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Testing cosmological models using state-of-the-art galaxy surveys

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TESTING COSMOLOGICAL MODELS USING STATE-OF-THE-ART GALAXY SURVEYS

Tese de Doutorado apresentada ao Instituto de Física Teórica do Câmpus de São Paulo, da Universidade Estadual Paulista “Júlio de Mesquita Filho”, como parte dos requisitos para obtenção do título de Doutor em Física, Especialidade Física Teórica.

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Dedico esta tese a minha mãe, Maria da Conceição Silva Rebouças.

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“O peito é infantaria do espírito”

Negro Leo, *Marcha para Longe*

Resumo

As últimas décadas viram gigantes avanços na cosmologia, tanto teóricos quanto experimentais. Há pouco mais de cem anos, Edwin Hubble obtia as primeiras evidências da expansão do Universo, através da luminosidade de "nébulas". Hoje, conseguimos modelar a abundância de elementos atômicos primordiais usando a teoria da Nucleosíntese do Big Bang, que usa a termodinâmica de fluidos cosmológicos para inferir a razão de massa entre elementos atômicos em estrelas. Consequimos também prever anisotropias da Radiação Cósmica de Fundo, previsões confirmadas por experimentos de alta resolução angular. Consequimos fazer o levantamento de milhões de galáxias, estudar correlações estatísticas na população levantada, observando efeitos cosmológicos previstos utilizando teoria de perturbação cosmológica. O sucesso de tais experimentos, entretanto, levantou enormes questões teóricas. Existem evidências de uma matéria escura, que se comporta como uma partícula massiva que não interage sob nenhuma interação fundamental conhecida no Modelo Padrão de Física de Partículas. Ainda mais, também existem evidências de que a expansão do Universo atualmente é acelerada. De acordo com a Relatividade Geral, isso só é possível devido a uma energia escura, um fluido de pressão negativa, que é a forma de energia mais abundante no Universo. A natureza dessa energia escura é desconhecida. O modelo mais simples que a descreve é de uma constante cosmológica, uma densidade de energia constante e igualmente distribuída pelo espaço. Finalmente, também existem evidências de uma época de expansão acelerada do Universo logo após o Big Bang, período conhecido como inflação, e cujo mecanismo ainda é desconhecido.

Estas e outras perguntas motivam uma ampla gama de experimentos cosmológicos com o intuito de entender melhor a natureza da matéria e energia escuras, além da inflação. Hoje em dia, contamos com uma ampla miríade de dados observacionais cada vez mais precisos, cada qual sensível a diferentes aspectos da teoria cosmológica e cada qual com sua previsão para parâmetros do modelo. Com o aumento gradual da precisão dos experimentos, alguns começaram a discordar entre si quanto à previsão de parâmetros. Tais discordâncias, conhecidas como tensões, podem algumas vezes ser aliviadas a partir de diferentes tratamentos de erros sistemáticos. Algumas tensões, como a tensão de Hubble, são tão graves que não possuem tratamento sistemático que consiga aliviá-las. A falta de soluções

às tensões motivou a investigação de modelos de energia escura alternativos, que consigam acomodar os dados discordantes. Nesta tese, apresento o modelo cosmológico Λ CDM, amplamente utilizado para prever observações de distâncias, das anisotropias da CMB, modelar a formação da estrutura em grande escala do Universo, dentre vários efeitos observáveis. Apresento também análise Bayesiana de dados cosmológicos, o procedimento padrão de como obter informação sobre o modelo cosmológico a partir da grande miríade de diferentes dados cosmológicos. Com o arcabouço teórico desenvolvido e as ferramentas em mão, investigo propriedades da energia escura, como sua equação de estado, sua abundância ao longo da história cósmica, suas possíveis interações com a matéria escura, seu efeito na formação de estruturas e sua capacidade de resolver tensões cosmológicas. Mais especificamente, eu discuto dois trabalhos originais desenvolvidos ao longo do meu doutorado: o primeiro investiga o paradigma de "Early Dark Energy" com uma modificação adicional na equação de estado da energia escura recente, e o segundo discute indicações de energia escura dinâmica usando dados recentes de medidas de distâncias.

Palavras Chaves: Energia Escura; Levantamentos de Galáxias; Radiação Cósmica de Fundo; Supernovas; Inferência Estatística.

Áreas do conhecimento: Física; Física Geral: Relatividade e Gravitação; Astrofísica Extragaláctica: Cosmologia.

Abstract

The last few decades have seen significant advances in cosmology, both theoretical and experimental. Just over a hundred years ago, Edwin Hubble obtained the first evidence of the expansion of the Universe through the luminosity of "nebulae". Today, we can model the abundance of primordial atomic elements using the Big Bang Nucleosynthesis theory, which uses the thermodynamics of cosmological fluids to infer the mass ratio of atomic elements in stars. We can also predict anisotropies in the Cosmic Microwave Background (CMB), predictions confirmed by high angular resolution experiments. We have conducted surveys of millions of galaxies, studying statistical correlations in the surveyed population and observing predicted cosmological effects using cosmological perturbation theory. The success of such experiments, however, has raised enormous theoretical questions. There is evidence of dark matter, which behaves like a massive particle that does not interact through any known fundamental interaction in the Standard Model of Particle Physics. Furthermore, there is evidence that the expansion of the Universe is currently accelerating. According to General Relativity, this is only possible due to dark energy, a negative pressure fluid that is the most abundant form of energy in the Universe. The nature of this dark energy is unknown. The simplest model that describes it is a cosmological constant, a constant and evenly distributed energy density throughout space. Finally, there is also evidence of a period of accelerated expansion of the Universe shortly after the Big Bang, known as inflation, whose mechanism is still unknown.

These and other questions motivate a wide range of cosmological experiments aimed at better understanding the nature of dark matter, dark energy, and inflation. Today, we have a vast array of increasingly precise observational data, each sensitive to different aspects of cosmological theory and each with its prediction for model parameters. As experimental precision gradually increases, some parameters' predictions have begun to disagree with one another. These disagreements, known as tensions, can sometimes be alleviated by different treatments of systematic errors. Some tensions, such as the Hubble tension, are so severe that no systematic treatment can alleviate them. The lack of solutions to these tensions has motivated the investigation of alternative dark energy models that can accommodate the conflicting data. In this thesis, I present the Lambda-CDM

(Λ CDM) cosmological model, widely used to predict distance observations, CMB anisotropies, model the large-scale structure formation of the Universe, among various observable effects. I also present Bayesian analysis of cosmological data, the standard procedure for obtaining information about the cosmological model from the vast array of different cosmological data. With the developed theoretical framework and tools in hand, I investigate properties of dark energy, such as its equation of state, its abundance throughout cosmic history, its possible interactions with dark matter, its effect on structure formation, and its capacity to resolve cosmological tensions. In particular, I discuss two original works done during my PhD: the first investigates Early Dark Energy with late-time equation of state modifications, and the second discusses hints of dynamical dark energy from recent geometric measurements.

Keywords: Dark Energy; Galaxy Surveys; Cosmic Microwave Background; Supernovae; Statistical Inference.

Knowledge areas: Physics; General Physics: Relativity and Gravitation; Extragalactic Astrophysics: Cosmology.

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Chapter 1

Introduction and Motivation

This chapter qualitatively explains what is cosmology, its main objects of study, the current state of the field, and the relevance of the research developed during my PhD. The ideas presented in this chapter will be carefully developed throughout the thesis.

Cosmology is the study of the Universe's evolution as it expands. The expansion of the Universe may be a difficult concept to grasp: the effects of the Universe's expansion can only be measured at very large scales, in distances typically of the order of 1Mpc (one megaparsec), or approximately 3×10^{22} m. For comparison, the distance between the Milky Way and Andromeda, the nearest galaxy, is approximately 765kpc away.

The expansion of the Universe is a gravitational effect that makes the physical spatial distance between two comoving points (i.e. points that have no relative motion) increases with time. This phenomenon affects different physical processes such as the formation of the first atomic elements, stars, galaxies, galaxy clusters and voids. It affects, for instance, how we perceive light from distant sources. The hypothesis of an expanding Universe was raised in the early twentieth century by physicists Alexander Friedmann and Georges Lemaître [1], and was developed by many great physicists such as James Peebles [2]. Since then, multiple predictions based on the Universe's expansion have been confirmed, such as the Hubble law for nearby astronomical objects [3], the existence of an almost isotropic Cosmic Microwave Background radiation [4] - as well as statistical properties of its anisotropies [5] -, the weak gravitational lensing of light in the large scale structure of the Universe [6], the relative abundance of light elements in stars [7], statistical properties of the spatial distribution of galaxies [8] - in particular the effect of Baryonic Acoustic Oscillations, or BAOs [9] - among many other observable effects. Today, the expansion of the Universe is unanimously accepted by the scientific community and continuously proven by new experiments.

General Relativity (GR) provides a theoretical framework that can describe the cosmological expansion effect in the spacetime geometry through the history of

the Universe. In GR, the geometrical properties of space and time are summarized by a metric tensor, whose components are $g_{\mu\nu}(\mathbf{r}, t)$ and are functions of the spatial position $\mathbf{r}$ and time t . The equations of motion for the metric tensor are the Einstein's field equations,

$$G_{\mu\nu} = 8\pi G T_{\mu\nu}. \quad (1.1)$$

The left hand side of Equation 1.1 is a complicated, nonlinear function of the metric components, its partial derivatives with respect to space and time, and its inverse. In the standard four spacetime dimensions, the components $g_{\mu\nu}$ are symmetric, leaving 10 independent components. The Einstein's field equations are a set of 10 nonlinear, coupled, second-order partial differential equations for the metric components. Due to the enormous complexity of the problem, in order to solve the Einstein's field equations, physicists rely on approximations and (sometimes bold) assumptions. The main assumption in cosmology is the so-called **cosmological principle**. To explain it, I use an analogy: the liquid content in a glass of water seems homogeneous. We know that water is formed by molecules, which in turn are formed by atoms, which are formed by more elementary particles. If we visualize a droplet of water in scales of nanometers, $1\text{nm} = 10^{-9}\text{m}$, we would observe that water is not homogeneous at all, but rather is made of a complex structure. Molecules interact with each other, forming intricate structures. Nevertheless, in scales much larger than the nanometer, a glass of water looks homogeneous. In the same way, the description of a single water molecule, composed by two hydrogen atoms and one oxygen atom, is intrinsically anisotropic: the molecule, for instance, has a nonzero electric dipole. However, in an ensemble of molecules, the dipoles are randomly distributed, in such a way that the average electric dipole over the ensemble is zero. The description of the average over the ensemble of particles is, therefore, isotropic: it shows no preferential spatial direction.

In the same way, the space is filled with numerous distinct components such as planets, stars, galaxies, black holes and an infinity of astronomical objects, all of them interacting gravitationally. However, at very large scales, the distribution of astronomical objects in the Universe seems homogeneous. The cosmological principle is an assumption that can be stated as: the properties of the Universe, when averaged over sufficiently large (but finite) scales, don't depend on the position or direction: they are homogeneous and isotropic. Properties of the Universe include the metric components, matter densities and velocities.

There is evidence supporting the cosmological principle. The Cosmic Mi-

microwave Background is a radiation signal that can be detected from any part of the Earth, pointing a detector to any direction in the sky. This electromagnetic radiation follows very perfectly a black body radiation distribution at temperature $T_{\text{CMB}} \approx 2.725\text{K}$ [10]. The temperature of this radiation is almost isotropic, with very small fluctuations of order $\Delta T / T_{\text{CMB}} \approx 10^{-5}$ [11, 5]. This indicates that the CMB photons, primordial photons created right after the Big Bang, were in thermal equilibrium everywhere, an indication of homogeneity. While there are tests of the cosmological principle using type Ia supernovae [12] and galaxy surveys [13, 14], these are very sensitive to astrophysical effects, and there is no decisive evidence against the principle. The cosmological principle is also closely related to the Einstein equivalence principle, which states that the Earth is not a privileged reference frame in the Universe. In practice, the Cosmological Principle greatly reduces the complexity of the Einstein's field equations: under the homogeneity assumption, the left and right-hand sides of Equation 1.1 depend only on time, and not on position.

Under the cosmological principle, the metric components $g_{\mu\nu}$ reduce to a single degree of freedom $a(t)$: the scale factor, a quantity that describes how the distance between any two given points change with time. We can interpret the scale factor in the following way: let A and B be two fixed points in space, and D_{AB} be the physical distance between the points. The expansion of the universe makes this distance change with time. The scale factor is defined such that, for arbitrary time instants t_1 and t_2 , the distance D_{AB} obeys the relation

$$\frac{D_{AB}(t_1)}{D_{AB}(t_2)} = \frac{a(t_1)}{a(t_2)} \quad \forall A, B. \quad (1.2)$$

It's common practice to normalize the scale factor today as $a(t_0) = 1$ ¹. Therefore, when specializing the Einstein's field equations to an isotropic, homogeneous and expanding space, we can determine how the scale factor varies in time. The solution of the Einstein's field equations reveals the expansion history of the Universe.

The energy-momentum tensor $T_{\mu\nu}$, appearing in the right-hand side of Equation 1.1, describes the distribution of energy and momentum across the Universe. For instance, part of the Universe is made by particles described by the Standard

¹Quantities with a 0 underscript, such as t_0 and a_0 , are evaluated "today", in the present time. Since the cosmological timescale is much larger than our human time scale, there is no issue with the fact that the definition of "today" or "now" varies continuously.

Model of Particle Physics. Quantum field theory provides a way to calculate the tensor $T_{\mu\nu}$ associated to the particle. At the largest scales, under the cosmological principle, much of the microphysics of the particles is "washed out", and only spatial-averaged quantities such as energy density ρ and pressure P affect the cosmological expansion. To describe cosmological contents of the Universe under the cosmological principle, we employ a coarse-grained fluid description in which particles are homogeneously distributed in space with an energy density and pressure that varies in time. The relation between energy density and pressure is dependent on the specific component. Ultrarelativistic particles (i.e. particles whose kinetic energy pc is much bigger than their rest mass energy mc^2) and massless particles are known to follow the relation $P = \rho/3$. Non-relativistic particles (i.e. particles whose kinetic energy is small compared to their rest mass energy) are pressureless, $P = 0$. Today, all visible matter in the universe is non-relativistic. Right after the Big Bang, when the temperature of the Universe was extremely high, these particles were ultrarelativistic. The transition between ultrarelativistic and non-relativistic behaviors occurs roughly when the temperature of the Universe cools down below the threshold $k_B T / mc^2 \approx 1$, where m is the mass of the particle.

The cosmological principle reduces the Einstein's field equations in 1.1 to two equations, named Friedmann equations, relating $a(t)$, $\rho(t)$ and $P(t)$,

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G\rho}{3}, \quad (1.3)$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P). \quad (1.4)$$

Due to energy conservation, energy density and pressure must obey the continuity equation,

$$\frac{d\rho}{dt} + 3H(\rho + P) = 0. \quad (1.5)$$

A cosmological model must specify the components of the Universe, that is, the fluids that contribute for the total energy density ρ . Most of the Standard Model particles, which we will call "baryonic matter"², have become non-relativistic very early in the history of the Universe. Massive neutrinos could still be relativistic if their mass is around $m_\nu \approx 2 \times 10^{-4} \text{eV}$, the mass corresponding to the CMB temperature. To this day, no constraints on the neutrino mass can rule out such

²In cosmology, baryonic matter refers to all Standard Model particles except for photons and neutrinos.

a small value. Photons and massless neutrinos - jointly referred to as radiation - obey the equation $P = \rho/3$ throughout all cosmological history, although the cosmological community is abandoning the massless neutrino paradigm.

The current consensual cosmological model, called Λ CDM, adds two extra components in the Universe in addition to radiation and baryonic matter: cold dark matter (CDM) and a cosmological constant (Λ), also known as dark energy. CDM behaves like non-relativistic matter, with $P = 0$, and the cosmological constant has a rather strange behavior: it follows $P = -\rho$. In the subsequent chapters, I will explain in more detail the motivations for having such strange components, as well as their behavior.

Evidence for cold dark matter was first observed in the rotational speed of astronomical objects [15]. The mass of a galaxy, for instance, can be estimated from its brightness and from the rotational speeds of stars in the galaxy due to gravity. In the first half of the twentieth century, many observations pointed out that the mass inferred from the gravitational effects is several times bigger than the mass inferred from the object's luminosity. This "non-luminous" mass was then called dark matter [16]. Since then, the existence of dark matter was confirmed by other methods. The CMB, for instance, can distinguish between dark matter and baryonic matter: the latter interacts with light via Thomson scattering, the former doesn't. This interaction leaves an imprint in the CMB temperature correlations. CMB measurements from the Planck collaboration point that approximately 30% of the Universe's energy density is due to non-relativistic matter, but only 5% is due to baryonic matter [5]. Gravitational lensing from galaxies is another effect able to measure the total mass of a galaxy. Since masses distort space, photon trajectories can make curves and circumvent massive objects. The more massive the lens is, the more light will bend: therefore, this lensing effect can also be used to infer the mass of a lens object, such as a galaxy. Finally, one main evidence for dark matter is the relative abundance of light elements in stars and galaxies, which can be predicted by the theory of Big Bang Nucleosynthesis [7]. Using the Boltzmann equation, we can compute, for instance, the abundance of helium that was formed from hydrogen atoms in the early Universe. We obtain the Helium mass fraction of $Y_{\text{He}} \approx 0.24$, compatible with an Universe with around 5% of baryonic matter.

