Energy Density of Non-Minimally Coupled Scalar Field Cosmologies

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ABSTRACT
Scalar fields coupled to gravity via $\xi R \Phi^2$ in arbitrary Friedmann-Robertson-Walker backgrounds can be represented by an effective flat space field theory. We derive an expression for the scalar energy density where the effective scalar mass becomes an explicit function of $\xi$ and the scale factor. The scalar quartic self-coupling gets shifted and can vanish for a particular choice of $\xi$. Gravitationally induced symmetry breaking and de-stabilization are possible in this theory.
I. Introduction

The study of classical and quantum fields in curved background spacetimes is by now a well established first step towards incorporating the influence of gravitation on both microscopic and large-scale physics. A major interest in this subject was spawned in the mid-seventies which saw a tremendous effort devoted towards the development of rigorous techniques for computing renormalized stress-energy tensors for quantum fields in various background geometries [1]. The knowledge of such tensors serves as the starting point for computing the back-reaction on the metric, an application of which is the semi-classical theory of black holes [2]. Apart from the stress-tensor renormalization program, cosmology has provided a strong motivation for delving into curved space field theory, most notably within the context of inflationary models [3] and the large-scale structure problem [4]. In both these areas, scalar fields play a decisive role. The inflationary epoch is believed to be driven by scalar field dynamics, usually via symmetry breaking. In the structure formation problem, (gauge-invariant) density perturbations are resolved into tensor, vector and scalar components. It is the dynamical equations for the scalar perturbation that reveal information on the growth and decay of density fluctuations [5].

In this paper, we take our cue from cosmology and consider the problem of scalar fields in Friedmann-Robertson-Walker (FRW) spacetimes. For our main result, we demonstrate that a scalar in an arbitrary expanding background, coupled with arbitrary strength to the scalar curvature ($\xi R \Phi^2$), is equivalent to a scalar with a time-dependent mass in a flat, Minkowski background. Moreover, the scalar quartic self-coupling in the effective theory is proportional to the FRW scalar quartic coupling, but rescaled by a term in-
volving $\xi$. The equivalence between curved-space and flat-space scalar field theory is established by computing the scalar field Hamiltonian, as this reveals the harmonic oscillator structure of quantum fields in FRW spaces, and allows us to make our curved space - to - flat space correspondences [6]. The benefit of the effective flat space representation will become apparent when we discuss implications for symmetry breaking in the early Universe and constraints on the non-minimal coupling from stability criteria.

Before launching into our analysis let us pause to briefly mention previous related work. Non-minimally coupled scalar field cosmologies have already been studied extensively by a number of authors. Two of the major topics that have been investigated are: (i) the cosmic no hair conjecture relating to the smoothing of anisotropies in the early Universe during inflation [7] and (ii) how nonminimal coupling affects inflation; it has been shown how variations in $\xi$ may or may not allow chaotic or power law inflation in various cosmologies [8]. Here we will address neither of these topics as our major interest is in the energy spectrum of the scalar fields. Our derivation of an energy spectrum for the scalar fields utilizes a Bogolyubov transformation and generates a conformally flat effective theory in the process. A flat space action can also be derived directly via a conformal transformation, but is less efficient for finding the energy spectrum. The lowest order effective action for gauge invariant cosmological perturbations is that of a real scalar with a time dependent mass in a flat background, ref. [23]. However, in addition to being a perturbative result, both the self-coupling and nonminimal coupling to gravity are not considered in those works. By contrast, our results are exact, and valid for arbitrary $\xi$ and $\lambda$, but do not involve gauge invariant perturbations about the FRW background.
II. Energy and Effective Mass

In treating the energy content of fields over curved backgrounds, a careful and consistent choice must be made as to which of various and possible field functionals actually represents the true, physical energy. For example, the canonical Hamiltonian, defined as the spatial integral of the Legendre-transformed Lagrange density, provides one possible candidate for an energy-like expression. Another candidate is furnished by the spatial integral of the pure timelike components of the stress-energy tensor, obtained from functionally differentiating the Lagrange density with respect to the background metric. In Minkowski space, there is no difference between the energies defined by one or the other of these two constructs. However, it is known that in expanding spacetimes, energy functionals derived via the canonical Hamiltonian and stress-energy tensor are generally not identical [9]. Moreover, in such backgrounds, inequivalent Hamiltonian energy expressions can be generated by means of successive canonical transformations. To avoid this ambiguity, we will define the energy via the stress-energy tensor. The latter has, after all, a direct physical significance as the source of the gravitational field.

