Lecture Notes on Non-minimally Coupled Scalar Fields

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1 Introduction and Motivation

The the most general action one can write for a scalar field in curved spacetime is

$$\mathcal{S} = \mathcal{S}_{\rm EH} + \mathcal{S}_\phi = \int d^4x\sqrt{-g}\left[\frac{M_P^2}{2}R - \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{1}{2}\xi R\phi^2 - V(\phi)\right] , \tag{1}$$

where $V(\phi)$ represents a general potential for ϕ which does not depend on R. Here, R is the Ricci scalar curvature and our metric sign convention is the mostly minus "west-coast" metric $(-+++)$ [1]. The parameter ξ controls the strength of the so-called *non-minimal coupling* (NMC) to of ϕ to gravity via the Ricci scalar R. The case $\xi = 0$ there corresponds to the minimally coupled scenario. Why do I want to consider a NMC scalar theory?

- Unlike the case for gauge fields and chiral fermions (where gauge and chiral symmetry completely fix the couplings of these fields to curvature), no symmetry forbids adding a direct coupling to the curvature of the form $R\phi^2$ in the case of scalars (as is the case with scalar masses). Indeed, the SM Higgs field should have this coupling, as it is a dimension-4 operator consistent with all symmetries of the SM and gravity.
- If one wants to consider conformal field theories, the action of a free scalar field in curved spacetime is not conformally invariant unless $\xi \neq 0$. Specifically, in 4D we must have $\xi = 1/6$ for the action to be invariant under conformal transformations. Again, this is in contrast to free vector and fermionic fields.
- The choice of minimal coupling is not stable quantum mechanically. Even if one sets $\xi = 0$ at some scale, non-zero ξ will be generated via renormalization group evolution in curved spacetime.

1.1 The Jordan Frame

Because we have introduced a direct coupling of ϕ to the curvature, one can also think of this as tensor-scalar theory defined by the action

$$\mathcal{S}_J = \int d^4x\sqrt{-g}\left[\frac{M_P^2}{2}f(\phi)R - \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - V(\phi)\right] , \tag{2}$$

where we have defined

$$f(\phi) = \left(1 - \frac{\xi\phi^2}{M_P^2}\right) . \tag{3}$$

[1] Specifically, our sign convention is (+,+,+) in the definition of Misner, Thorne, and Wheeler.

The action defined by Eq. (2) is sometimes said to define the so-called *Jordan frame*, where we appear to have a modified scalar-tensor theory of gravity.

2 Conformal Transformations and the Einstein Frame

It is common in the literature to study these theories in the so-called *Einstein frame*, defined by performing a conformal transformation that removes the $f(\phi)$ factor such that we have the canonical Einstein-Hilbert action. Specifically, we can do this by performing a conformal transformation of the metric tensor, defined as

$$g_{\mu\nu} \to \tilde{g}_{\mu\nu} = \Omega^2(x) g_{\mu\nu}\,, \tag{4}$$

where the scalar function $\Omega^2(x)$ is a continuous, non-vanishing, finite, real, but otherwise arbitrary function of $x = x^\mu$ [2].

2.1 Curvature Transformation Rules

From Eq. (4), the following transformation rules can be found in d spacetime dimensions

$$g_{\mu\nu} \to \Omega^{-2}\tilde{g}_{\mu\nu}\,, \qquad g^{\mu\nu} \to \Omega^2\, \tilde{g}^{\mu\nu}\,, \qquad g = \det(g_{\mu\nu}) \to \Omega^{-2d}\, \tilde{g}\,, \tag{5}$$

and (in 4-dimensions) the conformal transformation of the Ricci scalar is

$$R = \Omega^2 \tilde{R} + 6\,\Omega\tilde{\Box}\Omega - 6\,\tilde{g}^{\mu\nu}(\partial_\mu\Omega)(\partial_\nu\Omega) = \Omega^2\left[\tilde{R} + 6\,\tilde{\Box}\ln\Omega - 6\,\tilde{g}^{\mu\nu}(\partial_\mu \ln\Omega)(\partial_\nu \ln\Omega)\right]\,, \tag{6}$$

where we have used $\Omega^{-1}\tilde{\Box}\Omega = \tilde{\Box}\ln\Omega$.

