Pi_E\to\Pi_E,$$

$$\Pi_{\delta\phi}\to\Pi_{\delta\phi}+a^2\sqrt{\gamma}(\phi''-\mathcal{H}\phi')\lambda^0. \tag{7}$$

III. HAWKING-MOSS INSTANTONS

Let us first consider Hawking-Moss instantons [16], where the scalar field is everywhere a constant. It is well known that these have negative eigenmodes for $V_{,\phi\phi}<0$. The corresponding Lorentzian solution has $\phi'=0$ everywhere and so $V_{,\phi}$ must be zero. We notice immediately from Eq. (5) that the matter and metric degrees of freedom decouple and, from Eq. (7), that $\delta\phi$ has become a gauge invariant variable. Introducing conjugate momenta to the gravitational degrees of freedom and performing the integrals, we find that no gauge invariant combination of the fields and momenta that is not forced to be zero is left. This means that there are no real degrees of freedom described by the metric. Indeed Ψ_N is forced to be zero here, making one wary of any approach (such as that in [9,10]) pertaining to negative modes that relies on metric variables alone. Returning to the matter degree of freedom, we analytically continue into the Euclidean region as detailed in [7], leaving us with the action

$$\frac{1}{2}\int dX d^3x b^2 \sqrt{\gamma}(\delta\phi'^2 - \delta\phi\Delta_3\delta\phi + b^2 V_{,\phi\phi}\delta\phi^2), \quad (8)$$

where γ is now the determinant of the Euclidean metric, and the Euclidean background line element is $b^2(X)(dX^2 + \gamma_{ij}dx^i dx^j)$ with γ_{ij} the metric on the round three-sphere. All gradient terms are positive, so this action is bounded below for square-integrable variations of the scalar field. The first thing to note is that if $V_{,\phi\phi}>0$, then this action is positive definite and so the spacetime is perturbatively stable. If $V(\phi_0)$ is the global minimum of V, one might expect that this spacetime is non-perturbatively stable as well. We can see the existence of a negative mode for $V_{,\phi\phi}<0$ as follows. The eigenvalue equation associated with this action is of Sturm-Liouville form, but we have some freedom in specifying the measure, which we shall repeatedly exploit. $b^4\sqrt{\gamma}$ is a permissible choice, allowing us to just read off that $\delta\phi=\text{const}$ is an eigenmode with eigenvalue $V_{,\phi\phi}$. One might enquire if there is another negative mode. Rescaling $\delta\phi$ by a factor of b, the action operator takes Schrödinger form and choosing the measure to be $\sqrt{\gamma}$ gives us the Schrödinger equation with a $-(2-V_{,\phi\phi}/H^2)/\cosh^2 X + n^2$ potential with H^2 here defined to be $\kappa V_0/3$, and where $n^2=-\Delta_3+1$, with Δ_3 the Laplacian on S^3. This can be solved for the negative eigenvectors and eigenvalues (see [17] for example) in terms of hypergeometric functions. The number of negative modes is independent of the choice of measure. For $-4<V_{,\phi\phi}/H^2<0$ there is one, for $-10<V_{,\phi\phi}/H^2<-4$ there are six, and in general for $-N(N+3)<V_{,\phi\phi}/H^2<-(N-1)(N+2)$, where $N\in\mathcal{Z}^+$, there are $N(N+1)^2(N+2)/12$ negative modes. This counting agrees with an $O(5)$ spherical harmonic analysis. We see that as $V_{,\phi\phi}$ becomes more negative from zero five more modes suddenly cross zero at $V_{,\phi\phi}/H^2=-4$, meaning that the Hawking-Moss instanton cannot now have anything to do with tunneling. This is very interesting because one of the new negative modes is spatially homogeneous and antisymmetric in X. In fact it is the perturbative indication of the existence of a lower-action non-perturbative solution, namely the Coleman–De Luccia instanton for the same potential. $V_{,\phi\phi}/H^2<-4$ is the precise condition for the existence of a Coleman–De Luccia instanton [18], which has a lower action. We will show below that this itself has a negative mode, which may be viewed as the carryover of the lowest one of the Hawking-Moss instanton. The spectral flow is as follows. For small negative $V_{,\phi\phi}$, there is only one classical solution (the Hawking-Moss instanton) with one negative mode. As $V_{,\phi\phi}$ becomes more negative, one of the positive eigenvalues decreases to zero. As it crosses zero, a new classical solution is obtained by flowing down the new negative direction to a new saddle point, which retains the original negative mode but is stable in other directions. The spatially homogeneous negative modes gained by passing through $V_{,\phi\phi}/H^2=-N(N+3)$, $N>1$, correspond to the coming into existence of non-perturbative multibounce instantons. From spectral flow arguments one would expect these to possess N negative modes. The same arguments indicate that the lowest action Coleman–De Luccia instanton should only have one negative mode, and this is confirmed numerically as we discuss below.