Specializing to the case of a real scalar field, the variation of the action with respect to the metric results in a stress tensor:

\[
T_{\mu\nu}(\Phi) = \frac{2}{\sqrt{-g}} \frac{\delta A}{\delta g^{\mu\nu}} = (2\xi - \frac{1}{2})g_{\mu\nu}(g^{\alpha\beta}\partial_\alpha \Phi \partial_\beta \Phi) - (2\xi - 1)\partial_\mu \Phi \partial_\nu \Phi - 2\xi \Phi \nabla_\mu \nabla_\nu \Phi
\]

\[+ 2\xi g_{\mu\nu} \Phi \Box \Phi - \xi(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R)\Phi^2 + \frac{1}{2}m^2\Phi^2 g_{\mu\nu} + \frac{\lambda}{8} \Phi^4 g_{\mu\nu}, \tag{1}\]

where \(\nabla_\mu\) is the covariant derivative and \(\Box = \frac{1}{\sqrt{-g}} \partial_\mu (\sqrt{-g} g^{\mu\nu} \partial_\nu)\). We have taken the most general action for a real scalar field in an arbitrary curved
where $V(\Phi) = m^2\Phi^2 + \frac{\lambda}{4}\Phi^4$ [10]. This includes a possible nonminimal coupling to the metric, where $\xi$ is a real coupling constant and $R$ is the Ricci scalar curvature. This coupling can assume any real value; when $\xi = 0$, the scalar is said to be minimally coupled, when $\xi = 1/6$, the scalar is conformally coupled.

As our primary interest is in cosmological applications, we consider homogeneous isotropic Friedmann universes with zero spatial curvature [11], having as line element $ds^2 = dt^2 - a^2(t)dx \cdot dx$, where $a(t)$ is the scale factor. It is convenient to express the metric in terms of conformal coordinates $(\eta, x)$ where $\eta(t) = \int dt'/a(t')$ is conformal time and $C(\eta) = a^2(t)$ is the conformal scale factor. Then, the metric components are simply $g_{\mu\nu} = C(\eta)\text{diag}(1, -1, -1, -1)$. In these coordinates, the physical energy density is $E = T^0_0$, where

$$T_{00} = \frac{1}{2} \dot{\Phi}^2 + \left(\frac{1}{2} - 2\xi\right)\nabla\Phi \cdot \nabla\Phi - 2\xi\Phi (\ddot{\Phi} - \frac{\dot{C}}{2C} \dot{\Phi})$$

$$+ \left[\left(\frac{1}{2} - 2\xi\right)m^2C - \xi(R_{00} + (2\xi - \frac{1}{2})CR)\right] \Phi^2 + \lambda \left(\frac{1}{8} - \xi\right)C\Phi^4, \quad (3)$$

$\nabla$ denotes the ordinary flat gradient, the overdot represents $\frac{\partial}{\partial \eta}$, and we have used the equation of motion

$$(\Box + m^2 + \xi R + \frac{\lambda}{2}\Phi^2)\Phi = 0,$$  \quad (4)

in arriving at (3). The classical energy is obtained by integrating the energy density (in units where $\hbar = 1$)

$$E = \int d^3x \sqrt{-(3)g} T^0_0(\Phi), \quad (5)$$
over the spatial sections, while using the determinant of the three-metric of those subspaces.