Using these transformation rules, the action becomes (under an arbitrary Ω)

$$\tilde{\mathcal{S}} = \int d^4x\sqrt{-\tilde{g}}\left[\frac{M_P^2}{2} f(\phi)\,\Omega^{2-d}\left(\tilde{R} + 6\,\tilde{\Box}\ln\Omega - 6\,\tilde{g}^{\mu\nu}(\partial_\mu \ln\Omega)(\partial_\nu \ln\Omega)\right)\right. \tag{7}$$

$$\left. - \frac{1}{2}\Omega^{2-d}\,\tilde{g}^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \Omega^{-d}\,V(\phi)\right]\,. \tag{8}$$

2.2 Einstein Frame in 4-dimensions

The Einstein frame is defined by the Ω which transforms the coefficient of $M_P^2\tilde{R}/2$ to 1. The only dimensional dependence comes from the transformation of g, so the condition that defines the Einstein frame in d spacetime dimensions is $f(\phi)\Omega^{2-d} = 1$. Therefore, in 4-dimensions, we have

$$\Omega^2 = f(\phi)\,. \tag{9}$$

which means $\ln\Omega = \frac{1}{2}\ln f$ and $\partial_\mu \ln\Omega = \frac{1}{2}\partial_\mu \ln f = \frac{1}{2f}\partial_\mu f$. Thus, in the Einstein frame in $4d$ we have

$$\tilde{\mathcal{S}}_E = \int d^4x\sqrt{-\tilde{g}}\left[\frac{M_P^2}{2}\tilde{R} - \frac{3}{4f^2}M_P^2\,\tilde{g}^{\mu\nu}(\partial_\mu f)(\partial_\nu f) - \frac{1}{2f}\,\tilde{g}^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{1}{f^2}V(\phi)\right]\,. \tag{10}$$

[2] Sometimes people write $\Omega^2(x) = e^{2\omega(x)}$ since the exponential function (which is infinitely differentiable and has range $(0,\infty)$ for $\omega \in (-\infty,\infty)$) makes the aforementioned desired properties of $\Omega^2(x)$ explicit (and, as we will see, we end up with $\ln\Omega = \omega$ appearing in the results).

where we have thrown away a total derivative term $\# \times \tilde{\Box} \ln \Omega$. Trading the f derivatives for ϕ ones, we find

$$\tilde{\mathcal{S}}_E = \int d^4x \sqrt{-\tilde{g}} \left[\frac{M_P^2}{2} \tilde{R} - \frac{1}{2} \mathcal{K}^2(f) \, \tilde{g}^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - \frac{1}{f^2} V(\phi) \right] , \tag{11}$$

with

$$\mathcal{K}^2(f) = \frac{f + 6\xi(1-f)}{f^2} = \frac{1 + \xi(6\xi - 1)\phi^2/M_P^2}{\left(1 - \xi\phi^2/M_P^2\right)^2} . \tag{12}$$

Thus, we have Einstein gravity and a scalar degree of freedom with a non-minimal kinetic term. If we now define $\tilde{\phi}$ such that

$$\mathcal{K} \partial_\mu \phi = \partial_\mu \tilde{\phi} \qquad \Longrightarrow \qquad d\tilde{\phi} = \mathcal{K} d\phi \, , \tag{13}$$

where we have used the fact that the total differential is $d\phi = (\partial_\mu \phi) dx^\mu$, then we have an action with a canonically normalized kinetic term for $\tilde{\phi}$

$$\tilde{\mathcal{S}}_E = \int d^4x \sqrt{-\tilde{g}} \left[\frac{M_P^2}{2} \tilde{R} - \frac{1}{2} \, \tilde{g}^{\mu\nu} \partial_\mu \tilde{\phi} \partial_\nu \tilde{\phi} - \tilde{V}(\tilde{\phi}) \right] , \tag{14}$$

where $\tilde{V}(\tilde{\phi})$ is implicitly defined in terms of ϕ as

$$\tilde{V}(\tilde{\phi}) = \frac{V(\phi)}{\left(1 - \xi\phi^2/M_P^2\right)^2} , \tag{15}$$

and the field in the Einstein frame satisfies the usual Klein-Gordon equation

$$\tilde{\Box} \tilde{\phi} - \frac{\partial \tilde{V}}{\partial \tilde{\phi}} = \frac{1}{\sqrt{-\tilde{g}}} \partial_\mu \left(\sqrt{-\tilde{g}} \, \tilde{g}^{\mu\nu} \partial_\nu \tilde{\phi} \right) - \frac{\partial \tilde{V}}{\partial \tilde{\phi}} = 0 \, . \tag{16}$$