Strong evidence for dark energy was reported in 1998 by two research groups: the High- z supernovae search team led by Adam Riess [17], and the Supernovae Cosmology Project, led by Saul Perlmutter [18]. Type-IA Supernovae are explo-

sions of white dwarf stars. The physical mechanism behind these supernovae is well known, and the intrinsic luminosity from the explosions is roughly the same for all events. Therefore, type-IA supernovae can be treated as standard candles: we can infer the distance D_L to the supernovae based on their luminosity. We can also measure its redshift: the change in the light frequency due to the expansion of the Universe. Thus, we can study the relation between z and D_L . For nearby supernovae (i.e. those with redshift $z \ll 1$), this relation is the Hubble law,

$$D_L = \frac{1}{H_0} z, \quad (1.6)$$

where H_0 is the Hubble constant, the current expansion rate of the Universe, defined as $H_0 = \dot{a}(t_0)/a(t_0)$. For more distant objects, we can see a deviation from this linear approximation,

$$D_L = \frac{1}{H_0} (z + q_0 z^2 + \dots), \quad (1.7)$$

where q_0 is the current deceleration parameter of the Universe, defined as $q_0 = -a_0 \ddot{a}_0 / (\dot{a}_0)^2$. An Universe composed by radiation and non-relativistic matter has a strictly positive deceleration parameter: this is a consequence from the Friedmann Equations 1.3, as both the energy density and pressure for radiation and matter are positive. However, both teams found that distant supernovae pointed to a negative deceleration parameter. From the Friedmann equations, this can only happen if $\rho + 3P < 0$.

The final piece in all cosmological models, not just Λ CDM, is the existence of an accelerated expansion period, called inflation, right after the Big Bang [19]. Such an accelerated expansion solves the so-called horizon problem in the CMB. This problem can be stated shortly as: since the CMB photons were emitted early in the history of the Universe, two photons coming from opposite directions could not be in causal contact with each other, and thus could not be in thermal equilibrium. This goes against the evidence that the CMB is very isotropic. However, a period of accelerated expansion would solve this problem, putting all CMB photons in causal contact. The simplest inflation models are realized by a scalar field, named inflaton. Inflation is also a mechanism that provides initial inhomogeneities in the Universe. By calculating the quantum fluctuations of the inflaton in a de Sitter (i.e. exponentially expanding) spacetime, it can be shown that the power spectrum of the field fluctuations is nearly scale-invariant. These fluctuations are

imprinted in the inhomogeneities of the Universe, and can grow or decay during the expansion. CMB anisotropy power spectrum measurements are compatible with initial fluctuations from inflation.

Today, we are upon a data-driven era of precision cosmology. The great success of the Λ CDM model in describing such a myriad of data has led to increasingly ambitious and precise experiments able to pinpoint model parameters with percent-level precision. For instance, the PantheonPlus catalog of type Ia supernovae, calibrated with cepheid variable stars, give a current abundance of dark energy of $\Omega_\Lambda = \rho_{\Lambda,0}/\rho_{\text{tot},0} = 0.666 \pm 0.018$ and the current expansion rate of $H_0 = 73.3 \pm 1.1 \text{ km s}^{-1} \text{ Mpc}^{-1}$ [20]. CMB anisotropy data from the Planck collaboration also constrain the current baryonic matter density to be $\Omega_b h^2 = (\rho_{b,0}/\rho_{\text{tot},0})h^2 = 0.02233 \pm 0.00015^3$, the amplitude of inflation-induced perturbations to be $A_s \times 10^9 = 2.101^{+0.031}_{-0.034}$ and its spectral index, or tilt, as $n_s = 0.9649 \pm 0.0042$ [5]. Finally, the reionization optical depth, a parameter describing the effect of ionized gas in the CMB photons, is constrained by CMB polarization measurements to be $\tau = 0.0544 \pm 0.0073$. The enormous technical effort put in cosmological experiments has paid out: current experiments can place percent-level constraints on the six Λ CDM parameters.

A viable cosmological model must be able to consistently explain the myriad of current observational data. The current experimental precision, however, has revealed discrepancies between different experiments. For instance, the value of H_0 inferred the local distance ladder is [21]

$$H_0 = 73.3 \pm 1.04 \text{ km s}^{-1} \text{ Mpc}^{-1},$$

while the value inferred from Planck 2018 CMB anisotropies is

$$H_0 = 67.36 \pm 0.54 \text{ km s}^{-1} \text{ Mpc}^{-1}.$$

Making a simplistic interpretation of these constraints, the posterior distribution of H_0 from the SH0ES collaboration is a Gaussian centered at 73.3 with standard deviation 1.04. The mean of the Planck 2018 posterior distribution for H_0 is 67.34, which is more than five standard deviations away from the SH0ES mean. Assuming the posterior distribution from SH0ES, the probability of measuring the Planck 2018 mean value for H_0 is astronomically low, of order e^{-25} . There are statistical subtleties in making such an interpretation, but the fact is that the

³ $h = H_0 / (100 \text{ km s}^{-1} \text{ Mpc}^{-1})$

two measurements are in severe disagreement. This problem has been named the **Hubble tension**, and it stands as one of the most pressing problems in current physics.

A minor but persistent tension is also present between CMB and cosmic shear experiments. The σ_8 parameter represents the RMS of matter fluctuations inside a sphere of radius $R = 8\text{Mpc}/h$. This parameter affects the lensing of photons, being most constrained as the combination $S_8 = \sigma_8\sqrt{\Omega_m/0.3}$. CMB measurements from Planck place a constraint of [5]

$$S_8 = 0.846 \pm 0.017,$$

while cosmic shear measurements from the Dark Energy Survey constrain S_8 to be [8]

$$S_8 = 0.775^{+0.024}_{-0.026}.$$

Repeating the same simplistic interpretation of the H_0 tension, the difference in means is approximately 2.8σ . While this tension is less extreme, upcoming cosmic shear and CMB surveys will increase the precision, reducing the error bars and potentially aggravating this S_8 tension.

From a theoretical standpoint, there is no explanation for the nature of dark energy. A cosmological constant could in principle be explained by the vacuum energy of the fields comprising the Standard Model of Particle Physics. Performing this calculation, however, would yield a cosmological constant orders of magnitude larger than the current measured value. Much theoretical effort is being put into creating fundamental dark energy models and testing their predictions against state-of-the-art cosmological data.

Due to the tensions and the lack of theoretical support for a cosmological constant, it is important, to explore alternative dark energy models. Many of these are able to better fit the observed data and alleviate cosmological tensions [22]. Investigating alternative dark energy behaviors can provide information about the fundamental dark energy model, which could shed light on other problems in current physics. As of the time of writing, though, ΛCDM still stands as the standard model of cosmology.

My PhD research investigates alternative dark energy models in the context of cosmological tensions. I study scalar field models, fundamental components that can realize general dark energy dynamics in terms of a potential function $V(\phi)$, usually connected to particle physics. Phenomenological models try to

parametrize the dark energy density $\rho(a)$ or the dark energy equation of state $w(a)$, exploring determined dynamical behavior but having little theoretical support. Within these classes there are infinite possibilities, some of them able to alleviate cosmological tensions. For instance, the Early Dark Energy (EDE) model assumes a non-negligible amount of dark energy near recombination, at redshifts $z \approx 3000$: this addition can alleviate the H_0 tension without degrading the fit for late-time observables. I have studied them using cosmic shear data from the Dark Energy Survey, culminating in the analysis of Chapter 6 and the original work "Early dark energy constraints with late-time expansion marginalization" [23]. On the phenomenological side, my original work "Investigating Late-Time Dark Energy and Massive Neutrinos in Light of DESI Y1 BAO" tests parametrizations of the dark energy equation of state in the context of recent hints of dynamical dark energy from recent supernovae and BAO surveys [24]. Additionally, I have also contributed to the original work "Modeling nonlinear scales with the Comoving Lagrangian Acceleration method: Preparing for LSST Y1" [25], assessing the viability of building a suite of COLA simulations to construct an emulator of the nonlinear matter power spectrum for beyond- Λ CDM models. While the modelling of nonlinear effects represents a great challenge in the analysis of galaxy surveys with extended cosmological models, this work will not be discussed in this thesis. Furthermore, I am a member of two galaxy survey collaborations: the Dark Energy Survey (DES) and the Legacy Survey of Space and Time Dark Energy Collaboration (LSST-DESC). I am currently leading the analysis of an interacting dark energy model using the full observations from DES, and a project to forecast LSST constraints on the dark energy equation of state.

In this thesis, I study the theoretical basis of the Λ CDM model, describe the relevant datasets able to provide constraints on the cosmological model, list some alternative candidates to Λ CDM (non-exhaustively), discuss the data analysis techniques used to test dark energy models and present results from my PhD using various models and datasets. This PhD thesis is organized as follows. The first chapters review theoretical aspects of cosmological theory, observations and data analysis. Chapter 2 presents the Λ CDM model, the simplest model that explains all cosmological observations; Chapter 3 reviews recent and historical cosmological measurements and explains current cosmological tensions, the biggest challenges in cosmology today; Chapter 4 reviews modifications to the Λ CDM theory and their status; Chapter 5 explains the standard data analysis methods being utilized by the cosmological community today. The subsequent chapters present original

results developed during my PhD: Chapter 6 presents an analysis of combined Early Dark Energy and smooth dark energy at late-times; Chapter 7 presents the analysis of three different dark energy models using DESI 2024 BAO data, assessing constraints on the neutrino mass. Finally, Chapter 8 summarizes the thesis.

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Chapter 2

The Λ CDM Model

This chapter explains Λ CDM, the consensus model among the cosmological community. I start discussing the homogeneous and isotropic theory, a direct consequence of the Cosmological Principle. Using perturbation theory, I then insert small, inhomogeneous perturbations around the homogeneous solution. Such inhomogeneities are core theoretical aspects of present-day cosmological measurements.

Throughout this thesis, I use a spacetime metric with signature $(-, +, +, +)$.

2.1 Einstein Equations and The Cosmological Principle

The expansion of the Universe is described by General Relativity, summarized in the Einstein field equations,

$$G_{\mu\nu} = 8\pi G T_{\mu\nu}. \quad (2.1)$$

At face value, the field equations represent a set of 10 nonlinear, second-order partial differential equations for 10 functions $g_{\mu\nu}$ of 4 variables t, x, y, z . Finding exact solutions of the Einstein field equations is an extremely complex task. Fortunately, we can impose additional assumptions and symmetries that simplify the problem but restrict the applicability of the theory. The two most important assumptions, homogeneity and isotropy, are based on the cosmological principle.

The cosmological principle states that all spacetime properties, in particular the metric and matter distribution, when averaged over sufficiently large but finite distances, are homogeneous and isotropic. Homogeneity and isotropy greatly reduce the number of degrees of freedom in both metric and energy-momentum tensor. We can divide any rank-2 tensor $M_{\mu\nu}$ into four parts: its pure

time component M_{00} , its spatial-temporal components M_{0i} and M_{i0} , and the pure spatial components M_{ij} . For the energy-momentum tensor, we define $T_0^0 = -\rho$, the energy density of the fluid. T_0^i transforms as a vector in space, and since there are no isotropic vectors, $T_0^i = 0$. Finally, T_{ij} transforms as a rank-2 spatial tensor. It is known that the only rank-2 isotropic tensors are those proportional to the identity, and then we can define the fluid's pressure P as

$$T_j^i = P\delta_j^i. \quad (2.2)$$

Finally, the homogeneity condition implies that ρ and P are only functions of time, not position. Therefore, considering homogeneity and isotropy, the average matter content of the Universe can be described by two functions of time: its energy density $\rho(t)$ and its pressure $P(t)$. Its energy momentum tensor components are given by¹

$$T_\nu^\mu = \text{diag}(-\rho, P, P, P). \quad (2.3)$$

The same constraints also apply to the metric tensor $g_{\mu\nu}$: in particular, $g_{0i} = 0$ and $g_{ij} = a^2(t)\gamma_{ij}$, where $a(t)$ is the scale factor and γ_{ij} is the spatial metric. However, we also must impose that the spatial curvature is homogeneous: this condition sets a certain form for the spatial metric which will be derived in the next section.

2.2 The Homogeneous and Isotropic Cosmological Theory

2.2.1 The Geometry of the Universe

The Cosmological Principle implies that spatial curvature must be homogeneous. There are only three kinds of 3-dimensional spaces with constant curvature: planes (no curvature), spheres (positive curvature) and hyperbolae (negative curvature). The three of them can be jointly described by the metric

$$ds_{(3)}^2 = \frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2, \quad (2.4)$$

¹This definition changes with the metric signature.

where k is the spatial curvature, the inverse of the spatial curvature radius. A positive value of k refers to a sphere, a negative value refers to a hyperbola, and zero refers to the usual Euclidean space. A derivation of this spatial metric is presented in Appendix A.1. In cartesian coordinates, this metric can be written as

$$ds_{(3)}^2 = \frac{k(x_i dx^i)^2}{1 - kx_i x^i} + dx_i dx^i = \gamma_{ij} dx^i dx^j. \quad (2.5)$$

Throughout this thesis, I use γ_{ij} to denote the spatial metric. In the flat space, $\gamma_{ij} = \delta_{ij}$. To capture the expansion of the Universe, we introduce the scale factor $a(t)$ such that the physical distance element in the hypersurfaces of constant time t scales with time as

$$ds_{(3)}^2 = a^2(t) \left[\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right] = a^2(t) \gamma_{ij} dx^i dx^j. \quad (2.6)$$

Thus, we can express the spacetime metric as

$$ds^2 = -dt^2 + a^2(t) \left[\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right] = -dt^2 + a^2(t) \gamma_{ij} dx^i dx^j. \quad (2.7)$$

This metric is known as the curved FLRW² metric. From it, we identify two unknowns in cosmology:

- $a(t)$, the evolution of the scale factor in time, which determines the **expansion history of the Universe**;
- k , the spatial curvature of the Universe. While a flat space is commonly assumed, nothing prohibits $k \neq 0$, and the spatial curvature is always a considered hypothesis.

There are some useful reparametrizations of the FLRW metric 2.7. One of them consists in defining the **conformal time** τ via

$$d\tau = a dt. \quad (2.8)$$

Using the conformal time, we obtain the metric

$$ds^2 = a^2(\tau) (-d\tau^2 + \gamma_{ij} dx^i dx^j). \quad (2.9)$$

²As an homage to Alexander Friedmann, Georges Lemaître, Howard Robinson and Arthur Walker, prominent names in the conception of modern cosmology.

Another reparametrization consists in redefining the radial coordinate of the spatial metric, using an auxiliary coordinate χ as

$$d\chi = \frac{dr}{\sqrt{1 - kr^2}}. \quad (2.10)$$

Integrating the relation above, we find

$$\chi = \begin{cases} \frac{1}{\sqrt{k}} \arcsin(\sqrt{k}r), & \text{if } k > 0; \\ r, & \text{if } k = 0; \\ \frac{1}{\sqrt{|k|}} \operatorname{arcsinh}(\sqrt{|k|}r), & \text{if } k < 0. \end{cases} \quad (2.11)$$

It can be easily inverted to obtain the radial comoving distance r in terms of χ

$$r = S_k(\chi) = \begin{cases} \frac{1}{\sqrt{k}} \sin(\sqrt{k}\chi), & \text{if } k > 0; \\ \chi, & \text{if } k = 0; \\ \frac{1}{\sqrt{|k|}} \sinh(\sqrt{|k|}\chi), & \text{if } k < 0. \end{cases} \quad (2.12)$$

The function $S_k(\chi)$ is analytic in both χ and k , but this piecewise form is more useful in practice. Using the coordinates χ and τ , the FLRW metric can be written as

$$ds^2 = a^2(\tau)(-d\tau^2 + d\chi^2 + S_k^2(\chi)d\Omega^2), \quad (2.13)$$

where $d\Omega^2 = d\theta^2 + \sin^2\theta d\phi^2$ is the solid angle element. This form of the FLRW metric is useful for calculating photon trajectories.

2.2.2 Kinematics in an Expanding Universe

The 4-momentum of particles, $P^\mu = (E, P^i)$, must obey the geodesic equation

$$P^\mu \nabla_\mu P^\nu = 0 \rightarrow P^\mu \partial_\mu P^\nu + \Gamma_{\alpha\beta}^\nu P^\alpha P^\beta = 0, \quad (2.14)$$

where $\Gamma_{\alpha\beta}^\mu$ are the Christoffel symbols. Appendix A.2 presents the calculation of the Christoffel symbols. Assuming homogeneity, we have $\partial_i P^\nu = 0$, and thus

$$E \frac{dP^\nu}{dt} + \Gamma_{\alpha\beta}^\nu P^\alpha P^\beta = 0. \quad (2.15)$$

For the case $\nu = 0$, we use the computed Christoffel symbols to get

$$E \frac{dE}{dt} = -\Gamma_{ij}^0 P^i P^j = -a \dot{a} P^2 = -\frac{\dot{a}}{a} p^2, \quad (2.16)$$

where $P^2 = \gamma_{ij} P^i P^j$ is the magnitude of the comoving 3-momentum and we define the physical 3-momentum as $p^i = a P^i$, analogous to the relation between physical and comoving distances. The particles' momentum obey the on-shell energy-momentum relation

$$g_{\mu\nu} P^\mu P^\nu = -m^2 \rightarrow -E^2 + p^2 = -m^2 \rightarrow E^2 = p^2 + m^2, \quad (2.17)$$

where we identify the physical 3-momentum $a^2 \gamma_{ij} P^i P^j = p^2$. Therefore, $E dE = p dp$, and we can write

$$p \frac{dp}{dt} = -H p^2 \rightarrow \frac{dp}{dt} = -\frac{\dot{a}}{a} p \rightarrow p \propto a^{-1}. \quad (2.18)$$

The physical 3-momentum of particles decays with the scale factor. For massless particles, such as photons, $E = p$, and thus their energy is inversely proportional to the scale factor. Since the photons' energy is inversely proportional to its wavelength, this implies that the wavelength of photons increase linearly with the scale factor. Since red light has the biggest wavelength in the visible spectrum, we call this effect **cosmological redshift**, one of the main predictions of cosmology.