The passage to the quantum mechanical energy operator is achieved in the standard way by expanding the classical solutions of (4) in terms of a complete set of mode functions and imposing canonical commutation relations on the generalized Fourier coefficients [1]. The scalar field equation (for \( \lambda = 0 \)) is solved with the ansatz

\[
 u_k(\eta, \mathbf{x}) = N_k C^{-1/2} f_k(\eta) \frac{e^{i \mathbf{k} \cdot \mathbf{x}}}{(2\pi)^{3/2}},
\]

(6)

where \( f_k \) is a solution of

\[
 \ddot{f}_k + \left[ k^2 + m^2 C(\eta) + (\xi - \frac{1}{6}) R(\eta) C(\eta) \right] f_k = 0,
\]

(7)

and \( k = |\mathbf{k}| \). The associated mode expansion for \( \Phi \) is given by

\[
 \Phi = \int \frac{d^3k}{(2\pi)^{3/2}} (a(\mathbf{k})u_k + a^\dagger(\mathbf{k})u_k^*),
\]

(8)

where \([a(\mathbf{k}), a^\dagger(\mathbf{k}')] = \delta^3(\mathbf{k} - \mathbf{k}')\), and the other commutators vanish identically. The orthonormality of the mode functions \( u_k \) with respect to the (curved space) inner product (for a discussion of normalization see [1]; the reduction to flat space is given below)

\[
 (F, G) = -iC(\eta) \int d^3x \langle F \frac{\partial}{\partial \eta} G^* \rangle
\]

(9)

is expressed by the conditions \((u_k, u_p) = \delta^3(\mathbf{k} - \mathbf{p})\), \((u_k^*, u_p^*) = -\delta^3(\mathbf{k} - \mathbf{p})\), and \((u_k, u_p^*) = 0\). Inserting the mode solutions (6) into (9) fixes the \( k^{th} \) mode normalization constant

\[
 N_k^2 \left( f_k \dot{f}_k^* - \dot{f}_k f_k^* \right) = i.
\]

(10)
The polar representation of the function \( f_k \) is the starting point for a WKB analysis of the approximate solutions of (7) [12] and is also useful for making exact comparisons between curved-space results in field theory and their Minkowski space counterparts. In this representation we write

\[ f_k = A_k(\eta) e^{-iS_k(\eta)}, \tag{11} \]

where \( A_k, S_k \) are real amplitude and phase functions. Substituting this into (10) yields the important relation

\[ N_k^2 A_k^2 \dot{S}_k = \frac{1}{2}, \tag{12} \]

which we will have occasion to use later on. For example, in the Minkowski limit, the solutions of (7) are \( f_k \sim e^{\pm i\omega_k \eta} \) with \( A_k = 1 \) (without loss of generality) and constant phase, \( \dot{S}_k = \omega_k = (k^2 + m^2)^{1/2} \). In this limit, the mode normalization (12) reduces to \( N_k = \frac{1}{\sqrt{2\omega_k}} \), and \( E_k = \omega_k \), which one immediately recognizes as the standard results for flat space field theory [13].

Inserting the field operator (8) into (5) and (3) gives the energy operator. Unlike the familiar flat space result of the last paragraph, this involves second derivatives of the mode functions in (6), leading to intermediate steps which are straightforward but rather lengthy. We turn first to the quadratic part, for which we obtain

\[ \frac{E}{C^{1/2}} = \int \frac{d^3k}{(2\pi)^{3/2}} N_k^2 A_k^2 (Z_k a(k)a^\dagger(k) + Z_k^* a^\dagger(k)a(k) + W_k a(k)a(-k) + W_k^* a^\dagger(k)a^\dagger(-k)) \tag{13} \]

where

\[ Z_k = M^2 + \frac{1}{2}(\omega_k^2 + Y_k^2) + \left(\frac{1}{2} - 2\xi\right)k^2 - 2\xi \left[ F^*_{\infty} - \frac{C}{2C}(i\omega_k + Y_k) \right], \tag{14} \]
and

\[ W_k e^{2i\dot{S}_k} = M^2 + \frac{1}{2}(-i\omega_k + Y_k)^2 + \left(\frac{1}{2} - 2\xi\right)k^2 - 2\xi \left[ \mathcal{F}_k - \frac{\dot{C}}{2C}(-i\omega_k + Y_k) \right], \]

are complex functions of \( \eta \). Here, \( M^2 \) is a term combining the mass with a curvature dependent function [14],

\[ M^2 = \left(\frac{1}{2} - 2\xi\right)m^2C - \xi(R_{00} + (2\xi - \frac{1}{2})CR). \]