We can actually solve analytically for $\tilde{\phi}$ in terms of ϕ (up to an integration constant)

$$\pm \frac{\tilde{\phi}}{M_P} = \sqrt{6} \tanh^{-1} \left[\frac{\xi\phi/M_P}{\sqrt{\frac{1}{6} + \left(\xi - \frac{1}{6}\right) \xi\phi^2/M_P^2}} \right] - \sqrt{\frac{6\xi - 1}{\xi}} \sinh^{-1} \left[\sqrt{\frac{6\xi - 1}{\xi}} \frac{\xi\phi}{M_P} \right] , \tag{17}$$

however, this formula is difficult to invert. The function $\tanh^{-1}$ diverges when its argument goes to 1, which happens when $\xi\phi^2/M_P^2 \to 1$. Some interesting limits are

- $\xi = 0$: In this case, we simply have $\phi = \tilde{\phi}$ as the J and E frames are equivalent.
- $\xi = 1/6$: In this case, we have

$$\phi = \sqrt{6} M_P \tanh\left(\frac{\tilde{\phi}}{\sqrt{6} M_P} \right) \qquad \Longrightarrow \qquad \tilde{V}(\tilde{\phi}) = V(\phi(\tilde{\phi})) \cosh^4 \left(\frac{\tilde{\phi}}{\sqrt{6} M_P} \right) \tag{18}$$

- $\xi\phi^2/M_P^2 \gg 1$: In this case, we get

$$\phi = \frac{M_P}{\sqrt{\xi}} \exp\left(\frac{\tilde{\phi}}{\sqrt{6}M_P}\right) , \tag{19}$$

which if $V(\phi) = \lambda(\phi^2 - v^2)^2/4$ then yields the potential for Higgs inflation in the EF.

This frame is also interesting to study (will do it in future work), but given the difficulties inverting this formula in general (as well as potential singular points), it is also interesting to the study the theory in the Jordan frame.

2.3 Homework Problem

Show that $\xi = 1/6$ is required for $\mathcal{S}_\phi$ to be invariant under an arbitrary conformal transformation in $d = 4$ spacetime dimensions. Only look at $\mathcal{S}_\phi$, because $\mathcal{S}_{\text{EH}}$ is not conformally invariant!

3 Non-minimally Coupled Scalars in the Jordan Frame

We consider the action of a scalar field ϕ coupled to gravity in the most general way

$$\mathcal{S}_{\mathcal{J}} = \mathcal{S}_{\text{EH}} + \mathcal{S}_\phi = \int d^4x\sqrt{-g}\left[\frac{M_P^2}{2}R - \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{1}{2}\xi R\phi^2 - V(\phi) + \mathcal{L}_{\text{m}}\right] , \tag{20}$$

We'll study a flat but otherwise general Friedmann-Robertson-Walker (FRW) universe described by the following "α-time" metric used in CosmoLattice

$$ds^2 = -a(\eta)^{2\alpha}d\eta^2 + a(\eta)^2\delta_{ij}dx^i dx^j , \tag{21}$$

so we have $\sqrt{-g} = a(\eta)^{3+\alpha}$ and the Ricci scalar is

$$R = \frac{6}{a^{2\alpha}}\left[\frac{a''}{a} + (1-\alpha)\left(\frac{a'}{a}\right)^2\right] = \frac{6}{a^{2\alpha}}\left[\frac{a''}{a} + (1-\alpha)\mathcal{H}^2\right] , \tag{22}$$

where primes indicate derivatives with respect to the α-time variable η and $\mathcal{H}$ is the α-time Hubble rate $\mathcal{H} = a'/a$. This is related to the physical Hubble rate $H = \dot{a}/a$ by

$$\mathcal{H} = H\frac{dt}{d\eta} = Ha^\alpha , \tag{23}$$

where dots indicate derivatives w.r.t to cosmic time t.