2.2.3 The Components of the Universe

According to the Einstein's field equations, matter impacts the expansion of the Universe by the energy-momentum tensor, $T^{\mu\nu}$. Due to the cosmological principle, the energy-momentum tensor is determined by the energy density ρ and pressure P . Through Bianchi's identities, General Relativity also implies that the energy-momentum tensor is conserved,

$$\nabla_\mu T^{\mu\nu} = 0 \rightarrow \partial_\mu T^{\mu\nu} + \Gamma_{\mu\alpha}^\mu T^{\alpha\nu} + \Gamma_{\mu\alpha}^\nu T^{\alpha\mu} = 0. \quad (2.19)$$

Using the Christoffel symbols from Appendix A.2 and the fact that the energy-momentum tensor is diagonal, we get to the continuity equation for cosmological

fluids, which described how the energy density changes as the Universe expands

$$\begin{aligned}\partial_0 T^{00} + \Gamma_{i0}^i T^{00} + \Gamma_{ij}^0 T^{ij} &= 0, \\ \dot{\rho} + 3H\rho + a\dot{a}P/a^2 &= 0, \\ \frac{d\rho}{dt} + 3H(\rho + P) &= 0,\end{aligned}\tag{2.20}$$

where we define the Hubble factor as $H = \dot{a}/a$. Notice that we do not obtain an equation for the evolution of pressure. The microphysics of the matter fluid determines a relation between pressure and density, which can be expressed as

$$P = w\rho,\tag{2.21}$$

where w is the **equation of state** of the fluid. Assuming w is constant, we can solve for the density ρ as a function of the scale factor a

$$\frac{d\rho}{da}\dot{a} + 3\frac{\dot{a}}{a}(1+w)\rho = 0 \rightarrow \rho = \rho_0 a^{-3(1+w)},\tag{2.22}$$

where ρ_0 is the density today. Different kinds of fluids, such as radiation, dark matter and dark energy, have different equations of state. Since the energy-momentum tensor is additive, we can postulate that the total energy-momentum tensor $T_{\mu\nu}$ is the sum of several independent tensors $T_{(i)}^{\mu\nu}$, where i is the index of the component. Each of the components has its own density ρ_i and pressure P_i . Assuming that these components do not interact with each other, their energy-momentum tensors are separately conserved

$$\nabla_\mu T_{(i)}^{\mu\nu} = 0 \rightarrow \dot{\rho}_i + 3H(\rho_i + P_i) = 0.\tag{2.23}$$

This opens the possibility that the Universe is composed of multiple components that behave differently. For instance, it is known from statistical mechanics that radiation fluids, that is, ensembles of massless or ultrarelativistic particles, obey the relation $P = \rho/3$. This definition of radiation encompasses photons, massless neutrinos and massive neutrinos while they are ultrarelativistic. Other Standard Model particles have become nonrelativistic much early in the Universe's history. Notice that, if $w = 1/3$, then the energy density of radiation ρ scales with a^{-4} . This is consistent with the cosmological redshift discussed in the last Section. If the energy of ultrarelativistic particles scales with a^{-1} , then the energy density $\rho = E/V$ scales with a^{-4} , as the volume scales with a^3 .

For nonrelativistic particles, even though their physical 3-momentum P^i decays as a^{-1} , the momentum is only a small part of the total energy, which is mostly comprised by the rest-mass energy $E = m_0 c^2$, which is constant. This implies that ρ scales as a^{-3} and that the equation of state is $w = 0$. Dust is a general relativity jargon for this pressureless fluid.

After the Big Bang, all Standard Model particles are ultrarelativistic. As the Universe expands and cools down, the massive particles become nonrelativistic. This implies that their equation of state w smoothly transitions from $w = 1/3$ to $w = 0$. Cosmologists refer to massive Standard Model particles (except neutrinos) as **baryonic matter**, assumed to have $w = 0$. **Dark matter**, an exotic form of energy, behaves as massive particles with $w = 0$, but only interact with Standard Model particles through gravity. We are also going to see more exotic fluids: the curvature of the Universe effectively acts as a fluid with $w = -1/3$, a cosmological constant behaves as a fluid with $w = -1$, scalar fields can represent a fluid with varying equation of state w , among other possibilities.

The continuity equation has a thermodynamic interpretation. Each fluid is a thermodynamic system described by their internal energy U , their volume V and the number of particles N , such that

$$dU = -PdV + \mu dN + TdS. \quad (2.24)$$

The expansion of the Universe is an adiabatic process, that is, it does not alter the entropy: $dS = 0$. It also does not alter the number of particles, so $dN = 0$. Therefore, as the Universe expands, we have

$$dU = -PdV. \quad (2.25)$$

The energy density of a fluid is defined as $\rho = U/V$. Its derivative with respect to time is

$$\frac{d\rho}{dt} = \frac{1}{V} \frac{dU}{dt} - \frac{U}{V^2} \frac{dV}{dt} = -\frac{P}{V} \frac{dV}{dt} - \frac{\rho}{V} \frac{dV}{dt}. \quad (2.26)$$

The FLRW metric implies that the spatial volume scales as a^3 , or $V = V_0 a^3$, where V_0 is the fluid's volume today, and thus

$$\frac{1}{V} \frac{dV}{dt} = \frac{3a^2 \dot{a}}{a^3} = 3H. \quad (2.27)$$

Inserting this volume derivative into Equation 2.26, we obtain the same continuity

equation that was obtained via the Bianchi identity,

$$\frac{d\rho}{dt} = -3H(\rho + P). \quad (2.28)$$

2.2.4 The Friedmann Equations

We can proceed to calculate the Einstein field equations 2.1 assuming the FLRW metric 2.7. The general procedure consists in calculating the Christoffel symbols $\Gamma_{\alpha\beta}^{\mu}$, then the Ricci tensor $R_{\mu\nu}$ and finally the Einstein tensor $G_{\mu\nu}$. These lengthy computations are shown in Appendix A.2. We obtain the following components of the Einstein tensor

$$G_{00} = 3H^2 + \frac{3k}{a^2}, \quad (2.29)$$

$$G_{ij} = \left(-2\frac{\ddot{a}}{a} - H^2 - \frac{k}{a^2} \right) a^2 \gamma_{ij}. \quad (2.30)$$

We can proceed to calculate the time-time Einstein equation, $G_{00} = 8\pi GT_{00}$

$$\begin{aligned} 3H^2 + \frac{3k}{a^2} &= 8\pi G\rho \\ H^2 &= \left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G\rho}{3} - \frac{k}{a^2}. \end{aligned} \quad (2.31)$$

Equation 2.31 is the **Friedmann equation**, one of the central equations in cosmology. It relates the expansion rate $H = \dot{a}/a$ with the energy density of the Universe ρ . In summary, the more dense matter is, the faster the Universe will expand. The Friedmann equation can also be rewritten in terms of conformal time τ : defining $\mathcal{H} = a'/a$ and primes denoting derivatives with respect to τ , we get

$$\mathcal{H}^2 = \left(\frac{a'}{a} \right)^2 = \frac{8\pi G a^2 \rho}{3} - k. \quad (2.32)$$

We still have the spatial part of the Einstein equations, $G_{ij} = 8\pi GT_{ij}$. Due to

isotropy, we can simply take one of the diagonal terms, leading to

$$\begin{aligned} -2\frac{\ddot{a}}{a} - H^2 - \frac{k}{a^2} &= 8\pi G P \\ -2\frac{\ddot{a}}{a} - \frac{8\pi G \rho}{3} &= 8\pi G P \\ \frac{\ddot{a}}{a} &= -\frac{4\pi G}{3}(\rho + 3P). \end{aligned} \quad (2.33)$$

Equation 2.33 is the second Friedmann equation, relating the acceleration of the Universe's expansion $\ddot{a}$ with the matter pressure P and density ρ . In summary, if matter obeys the strong energy condition $\rho + 3P \geq 0$, the expansion of the Universe will be decelerating, $\ddot{a} < 0$.

The Λ CDM model assumes that the Universe is composed by photons, neutrinos, baryonic matter, cold dark matter and a cosmological constant. Photons and massless neutrinos are collectively denoted as **radiation** and have $w = 1/3$. Their current energy density is known from measurements of the Cosmic Microwave Background temperature $T_{\text{CMB}} \approx 2.7255$. Baryons and CDM, collectively denoted as **matter**, have $w = 0$. Finally, the cosmological constant has $w = -1$. Their energy densities scale as

$$\rho_r = \rho_{r,0} a^{-4}, \quad (2.34a)$$

$$\rho_b = \rho_{b,0} a^{-3}, \quad (2.34b)$$

$$\rho_c = \rho_{c,0} a^{-3}, \quad (2.34c)$$

$$\rho_\Lambda = \rho_{\Lambda,0}, \quad (2.34d)$$

where the subscripts indicate radiation, baryons, cold dark matter and the cosmological constant Λ , respectively, and $\rho_{i,0}$ is the current energy density of component i . Defining $\rho_{m,0} = \rho_{b,0} + \rho_{c,0}$, we can write the Friedmann equation as

$$H^2 = \frac{8\pi G}{3}(\rho_{r,0} a^{-4} + \rho_{m,0} a^{-3} + \rho_{\Lambda,0}) - \frac{k}{a^2}. \quad (2.35)$$

If we define $\rho_{k,0} = -3k/8\pi G$, we can rewrite the equation as

$$H^2 = \frac{8\pi G}{3}(\rho_{r,0} a^{-4} + \rho_{m,0} a^{-3} + \rho_{k,0} a^{-2} + \rho_{\Lambda,0}). \quad (2.36)$$

Thus, in the Friedmann equation, curvature effectively acts as a fluid with $w = -1/3$. Finally, one of the most important measurable quantities in cosmology is

the current expansion rate of the Universe, H_0 . From the Friedmann equation, we can obtain

$$H_0^2 = \frac{8\pi G}{3}(\rho_{r,0} + \rho_{m,0} + \rho_{k,0} + \rho_{\Lambda,0}). \quad (2.37)$$

We define the **critical energy density** ρ_{cr} as

$$\rho_{\text{cr}} = \frac{3H_0^2}{8\pi G}, \quad (2.38)$$

and the energy density parameters as $\Omega_i = \rho_{i,0}/\rho_{\text{cr}}$, so we can rewrite the Friedmann equation as

$$H^2 = H_0^2(\Omega_r a^{-4} + \Omega_m a^{-3} + \Omega_k a^{-2} + \Omega_\Lambda). \quad (2.39)$$

The parameters Ω_r , Ω_m , Ω_Λ and Ω_k are not independent, they must satisfy the relation

$$\Omega_r + \Omega_m + \Omega_\Lambda + \Omega_k = 1. \quad (2.40)$$

2.2.5 Measuring and Predicting Distances

Distances are one of the most important cosmological observables. The cosmological theory is able to predict the physical distance of an astronomical body with given redshift. Therefore, by comparing theory predictions against measured data, we can gain information about the theory, constraining its parameters.

Due to the expansion of the Universe, we observe distant bodies receding away from us. Because of the Doppler effect, the light emitted by these bodies will be measured with a different wavelength compared to the original wavelength emitted in the source frame. This difference is quantified by the redshift,

$$z = \frac{\lambda_{\text{obs}} - \lambda_{\text{emit}}}{\lambda_{\text{emit}}}, \quad (2.41)$$

where λ_{obs} and λ_{emit} are the observed and emitted wavelengths, respectively. Since the photon wavelength scales with a , we obtain the relation

$$z = \frac{\lambda_{\text{obs}}}{\lambda_{\text{emit}}} - 1 = \frac{a(t_{\text{obs}})}{a(t_{\text{emit}})} - 1 = \frac{1}{a(t_{\text{emit}})} - 1, \quad (2.42)$$

where $a(t_{\text{emit}})$ is the scale factor at photon emission time and $a(t_{\text{obs}}) = 1$ is the scale factor at observation time. Therefore, **by measuring the redshift of astronomical**

bodies, we can know the scale factor at the time of photon emission, assuming no peculiar velocities.

Redshifts are mainly measured in two ways. The most direct measurement is called the spectroscopic redshift. The received light is analyzed in a spectroscope, and its frequencies can be resolved. Since we know that hydrogen is the most common atomic element in the Universe, we can compare the spectroscopic lines with the hydrogen spectral lines, observing that they have been shifted by a constant amount. Spectroscopic redshift is a very precise measurement, but it's not the preferred method in surveys that measure the redshifts of millions of astronomical objects.

The second method is the photometric redshift. Although less precise than spectroscopic redshift, the photometric redshift of many objects can be easily measured. Photometric redshift is measured by making the light pass through different color filters. The Dark Energy Survey, for instance, has used 5 filters: gray, red, near-infrared and infrared (the so-called *griz* photometric system) are common in photometric surveys, but it's standard to add an additional filter, either in the ultraviolet region, forming the *ugriz* system, or in the far-infrared region, the *grizY* system [26].

Distances, on the other hand, are much harder to measure. There are two main distance measurements: **luminosity distance** and **angular diameter distance**. Luminosity distance is a measure of distance inferred by how bright the astronomical object looks. Using a charged coupled device (CCD), we can measure the luminous energy flux $\mathcal{F}$ of a luminous object,

$$\mathcal{F} = \frac{dE}{dA dt}, \quad (2.43)$$

where dE/dt is the energy per unit time entering the CCD lens area dA . Assuming no cosmological effects and the energy flux conservation, the measured flux must be equal to the source energy flux

$$\mathcal{F} = \frac{P_{\text{source}}}{4\pi D^2}, \quad (2.44)$$

where P_{source} is the source's energy emission rate per unit time and D is the distance to the source. Thus, we define the luminosity distance D_L from the

observer to the emitting body as

$$D_L^2 = \frac{P_{\text{source}}}{4\pi\mathcal{F}}. \quad (2.45)$$

We can only calculate the luminosity distance if we know the intrinsic luminosity of the source, P_{source} . Fortunately, there are **standard candles**: astronomical objects or events whose intrinsic luminosity is known. The first proposed standard candles were cepheid variable stars, following the work of Henrietta Swan Leavitt [27, 28]. In recent astronomy, Type Ia supernovae have become important standard candles that can be detected at high redshifts.

As stated, this definition assumed no cosmological effects on light: the luminosity distance is equal to the physical distance when this assumption is true. However, the observed energy flux cannot be equal to the emitted energy flux: during the photon trajectory, it redshifts, and its energy decreases with time until it is detected. Furthermore, if the source emits photons at a certain rate, we will receive these photons at a smaller rate because of the expansion. Imagine the photons being emitted by the source in a straight line, one by one, in regular intervals. As the Universe expands, the space between photons increases, and the time interval between photon receptions by the observer will be greater than the emission interval. Both these effects decrease the observed flux with respect to the emitted flux by factors of a . Taking both effects into account, we can rewrite the flux conservation as

$$\mathcal{F} = \frac{P_{\text{source}}}{4\pi D^2(1+z)^2}, \quad (2.46)$$

and we get the relation between luminosity distance and comoving distance D ,

$$D_L^2 = D^2(1+z)^2 \rightarrow D_L = (1+z)D. \quad (2.47)$$

Another distance measurement is the angular diameter distance. Suppose we observe an astronomical body at a certain region in the sky. This body occupies an angle $\delta\theta$ in the sky. If we know the actual size L of the body, we can then define the angular diameter distance D_A from the observer to the body as

$$D_A = \frac{L}{\delta\theta}. \quad (2.48)$$

This distance is simply related to the comoving distance D by the fact that, as the light from the body travels through the Universe, the physical distance to

the source increases, so we perceive a smaller angular size than that of a static Universe. Therefore

$$D_A = \frac{D}{1+z}. \quad (2.49)$$

The definitions imply a relation between angular and luminosity distances

$$D_L = (1+z)^2 D_A. \quad (2.50)$$

The CMB anisotropies provide a very precise measurement of an angular scale θ_* , related to the sound horizon at recombination $r_s(z_*)$, a physical scale related to the scattering between baryonic matter and photons. This angular scale θ_* is given by

$$\theta_* = \frac{r_s(z_*)}{D_A(z_*)}, \quad (2.51)$$

where $z_* \approx 1100$ is the recombination redshift and $D_A(z_*)$ is the angular diameter distance to that redshift.