IV. COLEMAN–De LUCCIA INSTANTONS

Let us now consider Coleman–De Luccia instantons [2]. We start in the open universe from Eq. (5). For $\Delta\neq 0$, we proceed as in Sec. 4 of Ref. [7] to Eq. (20) there. We do the B and Π_E integrals, effectively setting $\Pi_E=0$ in that expression. For $\Delta=0$, B and E no longer appear in Eq. (5), and we cannot define a Π_E. However, we can still introduce Π_ψ and $\Pi_{\delta\phi}$ and work forward to the same expression in terms of A, ψ, Π_ψ, $\delta\phi$, and $\Pi_{\delta\phi}$ as for $\Delta\neq 0$. So from now on we treat $\Delta=0$ and $\Delta\neq 0$ in a unified way. Ψ_N, as defined in Eq. (21) of Ref. [7], is singular for $\Delta=0$, and from our experience with the Hawking-Moss case above we know that spatially homogeneous fluctuations are significant when investigating negative modes. So we define the closely related variable

$$\Psi_l = (\Delta+3\mathcal{K})\psi + \frac{\mathcal{H}\kappa\Pi_\psi}{2a^2\sqrt{\gamma}} \quad (9)$$

where we have also taken the opportunity to multiply through by $\Delta+3\mathcal{K}$ in order to keep our fields local. This is gauge invariant and classically the same as $(\Delta+3\mathcal{K})\Psi_N$ since Π_E is constrained to be zero. In [7], introducing Π_N made the action independent of $\delta\phi$. This is classically equivalent to working in a gauge $\delta\phi=0$, and from the Hawking-Moss example we see that this is potentially awkward. So here we define

$$\delta\phi_l = (\Delta+3\mathcal{K})\delta\phi - \frac{\kappa\phi'\Pi_\psi}{2a^2\sqrt{\gamma}} \quad (10)$$

which is again local and gauge invariant. Using $\delta\phi_l$ and Ψ_l is classically equivalent to working in the gauge $\Pi_\psi=0$, which from Eqs. (6) and for $\mathcal{K}\neq 0$ is a good gauge everywhere. Integrating over A imposes the delta functional constraint on $\Pi_{\delta\phi}$, which is then integrated over, leaving the action in the simple form

$$\int d\tau d^3x \frac{a^2\sqrt{\gamma}}{\Delta+3\mathcal{K}} \times\left\{\frac{2}{\kappa\phi'}\Psi_l\delta\phi_l' + \frac{2(\mathcal{H}\phi'-\phi'')}{\kappa\phi'^2}\Psi_l\delta\phi_l + \frac{1}{2}\delta\phi_l^2 - \frac{1}{\kappa}[1+2(\Delta+3\mathcal{K})/\kappa\phi'^2]\Psi_l^2\right\}. \quad (11)$$

It is remarkable that in the $\Pi_\psi=0$ gauge, the Newtonian potential Ψ and the scalar field fluctuation $\delta\phi$ are the two remaining physical and canonically conjugate variables.