Some familiar examples of α-time choices

- $\alpha = 0$: Real or cosmic time
- $\alpha = 1$: Conformal time

To study this theory, we need the equations of motion for the scalar field, as well as the gravitational equations of motion (the Friedmann equations).

3.1 Equation of Motion for the Non-minimally Coupled Scalar Field

The equation of motion for ϕ is obtained via the variation of $\mathcal{S}_\phi$ with respect to ϕ, which gives the Euler-Lagrange equation

$$\begin{aligned} \partial_\mu \left(\sqrt{-g} \frac{\partial \mathcal{L}_\phi}{\partial(\partial_\mu \phi)} \right) - \sqrt{-g} \frac{\partial \mathcal{L}_\phi}{\partial \phi} &= 0 \,, \\ -\frac{1}{\sqrt{-g}} \partial_\mu \left(\sqrt{-g}\, g^{\mu\nu} \partial_\nu \phi \right) + \xi R \phi + \frac{\partial V}{\partial \phi} &= 0 \,, \\ \Box \phi - \xi R \phi - \frac{\partial V}{\partial \phi} &= 0 \,, \end{aligned} \tag{24}$$

where $\Box = g^{\mu\nu} \nabla_\mu \nabla_\nu$, which for scalars is equivalent to $\Box \phi = (-g)^{-1/2} \partial_\mu \left(\sqrt{-g}\, g^{\mu\nu} \partial_\nu \phi \right)$. Writing this out for our metric leads to the following equation of motion in α-time

$$\phi'' + (3 - \alpha) \frac{a'}{a} \phi' - a^{-2(1-\alpha)} \nabla^2 \phi = -a^{2\alpha} \left(\xi R \phi + \frac{\partial V}{\partial \phi} \right) . \tag{25}$$

3.2 Equations of Motion for Gravity: Einstein and Friedmann Equations

Given the FLRW metric in Eq. (21), the consistency of the Einstein equations requires that $T_{\mu\nu}$ takes the form of the energy-momentum tensor of a perfect fluid $T^\mu{}_\nu = \mathrm{diag}\,\{-\rho(\eta), p(\eta), p(\eta), p(\eta)\}$. We note that while fields can develop large spatial inhomogeneities, the homogeneous and isotropic pressure and energy density $p(\eta)$ and $\rho(\eta)$ should be understood as the result of a volume average over the inhomogeneous local field expressions. When the averaging volume is sufficiently large compared to the excitation scales of the fields, this procedure leads to a well-defined notion of a homogeneous and isotropic pressure and energy density within the given volume. In this case, taking spatial averages over the off-diagonal elements of $T_{\mu\nu}$ leads to vanishing results, consistent with homogeneity and isotropy within the considered volume. Under these conditions, the Einstein equations reduce to the Friedmann equations in α-time

$$\mathcal{H}^2 \equiv \left(\frac{a'}{a} \right)^2 = \frac{a^{2\alpha}}{3 m_p^2} \rho(\eta) \,, \tag{26}$$

$$\frac{a''}{a} = -\frac{a^{2\alpha}}{6 m_p^2} \Big[(1 - 2\alpha) \rho(\eta) + 3 p(\eta) \Big] \,, \tag{27}$$

where we defined $\mathcal{H} = a'/a$, which is related to the cosmic time Hubble rate H as $H = \mathcal{H}/a^\alpha$. We define the energy density and pressure as

$$\rho(\eta) = \rho_\phi(\eta) + \rho_{\rm m}(\eta) \equiv -g^{00} \langle T_{00} \rangle = a^{-2\alpha} \langle T^\phi_{00} \rangle + a^{-2\alpha} \langle T^{\rm m}_{00} \rangle \,, \tag{28}$$

$$p(\eta) = p_\phi(\eta) + p_{\rm m}(\eta) \equiv \frac{1}{3} g^{ij} \langle T_{ij} \rangle = \frac{1}{3a^2} \delta^{ij} \langle T^\phi_{ij} \rangle + \frac{1}{3a^2} \delta^{ij} \langle T^{\rm m}_{ij} \rangle \,, \tag{29}$$

with $\langle \ldots \rangle$ denoting volume averages.