In computing the derivatives of the \( u_k \), we have found it useful to define the following quantities

\[ Y_k = \ddot{A}_k A_k - \dot{C}^2 C, \]

and

\[ F_k = (-i\dddot{S}_k + \dot{Y}_k) + \left(-i\dddot{S}_k + Y_k\right)^2 \]

where \( \omega_k \equiv \dot{S}_k \) is the instantaneous frequency of the \( k^{th} \) mode [15].

The energy operator in (13) can be brought to diagonal form by means of a Bogolyubov transformation (a canonical transformation) [16]

\[ a(k) = \alpha_k b(k) + \beta_k b^\dagger(-k), \quad (17a) \]

\[ a^\dagger(k) = \alpha_k^* b^\dagger(k) + \beta_k^* b(-k), \quad (17b) \]

where the new operators \( b(k) \) obey canonical commutation relations, viz. \([b(k), b^\dagger(k')] = \delta^3(k - k')\), etc., provided the Bogolyubov coefficients satisfy

\[ |\alpha_k|^2 - |\beta_k|^2 = 1. \]

For the case at hand, we can parametrize this transformation by a single real angle by taking

\[ \alpha_k = \cosh(\theta_k) = \frac{1}{\sqrt{1 - L_k^2}}, \quad \text{and} \quad \beta_k = \sinh(\theta_k) = \frac{L_k}{\sqrt{1 - L_k^2}}, \]

where \( L_k = L_{-k} \) is a real function [17]. Applying the transformation (17) to (13), and absorbing the phase factor \( e^{2i\dot{S}_k} \) into the definition of \( W_k \), we find

\[ E \rightarrow E_{\text{number}} + E_{\text{squeeze}}, \]

(19)
where ($\Re$ denotes the real part)

$$E_{\text{number}} = \int d^3k \frac{2N_k^2 A_k^2 C^{-1/2}}{(1 - L_k^2)} \left((1 + L_k^2) \Re Z_k + 2L_k \Re W_k\right) b^\dagger(k) b(k), \quad (20)$$

and

$$E_{\text{squeeze}} = \int d^3k \frac{N_k^2 A_k^2 C^{-1/2}}{(1 - L_k^2)} \left(2L_k \Re Z_k + W_k + L_k^2 W_k^*\right) b(k) b(-k) + h.c. \quad (21)$$

The ‘squeeze’ term is so called because it is identical in form to multi-mode squeeze operators familiar from quantum optics [18] and leads to the phenomenon of gravitational squeezing as discussed in [19,20]. The other term has the familiar form of a weighted sum of number operators (after normal-ordering with respect to the $b$-vacuum [21]). Thus, diagonalization is achieved for the unique choice of time-dependent transformation angle corresponding to

$$L_k = \frac{-\Re Z_k + \left((\Re Z_k)^2 - |W_k|^2\right)^{1/2}}{W_k^*}. \quad (22)$$

For this choice, $E_{\text{squeeze}} = 0$ and $E = E_{\text{diag}} = E_{\text{number}}$. This solution is fixed by the requirement that $L_k \to 0$ as the background field is shut off, i.e., as $a(t) \to 1$. In this limit, the angle $\theta_k \to 0$, $\alpha_k \to 1$ and $\beta_k \to 0$, as expected.