We now have a choice in deciding which linear combination of $\delta\phi_l$ and Ψ_l to retain as our coordinate before continuing to the Euclidean region. Having made this choice we integrate out any remaining non-parallel combination and obtain a quadratic action for the coordinate of interest, which we continue to the Euclidean region. For a given background instanton, if the Euclidean action has positive definite derivative terms, it is bounded below for normalized square integrable fluctuations of that variable, and we have made a good choice for isolating negative modes. From our experience with Hawking-Moss an obvious choice is to take $\delta\phi_l$ itself. After analytic continuation to the Euclidean region, followed by a simple rescaling $Q=b\,\delta\phi_l/\phi'$, the action takes the form

$$\int \frac{dXd^3x\sqrt{\gamma}\phi'^2}{2(-\Delta_3-3)^2}\left(\frac{Q'^2}{1+\kappa\phi'^2/2(-\Delta_3-3)}+(-\Delta_3-3)Q^2\right). \tag{12}$$

Let us first briefly discuss the technicality of what happens when $(-\Delta_3-3)=0$, corresponding to $n=2$ (recall that the eigenvalues of the Laplacian on S^3 are $-n^2+1$, $n\in\mathcal{N}$). This action is infinite unless $Q=0$. One takes this to be a positive infinity since then it says that $(-\Delta_3-3)=0$ modes are infinitely suppressed. That this is correct can be seen by considering Eq. (5) for this mode in a closed universe with $\phi'\neq 0$. There is a degeneracy between ψ and E, resulting in only the sum $\psi+E$ affecting the three-metric. Then there are no gauge-invariant combinations of fields and momenta that are not forced to be zero. Note that $(-\Delta_3-3)=0$ modes do exist for the Hawking-Moss instanton but in that case $\phi'=V_{,\phi}=0$ everywhere.

Having dealt with this, we move on to the more interesting cases of $n=1$ and $n>2$. In the latter inhomogeneous case both the kinetic terms and the potential terms are positive definite, giving no possibility of negative modes. Now let us consider the potentially dangerous homogeneous $n=1$ mode. The kinetic term is positive definite as long as $1-\kappa\phi'^2/6>0$ across the entire instanton. This condition holds for a wide class of Coleman–De Luccia instantons, of both the thin-wall and the thick-wall variety. In this case we see the existence of the negative mode $Q=\text{const}$ by choosing the measure $\phi'^2\sqrt{\gamma}$. So a wide class of Coleman–De Luccia instantons are shown to have a negative mode. Incidentally we note that had we chosen a variable that had no $\delta\phi$ matter component, the homogeneous mode would have had negative definite kinetic term, as found in [9,10]. Then the action could be arbitrarily negative for square integrable fluctuations of the metric variable.

Having chosen a measure, one can numerically determine the other eigenmodes and eigenvalues of the operator. For Coleman–De Luccia instantons associated with potentials of Gaussian form $e^{-A\phi^2}$ for example, we have found no evidence of further negative modes about these lowest-action regular solutions. This is consistent with expectations based on spectral flow from the Hawking-Moss instanton as discussed above.

V. HAWKING-TUROK INSTANTONS

On singular instantons, as the scalar field tends to infinity, the condition $1-\kappa\phi'^2/6>0$ is certainly violated. However, this by itself does not mean that we should exclude them. Rather we should first consider the possibility that gravity on the instanton is sufficiently strong that a pure matter variable like Q does not provide a suitable description of the fluctuations. Indeed, going back to Eq. (11), we can define $\overline{Q}=\delta\phi_l+2(\mathcal{H}-\phi''/\phi')\Psi_l/\kappa\phi'$ to obtain, after analytic continuation,

$$\int \frac{dXd^3xb^2\sqrt{\gamma}}{2(-\Delta_3-3)^2}\left(\frac{(-\Delta_3-3)\overline{Q}'^2}{\phi'(1/\phi')''-\Delta_3-4}+(-\Delta_3-3)\overline{Q}^2\right). \tag{13}$$

This time we see that the kinetic term is positive definite both for $n=1$ and $n>2$ as long as $-4<\phi'(1/\phi')''<4$. Using the background field equations, we have

$$D(X)\equiv\phi'(1/\phi')''-4 = -b^2\left(2\kappa V+\frac{8\mathcal{H}V_{,\phi}}{\phi'}+V_{,\phi\phi}-\frac{2b^2V_{,\phi}^2}{\phi'^2}\right). \tag{14}$$