4 Energy-momentum tensor for the NMC scalar

The energy momentum tensor for ϕ is defined as

$$T^{\phi}_{\mu\nu} = -\frac{2}{\sqrt{-g}}\frac{\delta(\sqrt{-g}\mathcal{L}_\phi)}{\delta g^{\mu\nu}} = -2\frac{\delta\mathcal{L}_\phi}{\delta g^{\mu\nu}} + g_{\mu\nu}\mathcal{L}_\phi\,. \tag{30}$$

The result for the energy-momentum tensor is

$$T^{\phi}_{\mu\nu} = \underbrace{\partial_\mu\phi\partial_\nu\phi - g_{\mu\nu}\left(\frac{1}{2}g^{\rho\sigma}\partial_\rho\phi\partial_\sigma\phi + V(\phi)\right)}_{\text{minimally coupled}} + \underbrace{\xi(G_{\mu\nu} + g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu)\phi^2}_{\text{non}-\text{minimally coupled}}\,. \tag{31}$$

where we have used $\Box = \nabla^\sigma\nabla_\sigma = g^{\rho\sigma}\nabla_\rho\nabla_\sigma$. [Point out that the NMC coupled part contains curvature terms].

4.1 Homework Problem

Explicitly derive the previous equation for the energy-momentum tensor of a NMC scalar by variation of S_ϕ w.r.t to the inverse metric.

4.2 Energy Density

The energy density is given by $\rho_\phi = -T^0_0 = -g^{00}T_{00}$. The full expression for the energy in α-time is

$$\rho_\phi = \frac{1}{2a^{2\alpha}}\phi'^2 + \frac{1}{2a^2}(\nabla\phi)^2 + V(\phi) + \frac{1}{a^{2\alpha}}3\xi\mathcal{H}^2\phi^2 - \xi\frac{1}{a^2}\nabla^2\phi^2 + \frac{1}{a^{2\alpha}}6\xi\mathcal{H}\phi\phi'\,. \tag{32}$$

4.3 Pressure

The pressure is given as $p = g^{ij}T_{ij}/3$. Thus, the total pressure in α-time is

$$p_\phi = \frac{1}{2a^{2\alpha}}\phi'^2 - \frac{1}{6a^2}(\nabla\phi)^2 - V(\phi) + \xi\left(\frac{1}{a^{2\alpha}}\mathcal{H}^2 - \frac{R}{3}\right)\phi^2 + \xi\Box\phi^2 - \frac{1}{3a^2}\xi\nabla^2\phi^2 + \frac{1}{a^{2\alpha}}2\xi\mathcal{H}\phi\phi'\,. \tag{33}$$

4.4 Acceleration Equation

In principle, one can insert these expressions for the volumed-averaged energy and pressure into the second Friedmann equation

$$\frac{a''}{a} = -\frac{a^{2\alpha}}{6m_p^2}\Big[(1-2\alpha)\rho(\eta) + 3p(\eta)\Big]\,, \tag{34}$$

and solve this system. However, this involves the derivatives of a in a non-linear way as well as strange surface like terms that should vanish when volume averaged. Is there a better way?

5 Acceleration Equation Sourced by the Ricci Scalar

Using the definition of R, the α-time acceleration equation can be written as

$$\frac{a''}{a} + (1-\alpha)\mathcal{H}^2 = \frac{a^{2\alpha}}{6} R\,, \tag{35}$$

and taking the trace of the Einstein equation leads to the following relation

$$R = -\frac{T}{M_P^2} = \frac{1}{M_P^2}(\rho - 3p)\,. \tag{36}$$

Since the trace is a linear operator, we must have $T = T_\phi + T_m$, where T_m is the trace of the energy-momentum tensor describing the rest of the fields in the theory, e.g. the inflaton. Thus, we can write

$$-\,M_P^2 R = T_\phi + T_m\,, \tag{37}$$

However, since we do not solve the full Einstein equations on the lattice, we are always implicitly assuming $R = R(\eta)$. Therefore, this equation makes only if we take the spatial average of the RHS

$$-\,M_P^2 R = \langle T_\phi \rangle + \langle T_m \rangle\,. \tag{38}$$

This gives a clean way to compute R only in terms of the fields if I know T.