Finally, we must be able to provide theoretical predictions to these observables. We use the form of the FLRW metric in terms of the conformal time τ and auxiliary coordinate χ ,

$$ds^2 = a^2(\tau)[-d\tau^2 + d\chi^2 + S_k^2(\chi)d\Omega^2], \quad (2.52)$$

where

$$S_k(\chi) = \begin{cases} \chi, & \text{if } k = 0; \\ \frac{1}{\sqrt{\Omega_k}} \sin(\Omega_k \chi), & \text{if } k < 0; \\ \frac{1}{\sqrt{|\Omega_k|}} \sinh(\Omega_k \chi), & \text{if } k > 0. \end{cases} \quad (2.53)$$

Recall that the radial coordinate $r = S_k(\chi)$ is the metric distance. A radial photon trajectory would have $d\theta = 0, d\phi = 0, d\tau = d\chi$. Thus, the comoving distance χ to the source is

$$\chi = \int_{\tau_{\text{emit}}}^{\tau_{\text{now}}} d\tau = \int_{a_{\text{emit}}}^1 \frac{d\tau}{da} da \quad (2.54)$$

$$\chi = \int_{a_{\text{emit}}}^1 \frac{1}{a\dot{a}} da = \int_0^z \frac{dz'}{H(z')}. \quad (2.55)$$

Using the Friedmann equation 2.39, we can obtain

$$\chi(z) = \int_0^z \frac{dz'}{H_0 \sqrt{\Omega_r(1+z')^4 + \Omega_m(1+z')^3 + \Omega_k(1+z')^2 + \Omega_\Lambda}}, \quad (2.56)$$

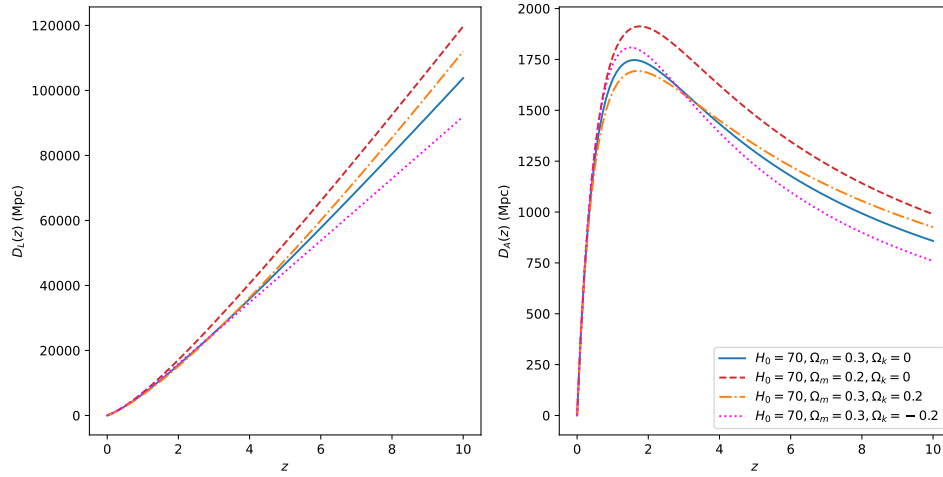


Figure 2.1: Examples of luminosity (left panel) and angular diameter (right panel) distances as a function of redshift for selected Λ CDM cosmologies.

and the luminosity and angular diameter distances are computed via

$$D_L(z) = (1+z)S_k(\chi(z)), \quad (2.57)$$

$$D_A(z) = \frac{S_k(\chi(z))}{1+z}. \quad (2.58)$$

2.3 The Inhomogeneous Universe

The universe is not homogeneous and isotropic. CMB temperature measurements indicate small fluctuations from isotropy, about 1 part in 10 thousand. The critical energy density today ρ_{cr} , when converted to matter density, evaluates at roughly 5 protons per cubic meter, which certainly doesn't describe galaxy clusters, let alone planets and stars. The background equations describe an average Universe. Now, we turn our attention to deviations from homogeneity.

2.3.1 Metric Perturbations

The FLRW metric with conformal time is

$$ds^2 = a^2(\tau)(-d\tau^2 + \gamma_{ij}dx^i dx^j), \quad (2.59)$$

where γ_{ij} is the spatial metric, which can be reduced to δ_{ij} if the space is flat. We will add small, position-dependent perturbations to this metric³ as

$$g_{\mu\nu} = \bar{g}_{\mu\nu}(\tau) + \delta g_{\mu\nu}(\tau, \mathbf{r}), \quad (2.60)$$

where $\bar{g}_{\mu\nu}$ is the FLRW metric and $\delta g_{\mu\nu}$ are the position-dependent perturbations. Breaking the assumptions of homogeneity and isotropy, we are now dealing with 10 extra degrees of freedom in the metric perturbations $\delta g_{\mu\nu}$. Assuming the deviations are small, we can approximate our equations to first order in $\delta g_{\mu\nu}$. It's important to notice that this is a bold statement: we assume that g is analytic with respect to the perturbations and that the derivative of the perturbations is of the same order of magnitude as the perturbations themselves. Finally, it's crucial to remark that linear perturbation theory is only a good approximation if the perturbations are much smaller than the background, homogeneous terms.

2.3.2 The Scalar-Vector-Tensor Decomposition

Without homogeneity and isotropy, linear perturbation theory adds 10 degrees of freedom to our theory. The Scalar-Vector-Tensor (SVT) decomposition is a technique to separate independent degrees of freedom in our perturbed tensors.

First of all, we can separate spatial and temporal parts of the metric perturbations: $\delta g_{00}, \delta g_{0i}, \delta g_{ij}$. We define each part of $\delta g_{\mu\nu}$ as

$$\delta g_{00} = -2a^2 A, \quad (2.61a)$$

$$\delta g_{0i} = -a^2 B_i, \quad (2.61b)$$

$$\delta g_{ij} = a^2 h_{ij}, \quad (2.61c)$$

such that the full metric can be written as

$$ds^2 = a^2(\tau) [-(1 + 2A)d\tau^2 - 2B_i d\tau dx^i + (\gamma_{ij} + h_{ij})dx^i dx^j]. \quad (2.62)$$

Next, every 3-vector B_i can be decomposed into a divergenceless part and a

³In reality, perturbation theory is based on expanding the metric in a power series: $g_{\mu\nu} = \bar{g}_{\mu\nu}(\tau) + \epsilon g_{\mu\nu}^{(1)} + \epsilon^2 g_{\mu\nu}^{(2)} + \dots$, where $g_{\mu\nu}^{(n)}$ is the n -th order correction in the metric and ϵ is the perturbation parameter that keeps track of the order of every term. Since we are in first order, it's not difficult to identify the order of any given term and linearize the equations, so we can present it in a more intuitive way in equation 2.60.

gradient part,

$$B_i = \hat{B}_i + \partial_i B, \text{ where } \partial_i \hat{B}^i = 0. \quad (2.63)$$

Note that B_i has 3 degrees of freedom which are divided into one scalar B and the other two in the divergenceless vector $\hat{B}_i$.

There is an analogous theorem for 3-tensors. The first part is to note that we can easily separate the trace of any rank 2 tensor.

$$h_{ij} = \frac{1}{3} \gamma_{ij} h_m^m + (H_T)_{ij} \implies (H_T)_m^m = 0 \quad (2.64)$$

I am going to denote the trace as $2H_L = h^l_l/3$. The traceless part can be decomposed as

$$(H_T)_{ij} = 2(\nabla_i \nabla_j - \frac{1}{3} \gamma_{ij} \nabla^2) H_T + (\nabla_i (\hat{H}_T)_j + \nabla_j (\hat{H}_T)_i) + 2(\hat{H}_T)_{ij}, \quad (2.65)$$

where ∇_i is the spatial covariant derivative and

$$\nabla_i (\hat{H}_T)^i = 0, \quad (2.66a)$$

$$\nabla_i (\hat{H}_T)^{ij} = 0, \quad (2.66b)$$

$$(\hat{H}_T)_i^i = 0. \quad (2.66c)$$

Again, note that h_{ij} has 6 degrees of freedom. These are now split as two scalar functions H_L and E , one transverse vector $\hat{E}_i$ with two free components, and one transverse-traceless tensor $\hat{E}_{ij}$ with two free components. To summarize, the tensor part of the metric perturbations can be written as

$$h_{ij} = 2H_L \gamma_{ij} + 2\nabla_{ij}^T H_T + (\nabla_i (\hat{H}_T)_j + \nabla_j (\hat{H}_T)_i) + 2(\hat{H}_T)_{ij}, \quad (2.67)$$

where, for brevity, we define the traceless second derivative as $\nabla_{ij}^T = \nabla_i \nabla_j - \nabla^2/3$.

The SVT decomposition is closely related to Fourier transforms and spherical tensors. The eigenfunctions of the spatial laplacian operator, ∇^2 , will be denoted as $Q_{\mathbf{k}}^{(0)}(\mathbf{r})$, and satisfy

$$\nabla^2 Q_{\mathbf{k}}^{(0)}(\mathbf{r}) = -k^2 Q_{\mathbf{k}}^{(0)}(\mathbf{r}). \quad (2.68)$$

In flat space, these functions are the exponentials, $Q_{\mathbf{k}}^{(0)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}}/(2\pi)^{3/2}$. For curved spaces, these functions assume more complicated forms, but luckily we are only interested in their linear independence, a property that generalizes to non-flat

spaces. They form a complete set of functions, and thus any scalar function can be written as

$$A(\tau, \mathbf{r}) = \int d^3k \tilde{A}(\tau, \mathbf{k}) Q_{\mathbf{k}}^{(0)}(\mathbf{r}), \quad (2.69)$$

where $\tilde{A}(\tau, \mathbf{k})$ is the amplitude of the $\mathbf{k}$ mode at an instant τ .

Vector functions can also be decomposed using the vector normal modes $Q_i^{(\pm 1)}(\mathbf{r})$ ⁴. In flat space, vector normal modes are related to circular polarizations,

$$Q_i^{(\pm 1)}(\mathbf{r}) = \frac{i}{\sqrt{2}}(\mathbf{e}_1 \pm i\mathbf{e}_2)_i e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (2.70)$$

where we chose $\mathbf{e}_1$ and $\mathbf{e}_2$ perpendicular to $\mathbf{k}$. The choice of circular polarizations is made so the modes are eigenfunctions of the angular part of the laplacian (i.e. spherical harmonics). These components also capture the vorticity of the vector field.

Since our space is 3-dimensional, there is also a third vector mode parallel to $\mathbf{k}$ (i.e. **longitudinal** mode) that can be built explicitly from the scalar mode,

$$Q_i^{(0)}(\mathbf{r}) = -\frac{1}{k} \nabla_i Q^{(0)}(\mathbf{r}). \quad (2.71)$$

In a flat space, this is equivalent to $Q_i^{(0)}(\mathbf{r}) = (\mathbf{e}_3)_i e^{i\mathbf{k} \cdot \mathbf{r}}$, choosing $\mathbf{e}_3$ in the direction of $\mathbf{k}$. The 3 vector modes $Q_i^{(0)}(\mathbf{r})$, $Q_i^{(\pm 1)}(\mathbf{r})$ are linearly independent vectors and complete sets of functions, and therefore can build any vector function in space. Finally, notice that the $Q_i^{(\pm 1)}(\mathbf{r})$ modes are transverse, that is, $\nabla_i Q_i^{(\pm 1)}(\mathbf{r}) = 0$, and the $Q_i^{(0)}(\mathbf{r})$ mode is a gradient. These facts are related to the decomposition made in Equation 2.63.

Any spatial tensor can be decomposed similarly. In particular, for rank 2 symmetric traceless tensors, we have two transverse modes $Q_{ij}^{(\pm 2)}(\mathbf{r})$, two mixed transverse-longitudinal modes that can be built from the transverse vector modes,

$$Q_{ij}^{(\pm 1)}(\mathbf{r}) = -\frac{1}{2k}(\nabla_i Q_j^{(\pm 1)}(\mathbf{r}) + \nabla_j Q_i^{(\pm 1)}(\mathbf{r})), \quad (2.72)$$

and one longitudinal mode built from the scalar mode

$$Q_{ij}^{(0)}(\mathbf{r}) = \left(\frac{1}{k^2} \nabla_i \nabla_j - \frac{1}{3} \gamma_{ij} \nabla^2 \right) Q^{(0)}(\mathbf{r}). \quad (2.73)$$

⁴From now on, I drop the subscript $\mathbf{k}$, leaving this dependence implicit.

Equations 2.72 and 2.73 are related to the SVT decomposition in Equation 2.65.

In summary, the Fourier $\mathbf{k}$ mode of a scalar function ($A, \delta\rho, H_L \dots$) is given by (usually the $\mathbf{k}$ can be denoted as a subscript or even be absent)

$$\delta\rho(\tau, \mathbf{r}) = \delta\rho(\tau, \mathbf{k}) Q^{(0)}(\mathbf{r}), \quad (2.74)$$

the $\mathbf{k}$ mode of a vector function will be given by

$$B_i(\tau, \mathbf{r}) = \sum_{m=-1}^1 B^{(m)}(\tau, \mathbf{k}) Q_i^{(m)}(\mathbf{r}), \quad (2.75)$$

and the $\mathbf{k}$ mode of a rank-2 tensor can be written as:

$$H_{Tij}(\tau, \mathbf{r}) = \sum_{m=-2}^2 H_T^{(m)}(\tau, \mathbf{k}) Q_{ij}^{(m)}(\mathbf{r}). \quad (2.76)$$

Longitudinal (0) degrees of freedom, also known as **scalar modes**, behave differently depending on their scale $\mathbf{k}$: they may oscillate with fixed amplitude, or grow in amplitude due to gravitational attraction. Usually, single transverse degrees of freedom (± 1), also known as **vector modes**, decay with the expansion of the universe. The transverse (± 2) degrees of freedom, or **tensor modes**, are related to gravitational waves.

Interlude: a fictional theory

I now illustrate the SVT decomposition with a simplistic fictional theory. Let $\mathbf{V}(\mathbf{r}, t)$ be a vector function and $A(\mathbf{r}, t)$ be a scalar function, both defined in the Euclidean spacetime and following the linear differential equations

$$A + \nabla \cdot \mathbf{V} = 0, \quad (2.77)$$

$$\frac{d\mathbf{V}}{dt} + \nabla A = 0. \quad (2.78)$$

One may perform a Fourier decomposition of the functions

$$A(\mathbf{r}, t) = \int \frac{d^3k}{(2\pi)^3} \tilde{A}(\mathbf{k}, t) e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (2.79a)$$

$$\mathbf{V}(\mathbf{r}, t) = \int \frac{d^3k}{(2\pi)^3} \tilde{\mathbf{V}}(\mathbf{k}, t) e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (2.79b)$$

$\tilde{\mathbf{V}}$ is a vector in k -space. We can choose $\hat{\mathbf{k}}$ as one of the basis vectors (the radial vector), and choose two perpendicular vectors to it, $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$. We can also define the circular polarization vectors $\hat{\pm} = (\hat{\mathbf{a}} \pm i\hat{\mathbf{b}})/\sqrt{2}$ and we have a basis. Thus, we can write

$$\tilde{\mathbf{V}} = V^{(0)}(\mathbf{k}, t)\hat{\mathbf{k}} + V^{(+1)}(\mathbf{k}, t)\hat{+} + V^{(-1)}(\mathbf{k}, t)\hat{-}. \quad (2.80)$$

For brevity, I will denote $V^{(+1)}(\mathbf{k}, t)\hat{+} + V^{(-1)}(\mathbf{k}, t)\hat{-} = V^{(\pm 1)}(\mathbf{k}, t)\hat{\pm}$. Inserting the Fourier decomposition in the scalar equation, we obtain

$$\int \frac{d^3k}{(2\pi)^3} [\tilde{A} + i\mathbf{k} \cdot \tilde{\mathbf{V}}] e^{i\mathbf{k} \cdot \mathbf{r}} = 0. \quad (2.81)$$

From our decomposition, we have

$$\mathbf{k} \cdot \tilde{\mathbf{V}} = kV^{(0)}(\mathbf{k}, t), \quad (2.82)$$

where k is the magnitude of $\mathbf{k}$. Hence, our scalar equation becomes

$$\int \frac{d^3k}{(2\pi)^3} [\tilde{A} + ikV^{(0)}] e^{i\mathbf{k} \cdot \mathbf{r}} = 0, \quad (2.83)$$

since the functions $e^{i\mathbf{k} \cdot \mathbf{r}}$ are linearly independent, the term in square brackets must vanish for all $\mathbf{k}$,

$$\tilde{A} + ikV^{(0)}. \quad (2.84)$$

Inserting the Fourier decomposition into the second equation, we obtain

$$\int \frac{d^3k}{(2\pi)^3} \left[\frac{d}{dt} V^{(0)}(\mathbf{k}, t)\hat{\mathbf{k}} + \frac{d}{dt} V^{(\pm 1)}(\mathbf{k}, t)\hat{\pm} + i\mathbf{k}\tilde{A}(\mathbf{k}, t) \right] = 0, \quad (2.85)$$

where the right-hand side is understood to be the null vector. Therefore, every component of the LHS vector must be zero, and we have three equations, one for each linearly independent vector,

$$\frac{d}{dt} V^{(0)}(\mathbf{k}, t) + ik\tilde{A}(\mathbf{k}, t) = 0 \quad (2.86)$$

and

$$\frac{d}{dt} V^{(\pm 1)}(\mathbf{k}, t) = 0. \quad (2.87)$$

We haven't relied on the orthonormality of the basis $\{\hat{\mathbf{k}}, \hat{\pm}\}$, only on the fact that they are linearly independent. We could have chosen, for instance, the basis

$\{i\mathbf{k}, \hat{\pm}\}$. Using this choice, we get the following equations:

$$\tilde{A} - k^2 V^{(0)} = 0; \quad (2.88a)$$

$$\frac{d}{dt} V^{(0)}(\mathbf{k}, t) + \tilde{A}(\mathbf{k}, t) = 0; \quad (2.88b)$$

$$\frac{d}{dt} V^{(\pm 1)}(\mathbf{k}, t) = 0. \quad (2.88c)$$

Both sets of equations are equivalent, the components are just defined differently. One has to be careful about the basis conventions, different authors may use different ones. One important thing to notice is that due to the linearity of the equations, **vector modes and scalar modes are completely independent**.

For tensors, things are exactly the same, only the basis we choose is the tensor product of the vector basis with itself. Any symmetric tensor can thus be decomposed into

$$\tilde{\mathbf{T}}(\mathbf{k}, t) = T^{(0)}(\mathbf{k} \otimes \mathbf{k}) + T^{(\pm 1)}(\mathbf{k} \otimes \hat{\pm}) + T^{(\pm 2)}(\hat{\pm} \otimes \hat{\pm}) \quad (2.89)$$

so the same procedure applies for tensor equations.

This formalism is still valid for the constant curvature spaces we study in cosmology, since the angular part doesn't change. The orthonormal set of eigenfunctions of $\nabla_\mu \nabla^\mu$ won't be the exponentials, but they exist and can provide a Fourier-like basis like discussed above, since for every point we pick vectors on the tangent space.