We see that if the potential has a maximum, then we must have $2\kappa V+V_{,\phi\phi}>0$ for $\overline{Q}$ to be a suitable variable. Let us examine the behavior of this term near the singularity. We have b^2 going like X, and ϕ goes like $-\sqrt{3/2\kappa}\ln X$. If V is polynomial, D goes like X times a term involving $\ln X$ factors. Now the solution of the eigenvalue operator for any eigenvalue is of the form $A\int D(X)/X\,dX+B$ near the singularity and we see that this has finite action for any A and B. This shows that the action alone does not in fact impose the boundary conditions for the $O(4)$ invariant perturbations of singular instantons. It is consistent with the fact that singular instantons cannot be regarded as unconstrained saddle points of the Euclidean action since the action varies across the class of singular instantons. They must be defined by introducing a constraint into the path integral which is later integrated over. This constraint determines the allowed $O(4)$ invariant modes. If one is interested in calculating a correlator which weights particularly strongly towards a given value for the constraint (for example if we are interested in correlating with the observed value of Ω today), it may be useful to only consider one sector and ignore the integration over the constraint. This is what is effectively done in [7,19] where a constraint is implicitly applied to give an acceptable value of Ω_0, and homogeneous fluctuations are ignored since they do not affect the microwave background correlations.

VI. REGULARIZED INSTANTONS

In the above section we saw that if V were polynomial in ϕ, then D went like X times a term involving $\ln X$ factors.

However, if V is asymptotically of the form $(e^{-\sqrt{2\kappa/3}\phi})^r$, with r an odd integer, then D goes like X^{r+1}, and the eigenfunctions have the form $AX^{r+1}+B$ near the singularity. Therefore with this form of potential the theory has good analytic behavior near the singularity. This suggests that with this type of potential there is special behavior and indeed this is the case. We see here the perturbative indication of the scenario of Kirklin, Turok and Wiseman [12]. There it is shown that singular instantons of potentials with the asymptotic form $(e^{-\sqrt{2\kappa/3}\phi})^r$, with r odd and greater than -3, may be viewed as true classical solutions of a theory related to the original theory by a conformal transformation which vanishes at the Einstein frame singularity. In terms of the new variables the metric is strictly Riemannian and the instantons are regular.

If we use this scheme to regularize the singular instantons occurring in a generic inflationary theory, we must modify the potential so that it tends to $(e^{-\sqrt{2\kappa/3}\phi})^r$ at large ϕ. The theory is then defined as the limit where this modification occurs at infinitely large ϕ. We must check that our results are insensitive to the details of how the limit is taken. We choose r positive because for $r=-1$, the function $D(X)$ vanishes making the kinetic term for the fluctuations ill defined.

In the regularized theory, the appropriate degrees of freedom are combinations of the conformal factor and the scalar field, residing on a regular Riemannian manifold. This manifold is taken to have the topology of RP^4, and the conformal factor is taken to be in the twisted sector. This enforces the conformal zero, corresponding to the singularity. On the non-contractible three-surface where the conformal factor is zero, one is free to specify the Riemannian three-metric, and this corresponds to information stored ''at the singularity'' in the original Einstein frame.

The appropriate action in this picture is one where the Riemannian three-metric is fixed on the conformal zero. In terms of Einstein frame variables, this action is just the standard first derivative action [20] including the usual Gibbons-Hawking boundary term. For $O(4)$ invariant solutions the boundary data may be taken to be the value of m on the three-surface, m_B, where m is the Riemannian frame radius given by $m\equiv be^{\sqrt{\kappa/6}\phi}$ in terms of Einstein frame variables. We treat the value of m_B at the conformal zero as a variable to be integrated over in the path integral. For m_B smaller than some value there is no classical solution. However, for larger m_B there are two solutions, one of higher and one of lower Euclidean action. The higher action solution corresponds to low values of the scalar field ϕ_0 at the beginning of the Lorentzian open universe. The lower action solution corresponds to a larger value for ϕ_0. As m_B is increased, the corresponding value of ϕ_0 increases to infinity, giving larger and larger amounts of inflation in the Lorentzian universe.