5.1 Trace of the Energy-Momentum Tensor

The trace of the energy-momentum tensor is defined as $T_\phi = g^{\mu\nu} T^\phi_{\mu\nu}$. Computing it in d spacetime dimensions, we find

$$T_\phi = \left(1 - \frac{d}{2}\right)\left(\partial^\mu\phi\partial_\mu\phi + \xi R\phi^2\right) - V\,d + \xi(d-1)\Box\phi^2\,, \tag{39}$$

Massaging this using the equation of motion and taking $d = 4$, we find

$$T_\phi = (6\xi - 1)\left(\partial^\mu\phi\partial_\mu\phi + \xi R\phi^2\right) - 4V + 6\xi\phi V_{,\phi}\,. \tag{40}$$

Interestingly, T is also a function of R. This is a funny feature of the energy-momentum tensor of NMC scalar fields.

5.2 Solving for the Ricci Scalar

We now go back to our expression for R

$$-\,M_P^2 R = \langle T_\phi \rangle + \langle T_m \rangle\,. \tag{41}$$

Substituting our result for T_ϕ gives

$$M_P^2 R = \langle (1 - 6\xi)\left(\partial^\mu\phi\partial_\mu\phi + \xi R\phi^2\right) + 4V - 6\xi\phi V_{,\phi} \rangle - \langle T_m \rangle \tag{42}$$

$$\left[M_P^2 + (6\xi - 1)\,\xi\langle\phi^2\rangle\right] R = (1 - 6\xi)\,\langle\partial^\mu\phi\partial_\mu\phi\rangle + 4\langle V\rangle - 6\xi\langle\phi V_{,\phi}\rangle - \langle T_m\rangle\,, \tag{43}$$

$$R = \frac{(1-6\xi)\,\langle\partial^\mu\phi\partial_\mu\phi\rangle + 4\langle V\rangle - 6\xi\langle\phi V_{,\phi}\rangle - \langle T_m\rangle}{M_P^2\,[1+(6\xi-1)\,\xi\langle\phi^2\rangle/M_P^2]}\,. \tag{44}$$

Let us define the dimensionless function

$$F(\phi) = \frac{1}{1+(6\xi-1)\,\xi\langle\phi^2\rangle/M_P^2}\,, \tag{45}$$

which has the nice property that it goes to 1 when $\xi = 0$ or $1/6$. Then we can write

$$R = \frac{F(\phi)}{M_P^2}\left[(1-6\xi)\,\langle\partial^\mu\phi\partial_\mu\phi\rangle + 4\langle V\rangle - 6\xi\langle\phi V_{,\phi}\rangle - \langle T_m\rangle\right]. \tag{46}$$

which is still a generally covariant expression for R. This formula is the key result of our method and is how we compute R on the lattice solely in terms of the fields.

5.3 Expression for R using the FRW α-time metric

Using our α-time FRW metric, we have

$$\frac{1}{2}\partial^\mu\phi\partial_\mu\phi = \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi = -\frac{1}{2a^{2\alpha}}\phi'^2 + \frac{1}{2a^2}(\nabla\phi)^2 = G_\phi - K_\phi \tag{47}$$

using the definitions of K and G from Ref. [1]. With these definitions, R can be expressed as

$$R = \frac{F(\phi)}{M_P^2}\left[2\,(1-6\xi)\left(\langle G_\phi\rangle - \langle K_\phi\rangle\right) + 4\langle V\rangle - 6\xi\langle\phi V_{,\phi}\rangle - \langle T_m\rangle\right], \tag{48}$$

6 Equations for the Lattice Implementation of NMC Scalars

The acceleration equation in terms of R

$$\frac{a''}{a} + (1-\alpha)\mathcal{H}^2 = \frac{a^{2\alpha}}{6}R\,, \tag{49}$$

together with the equation of motion for ϕ

$$\phi'' + (3-\alpha)\frac{a'}{a}\phi' - a^{-2(1-\alpha)}\nabla^2\phi = -a^{2\alpha}\left(\xi R\phi + \frac{\partial V}{\partial\phi}\right)\,, \tag{50}$$

spells out our evolution scheme for the lattice. The key point is that we only need to know R (or equivalently T) in terms of the fields to solve the NMC system. This that will allow us to spell out a simple and concise numerical scheme to evolve this system.