2.3.3 Energy-Momentum Tensor Perturbations

We must also include position-dependent perturbations in the energy-momentum tensor,

$$T_{\mu\nu}(\tau, \mathbf{r}) = \bar{T}_{\mu\nu}(\tau) + \delta T_{\mu\nu}(\tau, \mathbf{r}). \quad (2.90)$$

One way to see it is that metric perturbations cause matter perturbations (passive point of view), but this is not always the case. Some structure formation models predict persistent vector perturbations, and those must be caused by some internal

dynamics of the dark sector. We can parametrize the matter perturbations as

$$\delta T^0_0 = -\delta\rho, \quad (2.91a)$$

$$\delta T^i_0 = -(\bar{\rho} + \bar{P})v^i, \quad (2.91b)$$

$$\delta T^0_i = (\bar{\rho} + \bar{P})(v_i - B_i), \quad (2.91c)$$

$$\delta T^i_j = \delta P\delta^i_j + \bar{P}\Pi^i_j. \quad (2.91d)$$

There are 10 new degrees of freedom: $\delta\rho$ is the density perturbation, δP is the pressure perturbation, v^i is the velocity of the fluid; Π^i_j is the anisotropic stress, which can without loss of generality be made traceless. Each of those quantities can also be decomposed into scalar, vector and tensor modes. It is common to use the **density contrast**

$$\delta = \frac{\delta\rho}{\rho} \quad (2.92)$$

instead of the density perturbations $\delta\rho$.

Some components of the Universe have null or negligible perturbations, $\delta\rho_S \ll \delta\rho_C$, where C stands for clustering components. We call them **smooth components**. The two main examples in Λ CDM are curvature (thought of as a fluid with $w = -1/3$) and the cosmological constant, two fluids without any perturbations. Other fluids may have negligible perturbations, as we will see ahead.

2.3.4 Perturbed Conservation and Einstein Equations

Now, we want to write the conservation and Einstein equations, expanding them in linear perturbations. The process is the same as in the homogeneous case: we have to calculate the connection, Riemann tensor, etc. The calculations are longer because we are not working with homogeneity anymore, and there are more degrees of freedom, but reducing to linear order helps. Since this process is systematic and lengthy, we use a Mathematica package called xPand, a submodule from the xAct⁵ package. Its documentation is very thorough and should be sufficient to learn the basics of the package. For conciseness, I describe the process to obtain the perturbed Einstein and conservation equations using xPand in Appendix B. In the following, I summarize the main equations from cosmological perturbation theory.

In the remaining of the thesis, only scalar perturbations will be studied. Since

⁵<http://www.xact.es/index.html>

scalar perturbations are completely unaffected by the vector and tensor degrees of freedom, **I neglect the vector and tensor perturbations from now on.** Furthermore, I also assume **flat space**.

The perturbed FLRW metric is given by

$$ds^2 = a^2(\tau)[-(1 - 2A)d\tau^2 - 2\partial_i B dx^i d\tau + (\delta_{ij} - 2H_L \delta_{ij} + 2\partial_{ij}^T H_T)]. \quad (2.93)$$

The perturbed energy-momentum tensor is given by

$$\delta T^0_0 = -\delta\rho, \quad (2.94a)$$

$$\delta T^i_0 = -(\bar{\rho} + \bar{P})\partial^i v, \quad (2.94b)$$

$$\delta T^0_i = (\bar{\rho} + \bar{P})\partial_i(v - B), \quad (2.94c)$$

$$\delta T^i_j = \delta P \delta^i_j + \bar{P} \partial_{ij}^T \Pi. \quad (2.94d)$$

In Fourier space, the scalar conservation equations are

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = -(\bar{\rho} + \bar{P})(kv + 3H'_L), \quad (2.95a)$$

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [(\bar{\rho} + \bar{P})\frac{(v - B)}{k}] = \delta P - \frac{2}{3}\bar{P}\Pi + (\bar{\rho} + \bar{P})A. \quad (2.95b)$$

The Fourier-space scalar Einstein equations are

$$\left(2\frac{a''}{a} - 2\left(\frac{a'}{a}\right)^2 + \frac{d}{d\tau} - \frac{k^2}{3}\right)A - \left(\frac{d}{d\tau} + \mathcal{H}\right)\left(\frac{kB}{3} + H'_L\right) = 4\pi Ga^2\left(\delta P + \frac{\delta\rho}{3}\right), \quad (2.96a)$$

$$4\pi Ga^2\left(\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right)\right) = k^2\left(H_L + \frac{H_T}{3} + \frac{\mathcal{H}}{k^2}(kB - H'_T)\right), \quad (2.96b)$$

$$k^2\left(A + H_L + \frac{H_T}{3}\right) + \left(\frac{d}{d\tau} - 2\mathcal{H}\right)(kB - H'_T) = 8\pi Ga^2\bar{P}\Pi, \quad (2.96c)$$

$$\mathcal{H}A - H'_L - \frac{H'_T}{3} = 4\pi Ga^2(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right). \quad (2.96d)$$

2.3.5 The Gauge Problem

Both metric and matter perturbations are not coordinate independent. By changing the time slicing or the spatial threading, we can introduce or remove certain terms that we would relate to perturbations in equations 2.60 and 2.94.

I illustrate this dependence with one example. Suppose we keep the spatial coordinates but use a different time slicing $\tilde{\tau} = \tau + T(\mathbf{r}, \tau)$, where T is a small position-dependent function. We can calculate the metric component $\tilde{g}_{00}(\tilde{x})$ as

$$\tilde{g}_{00}(\tilde{x}) = \frac{\partial x^\mu}{\partial \tilde{x}^0} \frac{\partial x^\nu}{\partial \tilde{x}^0} g_{\mu\nu}(x). \quad (2.97)$$

In the tilde coordinate system, $\tilde{g}_{00}(\tilde{x}) = a^2(\tilde{\tau})(1 + 2\tilde{A})$. Since $\tilde{\tau} = \tau + T$, we can approximate at linear order

$$\tilde{g}_{00} = (a(\tau) + a'(\tau)T)^2(1 + 2\tilde{A}) \approx a^2(\tau)(1 + 2\mathcal{H}T)(1 + 2\tilde{A}) \approx a^2(\tau)(1 + 2\mathcal{H}T + 2\tilde{A}). \quad (2.98)$$

Plugging this result into Equation 2.97, we obtain

$$a^2(\tau)(1 + 2\mathcal{H}T + 2\tilde{A}) = a^2(\tau)(1 + 2A - 2T') \rightarrow \tilde{A} = A - T' - \mathcal{H}T. \quad (2.99)$$

If T is chosen such that $T' + \mathcal{H}T = A$, then $\tilde{A} = 0$: by a suitable coordinate redefinition, we were able to eliminate one of the perturbation degrees of freedom.

This is analogous to electromagnetism, where the vector potential A^μ has, in principle, four degrees of freedom, but there is also a freedom to redefine A^μ as $\tilde{A}^\mu = A^\mu + \partial^\mu \Lambda$ without changing the Maxwell equations. We say that A^μ has a **gauge degree of freedom**, which does not affect the physics. This gauge degree of freedom is eliminated by imposing some extra condition to A^μ which makes calculations easier. This condition must be satisfiable by fixing Λ .

We must identify the gauge degrees of freedom, determine how the perturbation variables transform with the gauge, and then fix the gauge degrees of freedom. Another possibility, which will not be explored in this work, is to find gauge-independent quantities and rewrite all equations in terms of those quantities.

Gauge Transformations

Let us analyze how perturbations change if we make a coordinate transformation of the form

$$x^\mu \rightarrow \tilde{x}^\mu = x^\mu + \xi^\mu(\tau, \mathbf{x}), \quad (2.100)$$

where ξ^μ are small, perturbative changes in the coordinates that we only need to consider linearly. We perform an SVT decomposition of ξ^μ : $\xi^0 = T$, $\xi^i = L^i = \nabla^i L$. Upon this coordinate transformation, the metric components transform as

$$\tilde{g}_{\mu\nu}(\tilde{x}) = \frac{\partial x^\alpha}{\partial \tilde{x}^\mu} \frac{\partial x^\beta}{\partial \tilde{x}^\nu} g_{\alpha\beta}(x), \quad (2.101)$$

and the energy-momentum transfer $T_{\mu\nu}$ transforms similarly. For the sake of conciseness, the computation of these coordinate transformations is presented in Appendix A.3. Using the SVT decomposition and Fourier modes, we can show that

$$\tilde{A} = A - T' - \mathcal{H}T, \quad (2.102a)$$

$$\tilde{B} = B + L' + kT, \quad (2.102b)$$

$$\tilde{H}_L = H_L - \frac{k}{3}L - \mathcal{H}T, \quad (2.102c)$$

$$\tilde{H}_T = H_T + kL, \quad (2.102d)$$

$$\delta\tilde{\rho} = \delta\rho - \bar{\rho}'T, \quad (2.102e)$$

$$\delta\tilde{P} = \delta P - \bar{P}'T, \quad (2.102f)$$

$$\tilde{v} = v + L'. \quad (2.102g)$$

The anisotropic stress Π is gauge-invariant.

Gauge Fixing and Commonly Used Gauges

Let us focus on scalar modes, where we have two degrees of freedom T and L to use. Let us assume we are working in a coordinate system x^μ with arbitrary scalar perturbations A , B , H_L , H_T . We can try to use T and L to change to a coordinate system $\tilde{x}^\mu$ where the new perturbations $\tilde{A}$, $\tilde{B}$, $\tilde{H}_L$ and $\tilde{H}_T$ are easier.

The **Newtonian gauge** imposes $\tilde{B} = \tilde{H}_T = 0$. Using Equations 2.102, we can

fix the gauge degrees of freedom,

$$H_T + kL = 0 \implies L = -\frac{H_T}{k}, \quad (2.103a)$$

$$B + L' + kT = 0 \implies kT = -B - L' = -B + \frac{H_T'}{k}, \quad (2.103b)$$

The remaining perturbations receive a new notation: $\tilde{A} = \Psi$, $\tilde{H}_L = \Phi$ ⁶. One advantage of this gauge is that the perturbed Einstein equations 2.96b and 2.96c resemble the Poisson equation for Newtonian gravity,

$$k^2\Phi = 4\pi Ga^2 \left[\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P})\frac{v}{k} \right], \quad (2.104a)$$

$$k^2(\Phi + \Psi) = 8\pi Ga^2 \bar{P}\Pi. \quad (2.104b)$$

Without anisotropic stress, one of the scalar perturbations is determined as $\Psi = -\Phi$. With anisotropic stress, the second equation becomes a simple algebraic relation between Ψ , Φ and Π .

In the **comoving gauge**, we impose $\tilde{v} - \tilde{B} = 0$ and $\tilde{H}_T = 0$. This is called the comoving gauge since the momentum density vanishes. Using Equations 2.102, we fix the gauge degrees of freedom as

$$H_T + kL = 0 \implies L = -\frac{H_T}{k} \quad (2.105a)$$

$$B + kT - v = 0 \implies T = \frac{v - B}{k} \quad (2.105b)$$

We denote the remaining metric perturbations as $\tilde{A} = \xi$, $\tilde{H}_L = \mathcal{R}$ and the density contrast in the comoving gauge is denoted by $\Delta = \delta\rho/\bar{\rho}$. If v is the total velocity, then this is the total comoving gauge. However, if v is the velocity of a given component, then this gauge is comoving to that specific component.

The comoving curvature perturbation $\mathcal{R}$ is a very important variable in cosmology because it's conserved for modes above the horizon and no stress. This can be seen by computing the Euler equation 2.95b and Einstein Equation 2.96d in the comoving gauge,

$$\delta P - \frac{2}{3}\bar{P}\Pi + (\bar{\rho} + \bar{P})\xi = 0, \quad (2.106a)$$

$$\mathcal{H}\xi - \mathcal{R}' = 0. \quad (2.106b)$$

⁶Different authors may swap Ψ and Φ

Inserting ξ into the Einstein equation, we get

$$\mathcal{R}' = \frac{\mathcal{H}}{\bar{\rho} + \bar{P}} \left[-\delta P + \frac{2}{3} \bar{P} \Pi \right]. \quad (2.107)$$

If stress fluctuations are negligible, then $\mathcal{R}' \approx 0$: the comoving scalar perturbation is conserved. Total stress should be negligible above the horizon (small k) because of causality: there is no time to perturbations to reach there. This makes $\mathcal{R}$ a very useful variable to work with, independently of gauge.

In the **synchronous gauge**, we impose no perturbations in the time part of the metric: $\tilde{A} = \tilde{B} = 0$. In order to find T, L , we have to solve the system of equations:

$$A - T' - \mathcal{H}T = 0 \implies aT' + a'T = aA \implies T = \frac{1}{a} \int d\tau aA + \frac{c_1}{a} \quad (2.108a)$$

$$B + L' + kT = 0 \implies L = - \int d\tau (B + kT) + c_2 \quad (2.108b)$$

And the remaining scalar perturbations are redefined to $\eta_T = -H_L - \frac{1}{3}H_T$ and $h_L = 6H_L$. One important thing to notice is that the gauge is not completely fixed, since there still are undetermined parameters c_1, c_2 . This is called residual gauge freedom. These constants are determined by initial conditions on the perturbations, as we will see later. Usually, these constants are used to set the CDM velocity to zero, simplifying the system of equations. However, this assumes CDM follows the Euler equation 2.95: changing the CDM velocity can break this assumption. If, however, the assumption holds, this choice makes the synchronous gauge comoving with CDM. The upside of this gauge is that the equations are numerically stable: the synchronous gauge is adopted in the numerical Einstein-Boltzmann solvers CAMB and CLASS.

The **spatially flat gauge** impose no perturbations on space: $\tilde{H}_L = \tilde{H}_T = 0$. We can easily check that:

$$L = -\frac{H_T}{k} \quad (2.109a)$$

$$\mathcal{H}T = H_L + \frac{1}{3}H_T \quad (2.109b)$$

In this gauge, the space has no scalar perturbations. This gauge is very useful to study inflaton fluctuations.

Examples of Gauge Transformations

Every gauge has pros and cons. Sometimes, you would like to work with a variable from a certain gauge in another gauge. For instance, comoving gauge variables can obey simple conservation laws, but the Newtonian gauge perturbations have a more clear physical interpretation, but the Einstein-Boltzmann numerical solver works in the synchronous gauge. Using Equations 2.102, one can perform transformations between any two gauges.

Let me illustrate gauge transformations by performing the change from the Newtonian gauge to the comoving gauge. Equations 2.102 imply that $L = 0$, $T = v_N/k$, where I use the subscripts C and N to denote comoving and Newtonian gauges respectively. In principle, $v_C \neq v_N$, but since $L = 0$, Equations 2.102 imply that the velocities are indeed the same, and we drop the subscript from now on. From the gauge transformation of H_L , we obtain

$$\mathcal{R} = \Phi - \mathcal{H} \frac{v}{k} \quad (2.110)$$

So we can compute $\mathcal{R}$, the comoving curvature perturbation, in terms of Newtonian gauge variables. We also have the other relations between Newtonian and comoving gauge variables,

$$\xi = \Psi - \frac{v'}{k} - \frac{\mathcal{H}v}{k} \quad (2.111a)$$

$$\delta\rho_C = \delta\rho_N - \bar{\rho}' \frac{v}{k} = \delta\rho_N + 3\mathcal{H}(\bar{\rho} + \bar{P}) \frac{v}{k} \quad (2.111b)$$

So we can rewrite the Einstein equations using mixed variables. The Poisson equation turns into

$$k^2\Phi = 4\pi G a^2 \delta\rho_C, \quad (2.112)$$

and Equation 2.96d in the Newtonian gauge can be used to write v in terms of the Newtonian potentials,

$$\frac{v}{k} = \frac{\mathcal{H}\Psi - \Phi'}{4\pi G a^2 (\bar{\rho} + \bar{P})}. \quad (2.113)$$

For single component universes, $\bar{P} = w\bar{\rho}$ and $\mathcal{H}^2 = 8\pi G a^2 \bar{\rho}/3$. Therefore:

$$\mathcal{H} \frac{v}{k} = \frac{\frac{8\pi G a^2 \bar{\rho}}{3} \Psi - \mathcal{H}\Phi'}{4\pi G a^2 \bar{\rho}(1+w)}. \quad (2.114)$$

Outside the horizon, total stress is negligible and the gravitational modes are

frozen: $\Phi' = 0$ and $\Psi \approx -\Phi$. Thus, we get:

$$\mathcal{H} \frac{v}{k} = -\frac{2}{3(1+w)} \Phi. \quad (2.115)$$

Inserting this relation into Equation 2.110, we obtain

$$\mathcal{R} = \Phi + \frac{2}{3(1+w)} \Phi = \frac{5+3w}{3+3w} \Phi. \quad (2.116)$$

Since $\mathcal{R}$ is conserved for superhorizon modes, we can calculate the ratios between the gravitational potential amplitudes in different epochs without calculating the transition between them. Between the matter-dominated and radiation-dominated epochs, we have

$$\mathcal{R} = \frac{5}{3} \Phi_{MD} = \frac{6}{4} \Phi_{RD} \implies \Phi_{MD} = \frac{9}{10} \Phi_{RD} \quad (2.117)$$

During the transition from radiation-dominated to matter-dominated epoch, the superhorizon gravitational potential modes are suppressed by a factor of 9/10.

Gauge-Invariant Quantities

Another way of analyzing gauge perturbations is by constructing gauge-invariant quantities. For instance, $\mathcal{R}$ and Δ can be used to construct gauge-invariant quantities

$$\mathcal{R} = H_L + \frac{1}{3} H_T - \mathcal{H} \frac{v-B}{k} \quad (2.118a)$$

$$\bar{\rho} \Delta = \delta\rho + 3(\bar{\rho} + \bar{P}) \mathcal{H} \frac{v-B}{k}, \quad (2.118b)$$

which reduce to their definitions in the comoving gauge. The advantage of using these variables is that it's easy to specialize them to any desired gauge.

2.3.6 Fluid Microphysics

The Stress Degrees of Freedom

In the background analysis, assuming homogeneity and isotropy, we had 3 degrees of freedom to solve for: $\bar{\rho}$, $\bar{P}$ and a . Einstein's equations gave only 2 independent equations to work with. The third equation was obtained when we

introduced the equation of state for our fluids, $\bar{P} = w\bar{\rho}$, determining the stress of the fluid and closing the system of equations. Different values for w change the behavior of $\bar{\rho}$ and a .