While the coefficient in (20) with $L_k$ given in (22) gives the correct energy eigenvalues, the resultant expression admits a tremendous algebraic simplification, though this fact is by no means a-priori obvious. To see how this comes about, we write the integrand of (13) as a $4$-by-$4$ matrix for each mode $k$

$$E_k = N_k^2 A_k^2 C^{-1/2} \begin{pmatrix} 0 & Z_k & W_k & 0 \\ Z_k^* & 0 & 0 & W_k^* \\ W_k & 0 & 0 & Z_k \\ 0 & W_k^* & Z_k^* & 0 \end{pmatrix}, \quad (23)$$
where the rows and columns of the array are labeled in the sequence \((a_k, a_k^\dagger, a_{-k}, a_{-k}^\dagger)\).

The determinant of this matrix is easily computed:

\[ \det \mathcal{E}_k = (N_k^2 A_k^2 C^{-1/2})^4 (|Z_k|^2 - |W_k|^2)^2. \quad (24) \]

On the other hand, as we have just demonstrated, the Bogolyubov transformation brings the energy operator into the diagonal (with respect to the number-operator basis) \[22] form given by

\[ \mathcal{E}_k = \begin{pmatrix}
0 & E_k & 0 & 0 \\
E_k & 0 & 0 & 0 \\
0 & 0 & 0 & E_k \\
0 & 0 & E_k & 0
\end{pmatrix}. \quad (25) \]

The canonical transformation (17a,b) is just a symplectic transformation which preserves the quadratic form \(|\alpha|^2 - |\beta|^2 = 1\). As the spectrum is invariant under this change of basis, we must have (using \(E_k\) to denote both the operator and its eigenvalue, without loss of generality)

\[ E_k = N_k^2 A_k^2 C^{-1/2} ||Z_k|^2 - |W_k|^2|^{1/2}. \quad (26) \]

The calculation of the energy levels is now straightforward and follows from substituting the expressions for \(Z_k\) and \(W_k\) into (26). The elimination of the second derivatives of the amplitude and phase functions which appear there is effected by means of the two identities

\[ A_k \ddot{S}_k + 2 \dot{A}_k \dot{S}_k = 0, \quad (27a) \]

and

\[ \left( \frac{\ddot{A}_k}{A_k} \right) - (\dot{S}_k)^2 + (k^2 + C[m^2 + (\xi - 1/6)R]) = 0, \quad (27b) \]
which result from substituting the polar functions (11) into the differential equation (7) [12]. Note the first equation can be integrated immediately to give

\[ A_k \sqrt{S_k} = b, \]

(28)

for some constant \( b \), and gives independent confirmation of the Wronskian constraint in (10). Comparison with (12) implies \( b = \frac{1}{\sqrt{2N_k}} \). After some additional algebra we find that

\[ |Z_k|^2 - |W_k|^2 = \omega^2_k (m^2 C + k^2 + \frac{3}{2} \xi (\dot{C}/C)^2), \]

(29)

which together with (12) and (26) yields the quadratic energy spectrum

\[ E_k = \left( m^2 + k_{\text{phys}}^2 + 6\xi (H(t)/c)^2 \right)^{1/2}, \]

(30)

which is our key result. Note that (30) is an exact result for a “free” scalar \((\lambda = 0)\), but nonminimally coupled to gravity \((\xi \neq 0)\) [23]. The physical wave vector \( k_{\text{phys}} = k/a(t) \) reflects the Doppler spread in the wavelength caused by the expansion/contraction of the background spacetime, and \( H = \frac{1}{a} \frac{da}{dt} \) is the Hubble constant. In the diagonal basis introduced in (17), the energy is given by

\[ E = \sum_k E_k b^*(k)b(k) + E_{\text{int}}(\lambda), \]

(31)

where \( E_{\text{int}} \) depends on the self-coupling. This result demonstrates that a free scalar field in a FRW background is equivalent to a system of harmonic oscillators in flat space, with the proviso that the oscillators have an effective, time-dependent, mass given by

\[ m_{\text{eff}}^2(\xi, t) \equiv m^2 + 6\xi (H/c)^2. \]

(32)