6.1 Natural Variables

It is convenient re-write the equations in terms of *natural variables*, by rescaling fields and coordinates as

$$\tilde\phi = \frac{1}{f_*}\phi\,,\quad d\tilde\eta = \omega_* d\eta\,,\quad d\tilde x_i = \omega_* dx_i\,. \tag{51}$$

with f_* some typical field amplitude and ω_* a characteristic (inverse) time scale of the problem to be studied. In terms of natural variables, we have

$$\tilde{R} = \omega_*^{-2} R \,, \qquad\qquad \widetilde{V} = \frac{1}{f_*^2 \omega_*^2} V \,. \tag{52}$$

Next, we reduce the order of the equation of motion for $\tilde{\phi}$ by introducing a conjugate momentum variable as

$$\tilde{\pi}_\phi = a^{3-\alpha} \tilde{\phi}' \,. \tag{53}$$

In the new variables, the evolution of the non-minimally coupled scalar field is governed by a system of coupled first-order differential equations, in terms of a *kernel* functional $\tilde{\mathcal{K}}_\phi$, as follows

$$\begin{cases} \tilde{\phi}' = a^{\alpha-3} \tilde{\pi}_\phi \,, \\ \tilde{\pi}_\phi' = \tilde{\mathcal{K}}_\phi[a, \tilde{\phi}, \{\tilde{\varphi}_{\rm m}\}, \tilde{R}] \,, \qquad \text{with} \qquad \mathcal{K}_\phi[a, \tilde{\phi}, \{\tilde{\varphi}_{\rm m}\}, \tilde{R}] \equiv a^{1+\alpha}\, \tilde{\nabla}^2 \tilde{\phi} - a^{3+\alpha} \left(\xi \tilde{R} \tilde{\phi} + \frac{\partial \tilde{V}}{\partial \tilde{\phi}} \right) \,. \end{cases} \tag{54}$$

Similarly, to evolve the scale factor we use the acceleration equation derived from the trace of the energy-momentum tensor. Defining the conjugate momentum of $a(\eta)$ as

$$\pi_a = a^{1-\alpha} a' \,, \tag{55}$$

we arrive to a system of coupled first-order differential equations depending on another kernel functional,

$$\begin{cases} a' = a^{\alpha-1} \tilde{\pi}_a \,, \\ \tilde{\pi}_a' = \tilde{\mathcal{K}}_a[a, \tilde{R}] \,, \qquad \text{with} \qquad \tilde{\mathcal{K}}_a[a, \tilde{R}] \equiv \frac{a^{2+\alpha}}{6} \tilde{R} \,. \end{cases} \tag{56}$$

To close the system, an expression for $\tilde{R}$ is needed in both kernels $\mathcal{K}_\phi$, $\mathcal{K}_a$. Changing variables in the expression for R above, we find that in terms of program variables and conjugate momenta, we have

$$\tilde{R} = \frac{f_*^2}{M_P^2} \left[\frac{2\,(1-6\xi) \left(\tilde{E}_G^{\tilde{\phi}} - \tilde{E}_K^{\tilde{\phi}} \right) + 4 \langle \tilde{V} \rangle - 6\xi \langle \tilde{\phi}\, \tilde{V}_{,\tilde{\phi}} \rangle + (\tilde{\rho}_{\rm m} - 3\tilde{p}_{\rm m})}{1 + (6\xi - 1)\, \xi \langle \tilde{\phi}^2 \rangle f_*^2 / M_P^2} \right] \,, \tag{57}$$

where we have used $\langle T_{\rm m} \rangle = 3p_{\rm m} - \rho_{\rm m}$ and introduced the volume-averaged kinetic $\tilde{E}_K^{\tilde{\phi}}$ and gradient $\tilde{E}_G^{\tilde{\phi}}$ energy densities

$$\tilde{E}_K^{\tilde{\phi}} = \frac{1}{2a^6} \langle \tilde{\pi}_{\tilde{\phi}}^2 \rangle \,, \qquad\qquad \tilde{E}_G^{\tilde{\phi}} = \frac{1}{2a^2} \sum_i \langle \tilde{\partial}_i \tilde{\phi} \partial_i \tilde{\phi} \rangle \,. \tag{58}$$