The same thing occurs in perturbation theory. Perturbations in metric and matter introduce 10+10 new degrees of freedom in our theory. We have 10 Einstein equations, and gauge fixing removes 4 degrees of freedom. Therefore, we still have 6 degrees of freedom to determine. These 6 degrees of freedom can be chosen to be the stress components of $\delta T_{\mu\nu}$: the isotropic stress δP , corresponding to the pressure perturbation; and the anisotropic stress $\bar{P}\Pi_{ij}$, which has 5 components $\bar{P}\Pi$, $\bar{P}\Pi^{(\pm 1)}$ and $\bar{P}\Pi^{(\pm 2)}$.

We can do the same counting but only looking to the scalar perturbations, and the results will be the same. We have 4 scalar degrees of freedom in the metric, A , B , H_L and H_T , and 4 degrees of freedom in the energy-momentum tensor, $\delta\rho$, v , δP and Π . However, we only have 4 Einstein equations 2.96 and 2 gauge variables L and T to fix, so only 2 scalar degrees of freedom remain. These can be chosen as the scalar stresses δP and $\bar{P}\Pi$. To close the system, we must relate these stresses to the density fluctuations $\delta\rho$. Determining these relations characterizes the fluid completely, and has a major influence on the evolution of perturbations.

The total stress will be defined in the comoving gauge by Equation 2.107 as

$$S = -\xi = \frac{\delta P}{\bar{\rho} + \bar{P}} - \frac{2}{3} \frac{\bar{P}\Pi}{\bar{\rho} + \bar{P}} \quad (2.119)$$

The total stress has components that behave differently. One is the anisotropic scalar stress,

$$S_{\Pi} = -\frac{8\pi G a^2 \bar{P}\Pi}{k^2} \quad (2.120)$$

which is gauge-invariant and can also enter the Einstein equations outside of the total stress S . Anisotropic stress can be thought of as a frictional force in response to metric shear and to the non-uniform motion of the fluid.

The δP term can be divided into two components: one is the adiabatic stress, defined by

$$S_a = \frac{\bar{P}'}{\bar{\rho}'(\bar{\rho} + \bar{P})} \delta\rho = \frac{\delta P_a}{\bar{\rho} + \bar{P}} \quad (2.121)$$

Adiabatic perturbations are predicted by inflation: they happen because the different points of the universe left inflation at different times, so the universal clock

has a perturbation $\delta\tau$ which is position-dependent. This is shown by

$$\delta P_a = \bar{P}(\tau + \delta\tau) - \bar{P} = \bar{P}'\delta\tau, \quad (2.122)$$

and conversely for the energy density,

$$\delta\rho = \bar{\rho}'\delta\tau. \quad (2.123)$$

Therefore, since $\delta\tau$ is the same for every component of the universe, we have:

$$\delta\tau = \frac{\delta\rho}{\bar{\rho}'} = \frac{\delta P}{\bar{P}'} \implies \frac{\delta\rho_J}{\bar{\rho}'_J} = \text{const for every species } J, \quad (2.124)$$

or, using the continuity equation and the density contrast,

$$\frac{\delta_J}{1 + w_J} = \text{const for every species } J. \quad (2.125)$$

The adiabatic stress is gauge-dependent. We define the adiabatic sound speed as

$$c_a^2 = \frac{\delta P_a}{\delta\rho} = \frac{\bar{P}'}{\bar{\rho}'}. \quad (2.126)$$

For non-interacting fluids with constant equation of state, $c_a^2 = w$. Baryons, which interact with light through Thomson and Compton scattering, have a nonzero adiabatic sound speed before recombination, whereas dark matter has no adiabatic sound speed.

The last stress is the non-adiabatic stress, or entropic stress, defined as the remaining part from δP ,

$$S_\Gamma = \frac{1}{\bar{\rho} + \bar{P}} (\delta P - \delta P_a) = \frac{1}{\bar{\rho} + \bar{P}} \left(\delta P - \frac{\bar{P}'}{\bar{\rho}'} \delta\rho \right). \quad (2.127)$$

Entropic stress can happen even if the density fluctuations are negligible. The total stress can be written as:

$$S = S_a + S_\Gamma + \frac{2}{3} \frac{k^2}{8\pi G a^2 (\bar{\rho} + \bar{P})} S_\Pi. \quad (2.128)$$

Parametrizing Stress

The entropic and anisotropic stresses must be parametrized in terms of the other fluid quantities. When creating such parametrizations, one must be consistent with the gauge transformation equations, Equations 2.102.

One of the first remarks is that the entropic stress is gauge-invariant: this can easily be seen from equations 2.102. Therefore, it must be related to another gauge-invariant fluid quantity. One natural candidate is the comoving density perturbation,

$$\delta\rho_C = \delta\rho + 3\mathcal{H}(\rho + P)\frac{v - B}{k}. \quad (2.129)$$

This way, one common choice [29] is to relate the entropic stress and the comoving density perturbation, and then

$$\delta P_\Gamma = \delta P - c_a^2 \delta\rho = (c_s^2 - c_a^2) \left(\delta\rho + 3\mathcal{H}(\rho + P)\frac{v - B}{k} \right), \quad (2.130)$$

where c_s^2 is the **effective sound speed** of the fluid.

In everyday liquid fluids, anisotropic stress is commonly caused by viscosity, an effect that damps perturbations. While this effect is naturally related to the fluid's velocity v , we must also impose the fact that Π is gauge-invariant. One choice is to add another equation to evolve the anisotropic stress,

$$w(\Pi' + 3\mathcal{H}\Pi) = 4c_v^2(kv - H_T'), \quad (2.131)$$

where c_v^2 is the viscosity parameter. This form of the anisotropic stress equation mimicks non-perfect fluids whose hierarchy truncates in the quadrupole.

With these choices, we can obtain two important equations throughout this thesis: the synchronous gauge fluid equations. First, let us assume the synchronous gauge conditions, $A = B = 0$ and define the synchronous gauge metric variables $\eta = -H_L - H_T/3$, $h = 6H_L$. The continuity and Euler equations become

$$\delta\rho' = -3\mathcal{H}(\delta\rho + \delta P) - (\rho + P) \left(kv + \frac{h'}{2} \right) \quad (2.132)$$

$$4\mathcal{H}(\rho + P)\frac{v}{k} + (\rho' + P')\frac{v}{k} + (\rho + P)\frac{v'}{k} = \delta P. \quad (2.133)$$

It is common to evolve the density contrast $\delta = \delta\rho/\rho$ instead of the full density

perturbation $\delta\rho$. To transform $\delta\rho'$ into δ' , we use the chain rule

$$\delta\rho' = (\rho\delta)' = \rho'\delta + \delta'\rho = -3\mathcal{H}(1+w)\rho\delta + \delta'\rho. \quad (2.134)$$

We can insert this back into the continuity equation, yielding

$$\rho\delta' = -3\mathcal{H}\delta P - (\rho + P) \left(kv + \frac{h'}{2} \right). \quad (2.135)$$

Dividing the equation by ρ , we obtain

$$\delta' = -3\mathcal{H}\frac{\delta P}{\rho} - (1+w) \left(kv + \frac{h'}{2} \right). \quad (2.136)$$

We may now insert our ansatz for the pressure perturbation, Equation 2.130, obtaining

$$\delta' = -3\mathcal{H}c_a^2\delta - 3\mathcal{H}(c_s^2 - c_a^2) \left(\delta + 3\mathcal{H}(1+w)\frac{v}{k} \right) - (1+w) \left(kv + \frac{h'}{2} \right); \quad (2.137)$$

$$\delta' = -3\mathcal{H}c_s^2\delta - 9\mathcal{H}^2(c_s^2 - c_a^2)(1+w)\frac{v}{k} - (1+w) \left(kv + \frac{h'}{2} \right). \quad (2.138)$$

Now, inserting the pressure perturbation into the Euler equation, we obtain

$$4\mathcal{H}(\rho + P)\frac{v}{k} + (\rho' + P')\frac{v}{k} + (\rho + P)\frac{v'}{k} = c_a^2\delta\rho + (c_s^2 - c_a^2)\delta\rho + (c_s^2 - c_a^2)3\mathcal{H}(\rho + P)\frac{v}{k} \quad (2.139)$$

Inserting $\rho' = -3\mathcal{H}(\rho + P)$ and multiplying the whole equation by k , we get

$$\mathcal{H}(\rho + P)v + P'v + (\rho + P)v' = kc_s^2\delta\rho + (c_s^2 - c_a^2)3\mathcal{H}(\rho + P)v. \quad (2.140)$$

Dividing by ρ , we get

$$\mathcal{H}(1+w)v + \frac{P'}{\rho'}\frac{\rho'}{\rho}v + (1+w)v' = kc_s^2\delta + 3\mathcal{H}(c_s^2 - c_a^2)(1+w)v. \quad (2.141)$$

$$\mathcal{H}(1+w)v - 3\mathcal{H}(1+w)c_a^2v + (1+w)v' = kc_s^2\delta + 3\mathcal{H}(c_s^2 - c_a^2)(1+w)v. \quad (2.142)$$

$$\mathcal{H}v - 3\mathcal{H}c_a^2v + v' = \frac{kc_s^2\delta}{1+w} + 3\mathcal{H}(c_s^2 - c_a^2)v. \quad (2.143)$$

After rearranging terms, we obtain

$$v' = -\mathcal{H}(1 - 3c_s^2)v + \frac{kc_s^2\delta}{1+w}. \quad (2.144)$$

Equations 2.138 and 2.144 are used in Einstein-Boltzmann solvers such as CAMB and CLASS to evolve the perturbation of dark energy fluids with dynamical equation of state.

In the density perturbation equation 2.138, the terms with the effective sound speed c_s^2 tend to suppress the perturbations. Dark energy fluids with $c_s^2 = 1$, such as quintessence (see Chapter 4), tend to have negligible perturbations inside the horizon. For this reason, they are called **smooth dark energy** models. Such models are analyzed in Chapter 6 and 7.

2.3.7 Initial Conditions

The perturbed Einstein and continuity equations, Equations 2.96 and 2.95, provide a number of differential equations to evolve in conformal time τ until today. In order to find the evolution of the perturbed metric and matter variables, we must provide a initial conditions for those variables. After inflation, the Universe was in a radiation-dominated era, and due to the accelerated expansion, all of the relevant k modes are outside of the horizon. We will see that these conditions alongside the Einstein equations imply that the initial conditions are adiabatic, i.e. following Equation 2.125.

Post-inflation Background

In background level, we want to find $a(\tau)$ by solving the Friedmann equation,

$$\mathcal{H} = \frac{\dot{a}}{a} = H_0 a (\Omega_r a^{-4} + \Omega_m a^{-3} + \Omega_K a^{-2} + \Omega_\Lambda)^{1/2}. \quad (2.145)$$

We may expand the solution $a(\tau)$ for $\tau \ll 1$,

$$a(\tau) = a(\tau = 0) + \dot{a}(\tau = 0)\tau + \frac{\ddot{a}}{2}\tau^2 + \dots \quad (2.146)$$

The coefficients can be found from the Friedmann equation. For instance, the first derivative is

$$\dot{a} = H_0 \sqrt{\Omega_r + \Omega_m a + \Omega_K a^2 + \Omega_\Lambda a^4} \implies \dot{a}(\tau = 0) = H_0 \sqrt{\Omega_r}. \quad (2.147)$$

The second derivative is

$$\ddot{a} = H_0 \frac{1}{2\sqrt{\Omega_r + \Omega_m a + \Omega_K a^2 + \Omega_\Lambda a^4}} (\Omega_m \dot{a} + 2\Omega_K a \dot{a} + 4\Omega_\Lambda a^3 \dot{a}), \quad (2.148)$$

which yields

$$\ddot{a}(\tau = 0) = \frac{H_0^2 \Omega_m}{2}. \quad (2.149)$$

We could continue this process indefinitely, even with help from software such as Mathematica, but we have a second-order solution for $a(\tau)$ at early, radiation-dominated times, right after inflation

$$a(\tau) = H_0 \sqrt{\Omega_r} \tau + \frac{H_0^2 \Omega_m \tau^2}{4} + \mathcal{O}(\tau^3). \quad (2.150)$$

And we could use this to set up an initial condition for a with minimal error for an arbitrary τ .

Initial Perturbations in an Universe with CDM and Photons

At perturbative level, the initial condition is a vector in the space of perturbation variables. Our goal is to explore the vector space of initial conditions that we can impose in perturbations. The process is almost exactly the same, but it's more complicated here since we have to deal with a system with a lot of equations. Here, Mathematica will definitely help with the manipulations.

The first thing to notice is that the synchronous gauge definitions $A = B = 0$ do not fully specify the coordinate system, leaving two undefined constants. We can use those constants to leave gauge modes out of the initial conditions, as we'll see ahead, but the main choice is to follow CDM so that $v_c = 0$.

As with the background, we want to obtain polynomial expansions for the solutions of the perturbation equations. This expansion assumes two hypotheses: early times and superhorizon modes. First, we are in a post-inflationary scenario, so $\tau \ll 1$. Second, all the relevant Fourier modes are outside the horizon so that $k/\mathcal{H} \ll 1$. Since $\mathcal{H} \approx 1/\tau$, we define the variable $x = k\tau$, and we want to expand for $x \ll 1$.

For an early universe with only photons and CDM, we have a system with six equations: 2 Einstein equations and 2 conservation equations for each component.

In synchronous gauge, the conservation equations are

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = -(\bar{\rho} + \bar{P})(kv + \frac{1}{2}h'_L) \quad (2.151a)$$

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [(\bar{\rho} + \bar{P})v] = k\delta P \quad (2.151b)$$

For pressureless CDM, $P = \delta P = 0$ and these equations reduce to:

$$\delta\rho'_c + 3\mathcal{H}\delta\rho_c = -\rho_c(kv_c + \frac{h'_L}{2}), \quad (2.152a)$$

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [\rho_c v_c] = 0. \quad (2.152b)$$

It's useful to rewrite this in terms of the density contrast $\delta = \delta\rho/\rho$,

$$\delta'_c = -kv_c - \frac{h'_L}{2}, \quad (2.153a)$$

$$v'_c + \mathcal{H}v_c = 0. \quad (2.153b)$$

The photon equations are similar, but now $\delta P_\gamma = \delta\rho_\gamma/3$ ⁷,

$$\delta\rho'_\gamma + 4\mathcal{H}\delta\rho_\gamma = -\frac{4}{3}\rho_\gamma(kv_\gamma + \frac{1}{2}h'_L), \quad (2.154a)$$

$$\frac{4}{3} \left(\frac{d}{d\tau} + 4\mathcal{H}\right) [\rho_\gamma v_\gamma] = \frac{k\delta\rho_\gamma}{3}. \quad (2.154b)$$

Again, we use the density contrast and obtain

$$\delta'_\gamma = -\frac{4}{3}kv_\gamma - \frac{2}{3}h'_L, \quad (2.155a)$$

$$v'_\gamma = k\frac{\delta_\gamma}{4}. \quad (2.155b)$$

Finally, we write the Einstein equations in the synchronous gauge without aniso-

⁷Photons have anisotropic stress, however, at early times, they are interacting with baryons through Thomson scattering and the tight coupling suppresses the photon anisotropic stress.

tropic stress and for a spatially flat universe

$$-\left(\frac{d}{d\tau} + \mathcal{H}\right) \left(\frac{1}{6}h'_L\right) = 4\pi Ga^2 \left(\delta P + \frac{\delta\rho}{3}\right), \quad (2.156a)$$

$$4\pi Ga^2 \left[\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P}) \left(\frac{v}{k}\right)\right] = k^2 \left[-\eta_T + \frac{3\mathcal{H}}{k^2} \left(\eta'_T + \frac{1}{6}h'_L\right)\right], \quad (2.156b)$$

$$-k^2\eta_T + 3 \left(\frac{d}{d\tau} - 2\mathcal{H}\right) \left(\eta'_T + \frac{1}{6}h'_L\right) = 0, \quad (2.156c)$$

$$\eta'_T = 4\pi Ga^2(\bar{\rho} + \bar{P}) \left(\frac{v}{k}\right). \quad (2.156d)$$

It's useful to write this in terms of the density contrasts and make $4\pi Ga^2 = 3\mathcal{H}^2/2\rho_T$, where ρ_T is the total energy density from all components,

$$-\left(\frac{d}{d\tau} + \mathcal{H}\right) \left(\frac{1}{6}h'_L\right) = \frac{\mathcal{H}^2}{2} \left(\frac{\rho_c}{\rho_T}\delta_c + 2\frac{\rho_\gamma}{\rho_T}\delta_\gamma\right), \quad (2.157a)$$

$$\frac{3\mathcal{H}^2}{2} \left(\frac{\rho_c}{\rho_T}\delta_c + \frac{\rho_\gamma}{\rho_T}\delta_\gamma + \frac{\rho_c}{\rho_T}\frac{v_c}{k} + \frac{4}{3}\frac{\rho_\gamma}{\rho_T}\frac{v_\gamma}{k}\right) = k^2 \left(-\eta_T + \frac{3\mathcal{H}}{k^2} \left(\eta'_T + \frac{1}{6}h'_L\right)\right), \quad (2.157b)$$

$$-k^2\eta_T + 3 \left(\frac{d}{d\tau} - 2\mathcal{H}\right) \left(\eta'_T + \frac{1}{6}h'_L\right) = 0, \quad (2.157c)$$

$$\eta'_T = \frac{3\mathcal{H}^2}{2k} \left(\frac{\rho_c}{\rho_T}v_c + \frac{4}{3}\frac{\rho_\gamma}{\rho_T}v_\gamma\right). \quad (2.157d)$$

These equations are not independent: only two of them are. Thus, I will choose Equations 2.157a and 2.157d to compose my system since they are equations that evolve η_T and h_L . If these two equations happen to be redundant, one can always go back and pick one of the two other equations.