It is slightly subtle to impose the required constraint because the single field degree of freedom we use is not δm. However, we express δm in terms of $\overline{Q}$ and its canonical conjugate, as given by its saddle-point value in the path integral. Consider working in the gauge $\delta\phi=0$. This is a good gauge near the singularity because ϕ is varying quickly there. Then δm goes like ψ, which in terms of our gauge-invariant local variables is proportional to $\Psi_l+\mathcal{H}\delta\phi_l/\phi'$. Now $\overline{Q}=\delta\phi_l+2(\mathcal{H}-\phi''/\phi')\Psi_l/\kappa\phi'$, and at the saddle point $\Psi_l=\kappa\phi'\overline{Q}'/2D(X)$. Consequently δm is proportional to $\overline{Q}-3\overline{Q}'/\mathcal{H}D(X)$ near the singularity. Our numerical code uses the auxiliary variable $P\equiv b^2\overline{Q}'/D(X)$ and works in proper Euclidean time. So the condition that we must impose on our eigenfunctions is that $\overline{Q}+3P/b^2\dot{b}=0$ at the singularity. It is straightforward to show that the most general solution of the $\overline{Q}$ eigenvalue equation has the behavior AX^2+B near $X=0$, and our boundary condition is a specific relation between A and B.

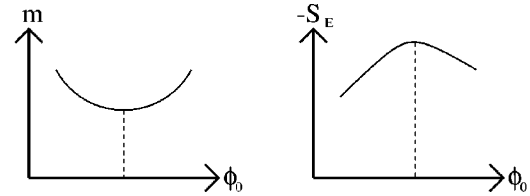

FIG. 1. The left sketch shows how m at the singularity varies with the value of ϕ at the regular pole. The right sketch shows how the appropriate action of the singular instanton varies with the value of ϕ at the regular pole.

We have investigated a number of potentials which behave appropriately at large ϕ. For example we have matched a ϕ^2 potential onto the $e^{-\sqrt{2\kappa/3}\phi}$ potential using a negative cubic term. One has to be slightly careful with the matching prescription so that one does not violate the $2\kappa V+V_{,\phi\phi}>0$ condition for $\overline{Q}$ to be a good variable at the turnover point. As long as the matching is done a long way further along the potential than where the runaway behavior starts, the results are in any case insensitive to the details of the matching.

Now as explained above there are two starting values of ϕ at the regular pole which lead to the same value of m_B at the singularity (see Fig. 1). The instanton with larger ϕ at the regular pole has lower action. Since for fixed m_B these are the only two extrema, one could anticipate that the larger ϕ solution would be stable and the lower ϕ solution unstable. We have confirmed this numerically.

Now as we vary m_B downwards the values of ϕ at the regular pole in the two solutions move closer and ultimately merge, in the unique solution with minimal m_B. The associated instanton is the one with the most negative action, and it is is like a critical point. Since two solutions—one unstable and one stable—are merging, one expects to find that the resulting configuration has a zero mode and this is indeed confirmed numerically.

As a result of this investigation we can build up a picture of the action-configuration space structure of the theory as shown in Fig. 2, and we can speculate as to what the structure might look like away from where we have been able to probe. For m_B above the critical value, there is a stable valley in m_B, ϕ space where the stability increases with increasing m_B. The instantons with lower action are con-

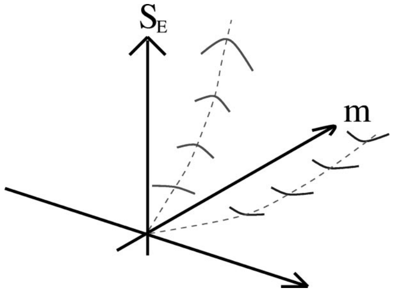

FIG. 2. A sketch of the dependence of the Euclidean action on the metric and scalar field configurations, about the constrained singular instantons, represented by the dashed lines. The dashed lines represent the instanton solutions at each m. The orthogonal direction shows the lowest eigendirection at fixed m. The lower action solution (larger ϕ) possesses no negative modes: the higher action solution possesses one. As m is lowered, the two solutions approach and merge, with a zero mode being produced. At smaller values of m there is no classical solution.

strained solutions which lie on the floor of this valley. However, at lower ϕ there is an unstable ridge, which is joined to the valley at the critical m_B. The implication is that even though the constrained instantons in the valley are stable, there are nonperturbative instabilities lurking at low ϕ, beyond the unstable ridge, and at low m_B, below the critical point. Hence it seems unlikely that the Euclidean path integral will be well defined nonperturbatively. It appears that at the very least projection operators onto certain subclasses of configuration space in the path integral are required.