We can write down an action leading to the same energy operator (31) if we identify the mass parameter appearing there with (32). The interacting
part can be incorporated immediately since the same transformation which diagonalized the quadratic sector keeps the quartic terms invariant (and these do not mix with the quadratic part). The effective quartic coupling can then be read off immediately from (3). The resultant effective field theory is given by [24]

\[ A_{\text{eff}} = \int d^4x \left( (\partial_t \phi)^2 - (\nabla_{\text{phys}} \phi)^2 - m_{\text{eff}}^2 \phi^2 - \frac{\lambda_{\text{eff}}}{4} \phi^4 \right), \tag{33} \]

where \( \lambda_{\text{eff}} = (1 - 8\xi)\lambda \), and \( \phi \) admits an expansion similar to (8) (when \( \lambda_{\text{eff}} = 0 \)) with \( a(k) \) replaced by \( b(k) \), and with different mode functions.

In passing, we comment briefly on the properties of a theory with an effective action given by (33), which has the \( Z_2 \) symmetry \( (\phi \rightarrow -\phi) \) [25]. For \( \lambda_{\text{eff}} > 0 \) the flat space theory undergoes spontaneous symmetry breaking (restoration) for \( m^2 < 0 \) (\( m^2 > 0 \)) and \( \xi > 0 \) (\( \xi < 0 \)) at a time \( \hat{t} \) when [26]

\[ |m^2| = 6|\xi|\left(\frac{H(\hat{t})}{c}\right)^2, \]

that is, when the Compton wavelength of the scalar is roughly the horizon size.

For \( \lambda_{\text{eff}} < 0 \) the flat space scalar theory is unstable but asymptotically free [27]. Finally, note there are two ways that (33) gives the action for a free flat space theory: when \( \lambda = 0 \) or when \( \xi = 1/8 \). Furthermore, for \( \lambda > 0 \), a conformally coupled scalar theory \( (\xi = 1/6) \) has \( \lambda_{\text{eff}} = -\lambda/3 \), and hence the theory is unstable.

III. Conclusions

The purpose of obtaining the results presented here has been to improve our understanding of the longest wavelength modes in cosmology, specifically, long wavelength (horizon size or longer) scalar density perturbations.
We have demonstrated that considerable care must be taken in the interpretation of such modes (beyond the standard considerations of gauge dependence). Previous work [12,15] has shown that the relation $\lambda = 1/\nu$ holds only in flat space and in some special cosmologies. Here, by studying the energy spectrum of classical scalar fields coupled to curvature, we have learned that Einstein’s relation $E = \omega$ (or $E = \sqrt{\omega^2 + m^2}$ for massive scalar fields) no longer holds in general, and what will be more important for the interpretation of the physics of large scale structures: the energy is no longer related in the standard way to the wavelength of the scalar fields that are not minimally coupled in any cosmology where the Hubble parameter is nonvanishing. A challenge for the future is to relate the results derived here for the classical fundamental scalar fields $\Phi$ in a homogeneous cosmology to the scalar density perturbation in a cosmological background. It would also be of interest to explore vector and tensor density perturbations in this approach [28].

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[26]. In general, 1-loop corrections give \( m^2 \) a temperature (i.e., time) dependence \( m^2(T) = m^2(0) + O(1) \times \lambda_{eff}^2 T^2 \); see L. Dolan and R. Jackiw, Phys. Rev. D9, 3320 (1974); S. Weinberg, Phys. Rev. D 9, 3357 (1974). Here we will ignore these corrections but in general, these effects must be taken into account, as can be easily done.

[27]. G. 't Hooft, talk at the Marseilles meeting, 1972 (unpublished).
One may expect (nongauged) classical fundamental vectors $v^\mu$ and tensors $t^\mu_\nu$ to couple to gravity via dimension four terms of the form $\xi_1 R^\mu v^\mu + \xi_2 R^\nu v^\nu v^\mu + \xi_3 R^\mu t^\mu + \xi_4 R^\mu t^\nu$ which in turn would contribute to vector and tensor density perturbations.