Notice that h_L only appears in the equations through h'_L . Thus, we define $\Theta = h'_L/k$ ⁸. We also define the variable $x = k\tau$ and $\tilde{\mathcal{H}} = \mathcal{H}/k$, the ratio between the horizon wavenumber and the mode wavenumber. This way, we have the

⁸CAMB defines $\mathcal{Z} = h'_L/2k$.

equations

$$\dot{\delta}_c = -v_c - \frac{\Theta}{2}, \quad (2.158a)$$

$$\dot{v}_c + \tilde{\mathcal{H}}v_c = 0, \quad (2.158b)$$

$$\dot{\delta}_\gamma = -\frac{4}{3}v_\gamma - \frac{2}{3}\Theta, \quad (2.158c)$$

$$\dot{v}_\gamma = \frac{\delta_\gamma}{4}, \quad (2.158d)$$

$$\dot{\Theta} + \tilde{\mathcal{H}}\Theta = -3\tilde{\mathcal{H}}^2 \left(\frac{\rho_c}{\rho_T}\delta_c + 2\frac{\rho_\gamma}{\rho_T}\delta_\gamma \right), \quad (2.158e)$$

$$\dot{\eta}_T = \frac{3\tilde{\mathcal{H}}^2}{2} \left(\frac{\rho_c}{\rho_T}v_c + \frac{4}{3}\frac{\rho_\gamma}{\rho_T}v_\gamma \right), \quad (2.158f)$$

where overdots denote derivatives with respect to x . We got a closed linear system of 6 ordinary differential equations for six variables. Thus far, these are the full perturbation equations without any approximations.

Now, we have to expand our background functions in τ . From the scale factor expansion,

$$a(\tau) = H_0\sqrt{\Omega_r}\tau + \frac{H_0^2\Omega_c\tau^2}{4}, \quad (2.159)$$

We obtain an expansion for the conformal Hubble factor,

$$\mathcal{H} = \frac{a'}{a} = \frac{H_0\sqrt{\Omega_r} + \frac{H_0^2\Omega_c\tau}{2}}{H_0\sqrt{\Omega_r}\tau + \frac{H_0^2\Omega_c\tau^2}{4}} = \frac{1}{\tau} \left(\frac{1 + \frac{H_0\Omega_c\tau}{2\sqrt{\Omega_r}}}{1 + \frac{H_0\Omega_c\tau}{4\sqrt{\Omega_r}}} \right). \quad (2.160)$$

Defining $\omega = \frac{H_0\Omega_c}{2\sqrt{\Omega_r}}$, we find

$$\mathcal{H} = \frac{1}{\tau}(1 + \omega\tau) \left(1 - \frac{\omega\tau}{2} + \frac{\omega^2\tau^2}{4} - \dots \right) \approx \frac{1}{\tau} \left(1 + \frac{\omega\tau}{2} \right) \quad (2.161)$$

The quantity ρ_c/ρ_T can be expanded as

$$\frac{\rho_c}{\rho_T} = \frac{\rho_c}{\rho_c + \rho_\gamma} = \frac{\Omega_c a^{-3}}{\Omega_c a^{-3} + \Omega_\gamma a^{-4}} = \frac{\Omega_c a}{\Omega_c a + \Omega_\gamma} = \frac{(a/a_{eq})}{1 + (a/a_{eq})} \quad (2.162)$$

where $a_{eq} = \Omega_\gamma/\Omega_c$ is the scale factor of CDM-radiation equality. Thus,

$$\frac{\rho_c}{\rho_T} \approx (a/a_{eq})(1 - (a/a_{eq})) \approx \frac{H_0\Omega_c}{\sqrt{\Omega_r}}\tau = 2\omega\tau \quad (2.163)$$

and

$$\frac{\rho_\gamma}{\rho_T} = 1 - \frac{\rho_c}{\rho_T} \approx 1 - 2\omega\tau. \quad (2.164)$$

If higher-order terms are needed, we may reevaluate these expansions. One concern for us is that $\omega \propto 1/\sqrt{\Omega_\gamma} \approx 10^2$, and for our first order approximation to be valid, we need $\omega\tau \ll 1$. We are in the regime where $a \ll a_{eq}$. This means that:

$$H_0\sqrt{\Omega_\gamma}\tau \ll \frac{\Omega_\gamma}{\Omega_m} \implies \omega\tau \ll \frac{1}{2} < 1 \quad (2.165)$$

which coincides with the validity condition of the expansion. As long as we are deep into the radiation era and far away from the matter dominated era, $\omega\tau \ll 1$.

Defining $\tilde{\omega} = \omega/k$ and employing the first order approximation in τ for the background functions, the equations now are

$$\frac{d\delta_c}{dx} = -v_c - \frac{\Theta}{2}, \quad (2.166a)$$

$$\frac{dv_c}{dx} + \frac{1}{x} \left(1 + \frac{\tilde{\omega}x}{2}\right) v_c = 0, \quad (2.166b)$$

$$\frac{d\delta_\gamma}{dx} = -\frac{4}{3}v_\gamma - \frac{2}{3}\Theta, \quad (2.166c)$$

$$\frac{dv_\gamma}{dx} = \frac{\delta_\gamma}{4}, \quad (2.166d)$$

$$\frac{d\Theta}{dx} + \frac{1}{x} \left(1 + \frac{\tilde{\omega}x}{2}\right) \Theta = -\frac{3}{x^2} (1 + \tilde{\omega}x) (2\tilde{\omega}x\delta_c + 2(1 - 2\tilde{\omega}x)\delta_\gamma), \quad (2.166e)$$

$$\frac{d\eta_T}{dx} = \frac{3}{2x^2} (1 + \tilde{\omega}x) (2\tilde{\omega}xv_c + \frac{4}{3}(1 - 2\tilde{\omega}x)v_\gamma). \quad (2.166f)$$

The factors of $1/x$ suggests that we should use $\ln x$ as preferred unit of time, so the divergences are eliminated. We are also going to redefine density contrast and velocities as

$$\tilde{\delta} = \delta/x, \quad (2.167a)$$

$$\tilde{v} = v/x^2. \quad (2.167b)$$

The extra $1/x$ factor in the velocity accounts for the fact that the velocity is a derivative of the density from the continuity equation. The derivatives in x can be

transformed as $\frac{d}{dx} = \frac{1}{x} \frac{d}{d \ln x}$. This way, the system of equations becomes

$$\frac{d\tilde{\delta}_c}{d \ln x} = -\tilde{\delta}_c - x^2 \tilde{v}_c - \frac{\Theta}{2}, \quad (2.168a)$$

$$\frac{d\tilde{v}_c}{d \ln x} = -\left(3 + \frac{\tilde{\omega}x}{2}\right) \tilde{v}_c, \quad (2.168b)$$

$$\frac{d\tilde{\delta}_\gamma}{d \ln x} = -\tilde{\delta}_\gamma - \frac{4x^2}{3} \tilde{v}_\gamma - \frac{2}{3} \Theta, \quad (2.168c)$$

$$\frac{d\tilde{v}_\gamma}{d \ln x} = -2\tilde{v}_\gamma + \frac{\tilde{\delta}_\gamma}{4}, \quad (2.168d)$$

$$\frac{d\Theta}{d \ln x} = -\left(1 + \frac{\tilde{\omega}x}{2}\right) \Theta - 3(1 + \tilde{\omega}x) (2\tilde{\omega}x\tilde{\delta}_c + 2(1 - 2\tilde{\omega}x)\tilde{\delta}_\gamma), \quad (2.168e)$$

$$\frac{d\eta_T}{d \ln x} = \frac{3x}{2}(1 + \tilde{\omega}x)(2\tilde{\omega}x\tilde{v}_c + \frac{4}{3}(1 - 2\tilde{\omega}x)\tilde{v}_\gamma). \quad (2.168f)$$

Let $\mathbf{u}(x) = (\tilde{\delta}_c, \tilde{\delta}_\gamma, \tilde{v}_c, \tilde{v}_\gamma, \Theta, \eta_T)$. We can write the system in matrix form,

$$\frac{d\mathbf{u}}{d \ln x} = A(x)\mathbf{u}, \quad (2.169)$$

where

$$A = \begin{pmatrix} -1 & 0 & -x^2 & 0 & -1/2 & 0 \\ 0 & -1 & 0 & -4x^2/3 & -2/3 & 0 \\ 0 & 0 & -3 - \tilde{\omega}x/2 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & -2 & 0 & 0 \\ -6\tilde{\omega}x(1 + \tilde{\omega}x) & -6(1 + \tilde{\omega}x)(1 - 2\tilde{\omega}x) & 0 & 0 & -1 - \tilde{\omega}x/2 & 0 \\ 0 & 0 & 3x^2(1 + \tilde{\omega}x)\tilde{\omega} & 2x(1 + \tilde{\omega}x)(1 - 2\tilde{\omega}x) & 0 & 0 \end{pmatrix} \quad (2.170)$$

A depends on x , but since it is analytical, we can write

$$A(x) = A_0 + A_1x + A_2x^2 + \dots \quad (2.171)$$

Where:

$$A_0 = \begin{pmatrix} -1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & -1 & 0 & 0 & -2/3 & 0 \\ 0 & 0 & -3 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & -2 & 0 & 0 \\ 0 & -6 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (2.172)$$

$$A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\tilde{\omega}/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -6\tilde{\omega} & 6\tilde{\omega} & 0 & 0 & -\tilde{\omega}/2 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \end{pmatrix} \quad (2.173)$$

And the second order matrix A_2 is incomplete, since we cut the τ expansion at first order in the background functions. If we want to go to the n th order in x , we need to go at least to n th order in τ .

Applying the superhorizon limit of $x \ll 1$, we can cut the expansion at the lowest relevant order that fully determines the system, which in principle would be the zeroth order. Thus, $A \approx A_0$ and the solution is given by

$$\mathbf{u}(x) = e^{A_0 \ln x} \mathbf{u}(0). \quad (2.174)$$

At zeroth order, the variable η_T leaves the system: its row and column at A_0 are null, so it does not interact with the other variables and remains undetermined. We will need to go to first order to determine its initial evolution. For the other variables, we need to find the eigenvalues and eigenvectors of the reduced A_0 (not considering the η_T row and column), which can easily be done with any linear algebra software⁹. The results for the (reduced) eigenvectors $\mathbf{u}$ and eigenvalues λ

⁹I used Mathematica and the calculations are in [this link](#)

are

$$\begin{cases} \mathbf{u}_{ad} = (-1/4, -1/3, 0, -1/36, 1) \text{ with } \lambda = 1, \\ \mathbf{u}_{-ad} = (1/4, 1/3, 0, -1/60, 1) \text{ with } \lambda = -3, \\ \mathbf{u}_{\text{iso cdm } v} = (0, 0, 1, 0, 0) \text{ with } \lambda = -3, \\ \mathbf{u}_{\text{iso } \gamma v} = (0, 0, 0, 1, 0) \text{ with } \lambda = -2, \\ \mathbf{u}_{\text{iso cdm}} = (1, 0, 0, 0, 0) \text{ with } \lambda = -1. \end{cases} \quad (2.175)$$

If the initial condition is one of the eigenvectors with eigenvalue λ , say $\mathbf{u}_\lambda$, then its early evolution can be approximated by

$$\mathbf{u}(x) = x^\lambda \mathbf{u}_\lambda. \quad (2.176)$$

Let's pay special attention to the first eigenvector, the only growing mode. The density contrasts of CDM and photons follow the relation

$$\frac{\delta_c}{1 + w_c} = \frac{\delta_\gamma}{1 + w_\gamma} \quad (2.177)$$

which is characteristic of adiabatic fluctuations. Also, in this mode, $v_c = 0$ and $\Theta = \dot{h}_L$ is nonzero, so we have an initial curvature perturbation which dictates the other perturbations.

The other initial eigenvectors have no initial curvature perturbation, so we call them isocurvature initial conditions. Adiabatic initial conditions are often assumed since single field inflation predicts adiabatic fluctuations, but isocurvature initial conditions can also be interesting.

Finally, we can go back to the original variables $\delta = x\tilde{\delta}$, $v = x^2\tilde{v}$ and use the approximate solution,

$$\mathbf{u}(x) = e^{\lambda \ln x} \mathbf{u}_{ad} + (0, 0, 0, 0, 0, \eta_0) = x^\lambda \mathbf{u}_{ad} + (0, 0, 0, 0, 0, \eta_0) = x \mathbf{u}_{ad} + (0, 0, 0, 0, 0, \eta_0) \quad (2.178)$$

which translates to

$$\delta_c = -\frac{(k\tau)^2}{4}, \quad (2.179a)$$

$$\delta_\gamma = -\frac{(k\tau)^2}{3}, \quad (2.179b)$$

$$v_c = 0, \quad (2.179c)$$

$$v_\gamma = \frac{(k\tau)^3}{36}, \quad (2.179d)$$

$$\Theta = k\tau. \quad (2.179e)$$

But what about η ? Our zeroth order approximation couldn't find an initial value to η , which is also needed. In order to find it, we need to go to the next order in $A(x) = A_0 + A_1x$. The trick to solve the system now is to expand the eigenvector in power series,

$$\mathbf{u}(x) = x^\lambda \mathbf{u}_\lambda + x^{\lambda+1} \mathbf{u}_1 + x^{\lambda+2} \mathbf{u}_2 + \dots \quad (2.180)$$

where $\mathbf{u}_n$ is the n -th order correction. We are looking for the first correction $\mathbf{u}_1$. Plugging the full solution into the differential equation and going up to first order in x , we find,

$$\frac{d\mathbf{u}}{d \ln x} = \lambda x^\lambda \mathbf{u}_\lambda + (\lambda + 1)x^{\lambda+1} \mathbf{u}_1 = (A_0 + A_1x)(x^\lambda \mathbf{u}_\lambda + x^{\lambda+1} \mathbf{u}_1). \quad (2.181)$$

Equating coefficients of equal powers of x , we find

$$A_0 \mathbf{u}_\lambda = \lambda \mathbf{u}_\lambda, \quad (2.182a)$$

$$A_1 \mathbf{u}_\lambda + A_0 \mathbf{u}_1 = (\lambda + 1) \mathbf{u}_1 \implies [(\lambda + 1)\mathbf{I} - A_0] \mathbf{u}_1 = A_1 \mathbf{u}_\lambda. \quad (2.182b)$$

We can find $\mathbf{u}_1$, by solving the linear system in Equation 2.182b with $\lambda = 1$,

$$(2\mathbf{I} - A_0) \mathbf{u}_1 = A_1 \mathbf{u}_{ad}. \quad (2.183)$$

This is a linear system and can in theory be solved easily in any linear algebra software. I once again used Mathematica. The solution for the first correction of the adiabatic mode is given by

$$\mathbf{u}_1 = \left(-\frac{9\tilde{\omega}}{20}, -\frac{3\tilde{\omega}}{5}, 0, -\frac{3\tilde{\omega}}{80}, \frac{27\tilde{\omega}}{10}, -\frac{1}{36} \right). \quad (2.184)$$

And now, in addition to more precise initial conditions for the matter components,

we have the solution for η_T ,

$$\delta_c = -\frac{(k\tau)^2}{4} - \frac{9\omega(k\tau)^3}{20k}, \quad (2.185a)$$

$$\delta_\gamma = -\frac{(k\tau)^2}{3} - \frac{3\omega(k\tau)^3}{5k} \quad (2.185b)$$

$$v_c = 0, \quad (2.185c)$$

$$v_\gamma = -\frac{(k\tau)^3}{36} - \frac{3\omega(k\tau)^4}{80k}, \quad (2.185d)$$

$$\Theta = k\tau + \frac{27\omega(k\tau)^2}{10} \implies h_L = \frac{(k\tau)^2}{2} + \frac{9\omega(k\tau)^3}{10}, \quad (2.185e)$$

$$\eta_T = \eta_0 - \frac{(k\tau)^2}{36}. \quad (2.185f)$$

In order to find η_0 , the zeroth order term that was missing from our calculations, we use Equation 2.157c to find that $\eta_0 = 1$.

After all of these lengthy calculations, we can ask ourselves: why are we doing this? The standard Λ CDM model assumes single-field inflation, which predicts purely adiabatic perturbations. If the initial conditions are not set precisely, we will be introducing non-adiabatic initial conditions by virtue of numerical error. This is concerning especially because among the other initial conditions, we have gauge modes, which are not physical.

Adding Baryons to the mix

Let's repeat the process, but now with an universe with baryons, CDM and photons. Deep into the radiation dominated epoch, before decoupling, baryons and photons interacted via Thomson scattering. At those times, the collision rate is very large: $\Gamma \approx n_e \sigma_T > H$, where n_e is the electron number density and σ_T is the Thomson scattering cross-section. Therefore, photons and baryons constantly exchange momentum in such a way that their bulk velocity becomes the same: $v_\gamma = v_b = v_{b\gamma}$. This is called the **tight coupling approximation**, valid as long as the interaction rate Γ is much greater than the Hubble factor H .

Since photons and baryons interact, their conservation equations are now coupled. Thomson scattering doesn't transfer energy, so the continuity equations are uncoupled, but it transfers momentum, so the Euler equations are coupled. The modified conservation equations can be written using the Boltzmann equation. When photons and baryons are tightly coupled, the momentum transfer rate (with

conformal time τ) is given by

$$C = an_e\sigma_T(v_b - v_\gamma) \quad (2.186)$$

on the photon Euler equation. If $v_b > v_\gamma$, then in average momentum is transferred from baryons to photons, and vice-versa.