VII. CONNECTIONS WITH PREVIOUS WORK

In this section we briefly show that the approach presented in this paper leads to the same results as in [7] for the computation of cosmic microwave background (CMB) background anisotropies about singular instantons. One needs to check that the spatially inhomogeneous modes allowed for one choice of path integral variable correspond to the equivalent modes allowed for the other choice of variable. For the inhomogeneous modes, Ψ_l and Ψ_N are equivalent, and we shall show that the q modes allowed in [7] give the same behavior in Ψ_N near the singularity as the allowed $\overline{Q}$ modes here give in Ψ_l. In [7], the unsuppressed q modes behaved as $X^{3/2}$, corresponding to Ψ_N tending to a constant. The suppressed mode had $q \to X^{-1/2}$, corresponding to Ψ_N diverging like $1/X^2$. The eigenvalue equation leading from Eq. (13) looks like $(X\overline{Q}')'=0$ near the singularity, with general solutions of the form $A \ln X + B$. Substituting back into the action we find that the $\ln X$ solution has infinite action and so is suppressed. At the saddle point we have Ψ_l behaving as $\overline{Q}'/X$ and we see that $\overline{Q} \to A \ln X$ corresponds to $\Psi_l \to 1/X^2$, whereas the unsuppressed mode $\overline{Q} \to B + O(X^2)$ corresponds to Ψ_l being finite. Hence both approaches select the same allowed modes and thus give equivalent correlators.

No such check is necessary for the non-singular instantons because in this case there is no boundary and all modes are allowed.

VIII. ALTERNATE "FIVE DIMENSIONAL" BOUNDARY CONDITION

For the special potential $V \propto e^{(\sqrt{2\kappa/3})\phi} = n^{-1}$, where here $n \equiv e^{(-\sqrt{2\kappa/3})\phi}$, Garriga showed [13] that singular Hawking-Turok instantons could be interpreted as "dimensional reductions" of a regular five-dimensional solution, which is just a round five sphere. He showed that the five dimensional action, when written in four dimensional variables, differs from the standard first-derivative four dimensional action by minus two thirds of the Gibbons-Hawking surface term. He also showed that for arbitrary potential V one reached the same conclusion if one introduced a brane (of negative tension) to regularize the singularity.

In this section we study the existence of negative modes for a form of the action motivated by Garriga's observation, for arbitrary scalar potential $V(\phi)$. Note that Garriga's five-dimensional example yields the specific potential $e^{(\sqrt{2\kappa/3})\phi}$. The exact solution here has $\phi' \propto 1/\sinh 2X$ and the function $D(X)$ which enters the kinetic term for the perturbations vanishes identically. We are unable therefore to prove existence of a negative mode in this case. Indeed this is perfectly consistent since from a five-dimensional view, the Garriga solution should have no negative modes. It is a round five-sphere and continues to five-dimensional de Sitter spacetime which is presumably stable in analogy with our treatment of the four-dimensional case.

The five dimensional line element is given in terms of the four-dimensional one ds_4^2 by $ds_5^2 = n^{-1} ds_4^2 + n^2 dy^2$ where $ds_4^2 = N^2 d\sigma^2 + b^2(\sigma) d\Omega_3^2$ and $0 < y \leqslant L$ runs around the fifth dimension, whose radius is $(L/2\pi)n = (L/2\pi)\exp[-\sqrt{2\kappa/3}\phi]$. Calculation of the five-dimensional Einstein action for gravity with a cosmological constant using this metric yields the action for four-dimensional Einstein gravity plus a minimally coupled scalar field ϕ with potential $V \propto e^{(\sqrt{2\kappa/3})\phi} = n^{-1}$.