In summary, Eqs. (54) and (56), together with the expression for $\tilde{R}$ in Eq. (57) (plus the equations of motion of the unspecified matter sector), represent a set of equations that completely characterizes the dynamics of a system with a scalar field non-minimally coupled to gravity in the Jordan frame. Generalization to multiple non-minimally coupled scalars is obtained straight forwardly by summing over the terms with non-minimal coupling in Eq. (57).

7 Discretization

In order to evolve our system of equations Eqs. (54), (56) and (57) in a way that fully captures the spatial dependence of the fields, we need to choose a time evolution scheme and to introduce a spatial discretization prescription. We use a lattice with N sites per dimension with periodic boundary conditions. We will consider the lattice sites to represent comoving coordinates. If the (comoving) length of the grid is L, the resulting (comoving) lattice spacing between sites is $\delta x = L/N$. We work with finite differences and use the following notation for the forward and backward derivatives

$$\nabla_i^{\pm} f(\mathbf{n}) = \frac{\pm f(\mathbf{n}) \mp f(\mathbf{n} \pm \hat{\imath})}{\delta x}\,, \tag{59}$$

where f is an arbitrary scalar function defined on the lattice sites $\mathbf{n} = (n_1, n_2, n_3)$, and $\hat{\imath}$ represents a displacement vector of one unit in the i-th direction. We discretize the gradient terms using forward differences and the Laplacian using a symmetric discretization

$$\sum_i \langle \partial_i \phi \partial_i \phi \rangle \quad \longrightarrow \quad \sum_i \langle \nabla_i^+ \phi \nabla_i^+ \phi \rangle\,, \tag{60}$$

$$\vec{\nabla}^2 \phi \quad \longrightarrow \quad \sum_i \nabla_i^- \nabla_i^+ \phi\,. \tag{61}$$

7.1 Discrete Kernels

We are now in a position to define the evolution equations by introducing the discrete kernels

$$\tilde{\mathcal{K}}_\phi \left[a, \tilde{\phi}, \{\tilde{\varphi}_{\rm m}\}, \tilde{R}\right] = a^{1+\alpha} \tilde{\nabla}_i^- \tilde{\nabla}_i^+ \tilde{\phi} - a^{3+\alpha} \left(\xi \tilde{R} \tilde{\phi} + \frac{\partial \tilde{V}}{\partial \tilde{\phi}} \right)\,, \tag{62}$$

$$\tilde{\mathcal{K}}_a \left[a, \tilde{R}\right] = \frac{a^{2+\alpha}}{6} \tilde{R}\,, \tag{63}$$

which we have already written in terms of natural field and spacetime variables, c.f. Eq. (51). We have also introduced dimensionless discrete derivatives $\tilde{\nabla}$ given by Eq. (59) in terms of the dimensionless lattice spacing $\delta\tilde{x} = \tilde{L}/N = \omega_* \delta x$, with $\tilde{L} = \omega_* L$.

7.2 Non-symplectic Evolvers are Required

At this point, it is important to realize that $\tilde{R} = \tilde{R}[\tilde{\phi}, \tilde{\pi}_\phi, \{\tilde{\varphi}_{\rm m}\}, \{\tilde{\pi}_{\varphi_{\rm m}}\}]$ depends on all fields and conjugate momentum variables, and hence the kernel for the non-minimally coupled field $\tilde{\phi}$ depends on its own conjugate momentum. Because of this, preferred symplectic algorithms such as *staggered Leapfrog*, *velocity-* or *position-Verlet*, cannot be used. We can instead use *Runge-Kutta* (RK) methods, in particular explicit RK algorithms. We have adapted the well known *mid-point method* to our set of equations, corresponding to a second order RK method.

References

[1] D. G. Figueroa, A. Florio, F. Torrenti, and W. Valkenburg, *CosmoLattice*, `arXiv:2102.01031`.