The embedding in five dimensions yields a natural regularization of the singularity. Rewriting the line element as $d\chi^2 + m^2(\chi) d\Omega_3^2 + n^2 dy^2$, we see that the five-dimensional metric is actually perfectly regular when n vanishes as long as $dn/d\chi$ tends to $2\pi/L$ there, since then the singularity is just the usual two-dimensional polar coordinate singularity which may be removed by changing to Cartesian coordinates. We shall explore the consequences of applying this boundary condition in the general case.

Setting $d\tilde{\sigma} = N d\sigma$, the four-dimensional Euclidean Einstein–scalar-field action is

$$\mathcal{S}_{\rm Ein} = S_3 \int d\tilde{\sigma} \left(\frac{1}{2}\dot{\phi}^2 b^3 + V(\phi) b^3 - 3M_{Pl}^2 b (1 - b\ddot{b} - \dot{b}^2) \right), \tag{15}$$

where $S_3 = 2\pi^2$ is the volume of the unit three sphere and overdots denote derivatives with respect to $\tilde{\sigma}$. The last term in the integrand is $(-1/2\kappa)R$, with R the Ricci scalar. We shall be interested in rewriting this term in various ways differing by surface terms. First we integrate by parts to remove the second derivatives to obtain the action appropriate to fixed values for the three-metric and scalar field on the boundary, as discussed by Dirac [20]:

$$\mathcal{S}_{\rm Dir}=S_3\int\left(\frac{1}{2}\dot{\phi}^2b^3+V(\phi)b^3-3M_{Pl}^2b(\dot{b}^2+1)\right)$$
$$=\mathcal{S}_{\rm Ein}-3M_{Pl}^2S_3[b^2\dot{b}]. \tag{16}$$

The last term is the Gibbons-Hawking boundary term. Reexpressing this action in terms of the fields m, n, and the coordinate χ, we find

$$\mathcal{S}_{\rm Dir}=S_3\int d\chi m[V(n)n^2m^3-3M_{Pl}^2(m'^2n+mm'n'+1)]$$
$$=\mathcal{S}_{\rm Ein}-\frac{3}{2}M_{Pl}^2[m^3n'], \tag{17}$$

where here a prime denotes a derivative with respect to χ and we have used the fact that $n=0$ on the boundary. This action is clearly stationary under variations satisfying $\delta m=0$ on the boundary.

If instead we adopt the boundary condition suggested by Garriga's construction, we fix $n'=2\pi/L$ at the boundary. The appropriate action is obtained from Eq. (17) by integration by parts,

$$\mathcal{S}_{n'}=S_3\int m[V(n)n^2m^3-M_{Pl}^2(3m'^2n+3-m^3n'')]$$
$$=\mathcal{S}_{\rm Ein}-\frac{1}{2}M_{Pl}^2[m^3n'], \tag{18}$$

and we see that the Gibbons-Hawking term has been reduced by a factor of 3.

For simple monotonic scalar potentials, the action appropriate to the $\delta n'=0$ boundary condition is monotonically decreasing as ϕ_0 decreases towards the potential minimum. If the potential minimum is zero, the action for the constrained instantons tends to minus infinity. This is quite different from the behavior of the action appropriate to the $\delta m=0$ boundary condition. The latter action has two solutions at fixed m_B above some minimal value. As we showed above the lower action solution has no negative modes, giving us a picture of configuration space in which the lower action solutions comprise a stable valley running up towards $\phi_0\to\infty$. In contrast, since for generic potentials there is a unique solution for each value of n' at the singularity [12], and since we know that the Euclidean action is unbounded below, we might suspect that the action-configuration space structure takes the form of a single unstable ridge. We shall see that this picture is indeed correct.

We need to rewrite the condition that the five dimensional metric be regular in terms of our perturbation fields. To do so, we rewrite the four dimensional line element in terms of comoving coordinate X as in the previous sections. Then we divide the last term in the five dimensional line element by the first and take the square root. We find the condition that as X tends to zero, $b_0^{-1}(1+A)^{-1}e^{-(\sqrt{\kappa/6})\phi}(e^{(-\sqrt{2\kappa/3})\phi})'$ should tend to $2\pi/L$ where primes now refer to X derivatives, $b_0(X)$ is the unperturbed scale factor and the scalar field now includes the infinitesimal perturbation $\delta\phi$. It is convenient to pick a gauge where $\delta\phi=0$, which is possible near the singularity. In this gauge, in order to preserve five dimensional regularity we must have $A=0$ at the singularity. Expressed in canonical variables, this condition becomes $\Pi_{\delta\phi}/(a^2\phi')=0$. In the path integral, the G_{00} constraint is imposed as a delta functional and the condition on $\Pi_{\delta\phi}$ implies $(\kappa\mathcal{H}\Pi_\psi/\phi'+6\mathcal{K}\sqrt{\gamma}\psi/\phi')/(a^2\phi')=0$, which from Eq. (9) and for the homogeneous mode becomes after Euclideanization $\Psi_l/\phi'^2\sim X^2\Psi_l=0$ at $X=0$.

Having established the boundary condition $X^2\Psi_l=0$ appropriate to five dimensional regularity, we translate this into a boundary condition for the fluctuation variable $\bar{Q}$ appropriate to the negative mode computation. We find that $X^2\Psi_l\sim\kappa X^2\phi'\bar{Q}'/2D(X)\sim X^{-1}\bar{Q}'$. For the regularized instantons, the general solution for the mode equation for $\bar{Q}$ is specified by its expansion $\bar{Q}\sim AX^2+B$ near $X=0$, and the boundary condition therefore reads $A=0$. It is easy to see that a negative mode always exists for this boundary condition. From Eq. (13) and taking the measure to be $b^2\sqrt{\gamma}$, if we set $\bar{Q}=$const, the action is negative. The ansatz clearly satisfies the boundary condition. Therefore there is at least one negative mode. From a numerical study, we find that for a simple quadratic potential, regularized at large ϕ as above, there is in fact only one negative mode.

To summarize, the condition of five dimensional regularity may be imposed as a boundary condition. However, it does not eliminate the negative modes, therefore leaving the Euclidean path integral as ill defined at a fundamental level.

IX. CONCLUSIONS

In this paper we have given a detailed investigation of spatially homogeneous fluctuations of cosmological instantons. We showed how a Hamiltonian treatment, with an appropriate choice of variable, produces a Euclidean action which is bounded below for normalized fluctuations. First, we investigated Hawking-Moss and Coleman–De Luccia instantons, and showed that the lowest action solution in each case possesses a negative mode. For the ''thin-wall'' Coleman–De Luccia case where the instantons ''almost'' interpolate between the true and false vacua, this supports their use in tunneling roles as discussed in [4,21]. In that approach it is necessary that the potential may be obtained by analytically distorting one for which the action is positive definite for all configurations. In the ''thick-wall'' case, and certainly for Hawking-Moss instantons, where gravitational effects are important, it is not clear that this is possible. Thus even though we have found that these instantons do possess a single negative mode, the assertion that these instantons are useful for describing the decay of one spacetime to another requires further understanding.

Our investigation of singular instantons indicates the importance of a well-defined regularization. In contrast to the situation for the inhomogeneous modes [7], the Euclidean action does not uniquely select a boundary condition for the homogeneous modes. It is therefore essential to choose a regularization within which the relevant boundary condition is defined. We have investigated two such frameworks. The first is the RP^4 construction of [12], according to which we find that instantons with large starting values ϕ_0 of the inflaton field have no negative modes to quadratic order. The second is the regularization motivated by Garriga's five dimensional construction. Here we find that a negative mode is always present.

Since in all the cases studied here the instantons have perturbations which decrease their action, their use in an unconstrained path integral to determine the quantum state of the universe is questionable. In the case of the instantons describing tunneling, a constraint is needed to set the system in an initial unstable state. The constraints introduced in the RP^4 construction remove negative modes perturbatively, but as we have argued, probably do not remove them nonperturbatively. It therefore seems essential that an additional constraint be introduced which effectively projects onto certain subsets of states, and excludes the configurations of arbitrarily negative Euclidean action. This might be justified if we are only interested in correlators of certain subsets of observables, for example, as opposed to the unconstrained Euclidean partition function. How the appropriate projections are to be defined and introduced is an important topic for future work.

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