Photons' and baryons' momenta are differently related to their velocity:

$$q_\gamma = (\rho_\gamma + P_\gamma)v_\gamma = \frac{4}{3}\rho_\gamma v_\gamma, \quad (2.187a)$$

$$q_b = (\rho_b + P_b)v_b = \rho_b v_b. \quad (2.187b)$$

If Thomson scattering causes photons to lose their bulk velocity by Δv_γ , then the momentum loss of photons is $\Delta q = 4\rho_\gamma\Delta v_\gamma/3$. This momentum Δq is transferred to baryons, which in turn increase their velocity by

$$\Delta v_b = \frac{\Delta q}{\rho_b} = \frac{4\rho_\gamma}{3\rho_b}\Delta v_\gamma. \quad (2.188)$$

This way, the Euler equation for baryons will have a term

$$C = -\frac{4\rho_\gamma}{3\rho_b}an_e\sigma_T(v_b - v_\gamma), \quad (2.189)$$

where the minus sign is due to momentum conservation. This way, the Euler equations for photons and baryons become

$$v'_b + \mathcal{H}v_b = -\frac{4\rho_\gamma}{3\rho_b}an_e\sigma_T(v_b - v_\gamma), \quad (2.190a)$$

$$v'_\gamma - \frac{k\delta_\gamma}{4} = an_e\sigma_T(v_b - v_\gamma). \quad (2.190b)$$

Right after inflation, Thomson scattering is so intense that their bulk velocities are the same. They can be treated as a single fluid: the baryon-photon plasma, whose momentum is conserved. We can find the total conservation equation by summing both of the Euler equations (with the appropriate factor of $4\rho_\gamma/3\rho_b$),

$$v'_b + \frac{4\rho_\gamma}{3\rho_b}v'_\gamma + \mathcal{H}v_b - \frac{k\rho_\gamma\delta_\gamma}{3\rho_b} = 0. \quad (2.191)$$

Now we can impose the tight coupling condition $v_b = v_\gamma = v_{b\gamma}$ to find

$$\left(1 + \frac{4\rho_\gamma}{3\rho_b}\right) v'_{b\gamma} = -\mathcal{H}v_{b\gamma} + \frac{k\rho_\gamma}{3\rho_b}\delta_\gamma. \quad (2.192)$$

Now there is another function of interest, ρ_γ/ρ_b , to expand in τ . Its expansion for $\tau \ll 1$ is also easy,

$$\frac{\rho_\gamma}{\rho_b} = \frac{\Omega_r a^{-4}}{\Omega_b a^{-3}} = \frac{\Omega_r}{\Omega_b a} = \frac{\Omega_r}{\Omega_b} \frac{1}{H_0 \sqrt{\Omega_r} \tau + \frac{H_0^2 \Omega_m \tau^2}{4}}. \quad (2.193)$$

Since I want to go only to first order in τ , we get

$$\frac{\rho_\gamma}{\rho_b} = \frac{1}{\omega_b \tau} \frac{1}{1 + \frac{\omega \tau}{2}} \approx \frac{1}{\omega_b \tau} \left(1 - \frac{\omega \tau}{2}\right), \quad (2.194)$$

where $\omega_b = \frac{H_0 \Omega_b}{\sqrt{\Omega_r}}$. Defining the baryon-matter fraction as $r_b = \rho_b/\rho_m = \Omega_b/\Omega_m$ and $r_c = 1 - r_b$, we find $\omega_b = 2r_b \omega$, where $\omega = \frac{H_0 \Omega_m}{2\sqrt{\Omega_r}}$. The Hubble factor expansion is the same as before, but now with $\Omega_m = \Omega_b + \Omega_c$,

$$\mathcal{H} \approx \frac{1}{\tau} \left(1 + \frac{\omega \tau}{2}\right). \quad (2.195)$$

The energy fractions to be inserted in the Einstein equations are

$$\frac{\rho_c}{\rho_T} = \frac{\rho_c}{\rho_m + \rho_\gamma} = \frac{\Omega_c a^{-3}}{\Omega_m a^{-3} + \Omega_r a^{-4}} = r_c \frac{a/a_{eq}}{1 + a/a_{eq}} = 2r_c \omega \tau. \quad (2.196)$$

In the same way, we get

$$\frac{\rho_b}{\rho_T} = 2r_b \omega \tau, \quad (2.197)$$

$$\frac{\rho_\gamma}{\rho_T} = 1 - 2\omega \tau. \quad (2.198)$$

Thus, with baryons, the full system of equations is

$$\frac{d\tilde{\delta}_c}{d\ln x} = -\tilde{\delta}_c - x^2\tilde{v}_c - \frac{\Theta}{2}, \quad (2.199a)$$

$$\frac{d\tilde{v}_c}{d\ln x} = -2\tilde{v}_c - \tilde{\mathcal{H}}x\tilde{v}_c, \quad (2.199b)$$

$$\frac{d\tilde{\delta}_b}{d\ln x} = -\tilde{\delta}_b - x^2\tilde{v}_{b\gamma} - \frac{\Theta}{2}, \quad (2.199c)$$

$$\frac{d\tilde{\delta}_\gamma}{d\ln x} = -\tilde{\delta}_\gamma - \frac{4x^2}{3}\tilde{v}_{b\gamma} - \frac{2}{3}\Theta, \quad (2.199d)$$

$$\frac{d\tilde{v}_{b\gamma}}{d\ln x} = -2\tilde{v}_{b\gamma} - \frac{\tilde{\mathcal{H}}x}{1 + \frac{4\rho_\gamma}{3\rho_b}}\tilde{v}_{b\gamma} + \frac{\rho_\gamma}{3\rho_b \left(1 + \frac{4\rho_\gamma}{3\rho_b}\right)}\tilde{\delta}_\gamma, \quad (2.199e)$$

$$\frac{d\Theta}{d\ln x} = -x\tilde{\mathcal{H}}\Theta - 3x^2\tilde{\mathcal{H}}^2 \left(\frac{\rho_c}{\rho_T}\tilde{\delta}_c + \frac{\rho_b}{\rho_T}\tilde{\delta}_b + 2\frac{\rho_\gamma}{\rho_T}\tilde{\delta}_\gamma \right), \quad (2.199f)$$

$$\frac{d\eta_T}{d\ln x} = \frac{3x^3\tilde{\mathcal{H}}^2}{2} \left(\frac{\rho_c}{\rho_T}\tilde{v}_c + \frac{\rho_b}{\rho_T}\tilde{v}_{b\gamma} + \frac{4}{3}\frac{\rho_\gamma}{\rho_T}\tilde{v}_{b\gamma} \right). \quad (2.199g)$$

Now we need to insert the background expansions to first order in τ . We have (already converting to x),

$$x\tilde{\mathcal{H}} = 1 + \frac{\tilde{\omega}x}{2}, \quad (2.200a)$$

$$(x\tilde{\mathcal{H}})^2 = 1 + \tilde{\omega}x, \quad (2.200b)$$

$$\frac{4\rho_\gamma}{3\rho_b} = \frac{4}{3\tilde{\omega}_bx} \left(1 - \frac{\tilde{\omega}x}{2} \right), \quad (2.200c)$$

$$\frac{\tilde{\mathcal{H}}x}{1 + \frac{4\rho_\gamma}{3\rho_b}} = \frac{1 + \frac{\tilde{\omega}x}{2}}{1 + \frac{4}{3\tilde{\omega}_bx} \left(1 - \frac{\tilde{\omega}x}{2} \right)} \approx \frac{3\tilde{\omega}_bx}{4}, \quad (2.200d)$$

$$\frac{\rho_\gamma/\rho_b}{1 + \frac{4\rho_\gamma}{3\rho_b}} \approx \frac{\frac{1}{\tilde{\omega}_bx} \left(1 - \frac{\tilde{\omega}x}{2} \right)}{1 + \frac{4}{3\tilde{\omega}_bx} \left(1 - \frac{\tilde{\omega}x}{2} \right)} \approx \frac{3}{4} \left(1 - \frac{3}{4}\tilde{\omega}_bx \right), \quad (2.200e)$$

$$\frac{\rho_c}{\rho_T} \approx 2r_c\tilde{\omega}x, \quad (2.200f)$$

$$\frac{\rho_b}{\rho_T} \approx 2r_b\tilde{\omega}x, \quad (2.200g)$$

$$\frac{\rho_\gamma}{\rho_T} \approx 1 - 2\tilde{\omega}x. \quad (2.200h)$$

So the system becomes

$$\frac{d\tilde{\delta}_c}{d \ln x} = -\tilde{\delta}_c - x^2 \tilde{v}_c - \frac{\Theta}{2}, \quad (2.201a)$$

$$\frac{d\tilde{v}_c}{d \ln x} = -2\tilde{v}_c - \left(1 + \frac{\tilde{\omega}x}{2}\right) \tilde{v}_c, \quad (2.201b)$$

$$\frac{d\tilde{\delta}_b}{d \ln x} = -\tilde{\delta}_b - x^2 \tilde{v}_{b\gamma} - \frac{\Theta}{2}, \quad (2.201c)$$

$$\frac{d\tilde{\delta}_\gamma}{d \ln x} = -\tilde{\delta}_\gamma - \frac{4x^2}{3} \tilde{v}_{b\gamma} - \frac{2}{3} \Theta, \quad (2.201d)$$

$$\frac{d\tilde{v}_{b\gamma}}{d \ln x} = -2\tilde{v}_{b\gamma} - \frac{3r_b \tilde{\omega}x}{2} \tilde{v}_{b\gamma} + \frac{1}{4} \left(1 - \frac{3r_b \tilde{\omega}x}{2}\right) \tilde{\delta}_\gamma, \quad (2.201e)$$

$$\frac{d\Theta}{d \ln x} = - \left(1 + \frac{\tilde{\omega}x}{2}\right) \Theta - 3(1 + \tilde{\omega}x) (2r_c \tilde{\omega}x \tilde{\delta}_c + 2r_b \tilde{\omega}x \tilde{\delta}_b + 2(1 - 2\tilde{\omega}x) \tilde{\delta}_\gamma), \quad (2.201f)$$

$$\frac{d\eta_T}{d \ln x} = \frac{3}{2}x(1 + \tilde{\omega}x) \left(2r_c \tilde{\omega}x \tilde{v}_c + 2r_b \tilde{\omega}x \tilde{v}_{b\gamma} + \frac{4}{3}(1 - 2\tilde{\omega}x) \tilde{v}_{b\gamma}\right). \quad (2.201g)$$

Now, defining the system vector as $\mathbf{u} = (\tilde{\delta}_c, \tilde{\delta}_b, \tilde{\delta}_\gamma, \tilde{v}_c, \tilde{v}_{b\gamma}, \Theta, \eta_T)$, we have

$$\frac{d\mathbf{u}}{d \ln x} = A(x)\mathbf{u}, \quad (2.202)$$

where

$$A = \begin{pmatrix} -1 & 0 & 0 & -x^2 & 0 & -1/2 & 0 \\ 0 & -1 & 0 & 0 & -x^2 & -1/2 & 0 \\ 0 & 0 & -1 & 0 & -4x^2/3 & -2/3 & 0 \\ 0 & 0 & 0 & -3 - \tilde{\omega}x/2 & 0 & 0 & 0 \\ 0 & 0 & (1 - \frac{3r_b\tilde{\omega}x}{2})/4 & 0 & -2 - 3r_b\tilde{\omega}x/2 & 0 & 0 \\ -6r_c\tilde{\omega}x(1 + \tilde{\omega}x) & -6r_b\tilde{\omega}x(1 + \tilde{\omega}x) & -6(1 + \tilde{\omega}x)(1 - 2\tilde{\omega}x) & 0 & 0 & -1 - \tilde{\omega}x/2 & 0 \\ 0 & 0 & 0 & 3r_c\tilde{\omega}x^2(1 + \tilde{\omega}x) & 3r_c\tilde{\omega}x^2(1 + \tilde{\omega}x) + 2x(1 + \tilde{\omega}x)(1 - 2\tilde{\omega}x) & 0 & 0 \end{pmatrix} \quad (2.203)$$

Again, we can expand A up to first order in x (superhorizon limit): $A = A_0 + A_1 x$, where

$$A_0 = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & -1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & -1 & 0 & 0 & -2/3 & 0 \\ 0 & 0 & 0 & -3 & 0 & 0 & 0 \\ 0 & 0 & 1/4 & 0 & -2 & 0 & 0 \\ 0 & 0 & -6 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (2.204)$$

$$A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tilde{\omega}/2 & 0 & 0 & 0 \\ 0 & 0 & -3r_b\tilde{\omega}/8 & 0 & -3r_b\tilde{\omega}/2 & 0 & 0 \\ -6r_c\tilde{\omega} & -6r_b\tilde{\omega} & 6\tilde{\omega} & 0 & 0 & -\tilde{\omega}/2 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \end{pmatrix} \quad (2.205)$$

And now it's simply a matter of diagonalizing A_0 and solve the linear system for the first correction. The eigenvectors of A are:

$$\left\{ \begin{array}{l} \mathbf{u}_{ad} = (-1/4, -1/4, -1/3, 0, -1/36, 1, \eta_0) \text{ with } \lambda = 1 \\ \mathbf{u}_{-ad} = (1/4, 1/4, 1/3, 0, -1/12, 1, \eta_0) \text{ with } \lambda = -3 \\ \mathbf{u}_{\text{iso cdm v}} = (0, 0, 0, 1, 0, 0, \eta_0) \text{ with } \lambda = -3 \\ \mathbf{u}_{\text{iso } \gamma \text{ v}} = (0, 0, 0, 0, 1, 0, \eta_0) \text{ with } \lambda = -2 \\ \mathbf{u}_{\text{iso cdm}} = (1, 0, 0, 0, 0, 0, \eta_0) \text{ with } \lambda = -1 \\ \mathbf{u}_{\text{iso bar}} = (0, 1, 0, 0, 0, 0, \eta_0) \text{ with } \lambda = -1 \end{array} \right. \quad (2.206)$$

Again, the only growing mode is the adiabatic mode. For the first correction of the adiabatic mode, we have

$$\mathbf{u}_1 = \tilde{\omega} \left(\frac{1}{10}, \frac{1}{10}, \frac{2}{15}, 0, \frac{1+5r_b}{120}, -\frac{3}{5}, 0 \right) + \left(0, 0, 0, 0, 0, 0, -\frac{1}{36} \right). \quad (2.207)$$

The initial conditions are:

$$\delta_c = -\frac{(k\tau)^2}{4} \quad (2.208a)$$

$$\delta_b = -\frac{(k\tau)^2}{4} \quad (2.208b)$$

$$\delta_\gamma = -\frac{(k\tau)^2}{3} \quad (2.208c)$$

$$v_c = 0 \quad (2.208d)$$

$$v_{b\gamma} = -\frac{(k\tau)^3}{36} \quad (2.208e)$$

$$\Theta = k\tau \implies h_L = \frac{(k\tau)^2}{2} \quad (2.208f)$$

$$\eta_T = 1 - \frac{(k\tau)^2}{36} \quad (2.208g)$$

I can calculate the first corrections to all different modes. For instance, for $\mathbf{u}_{\text{iso bar}} = (0, 1, 0, 0, 0, 0, 0)$, the first correction is:

$$\mathbf{u}_1 = r_b \tilde{\omega}(-1, -1, -4/3, 0, -1/6, 2, 0). \quad (2.209)$$

In this mode, η_T is still not determined in first order, so I would need to go to second order. The baryon isocurvature mode yields the following initial conditions (I put the η solution for completion):

$$\delta_c = -r_b \omega \tau \quad (2.210a)$$

$$\delta_b = 1 - r_b \omega \tau \quad (2.210b)$$

$$\delta_\gamma = -\frac{4r_b \omega \tau}{3} \quad (2.210c)$$

$$v_c = 0 \quad (2.210d)$$

$$v_{b\gamma} = -\frac{r_b \tilde{\omega} (k\tau)^2}{6} \quad (2.210e)$$

$$\Theta = 2r_b \tilde{\omega} \implies h_L = 2r_b \omega \tau \quad (2.210f)$$

$$\eta_T = -\frac{r_b \omega \tau}{3} \quad (2.210g)$$

For the CDM isocurvature mode, $\mathbf{u}_{\text{iso cdm}} = (1, 0, 0, 0, 0, 0, 0)$, the result is very much similar, except that r_b is changed with r_c :

$$\mathbf{u}_1 = r_c \tilde{\omega}(-1, -1, -4/3, 0, -1/6, 2, 0) \quad (2.211)$$

and the initial conditions are:

$$\delta_c = 1 - r_c \omega \tau \quad (2.212a)$$

$$\delta_b = r_c \omega \tau \quad (2.212b)$$

$$\delta_\gamma = -\frac{4r_c \omega \tau}{3} \quad (2.212c)$$

$$v_c = 0 \quad (2.212d)$$

$$v_{b\gamma} = -\frac{r_c \tilde{\omega}(k\tau)^2}{6} \quad (2.212e)$$

$$\Theta = 2r_c \tilde{\omega} \implies h_L = 2r_c \omega \tau \quad (2.212f)$$

$$\eta_T = -\frac{r_c \omega \tau}{3} \quad (2.212g)$$

2.3.8 Inflation and the Primordial Power Spectrum

During inflation, not only the horizon shrink, but the quantum fluctuations of the inflaton field have sourced the initial metric and matter perturbations. Since these quantum fluctuations are stochastic, we cannot predict the values of the fluctuations, only their correlations.

The inflaton is a scalar field (see Section 4.2.1 for more details) that undergoes a slow-roll phase, causing the Universe's expansion to accelerate. We can write the field as a sum of the homogeneous part and the small, position-dependent perturbations,

$$\phi = \bar{\phi}(t) + \frac{f(\mathbf{r}, t)}{a}. \quad (2.213)$$

The homogeneous part of the field follows the Klein-Gordon equation,

$$\bar{\phi}'' + 2\mathcal{H}\bar{\phi}' + a^2 V'(\phi) = 0, \quad (2.214)$$

where $V'(\phi)$ is the derivative of the potential with respect to ϕ . The calculation of the field perturbations is made easier by a suitable choice of gauge: the spatially flat gauge, which imposes $H_L = H_T = 0$. In this gauge, assuming the field is slowly rolling, the metric perturbations A and B are suppressed. Also, during slow roll, the potential term is negligible when compared to the Hubble friction term. Therefore, the field perturbations f follow the Mukhanov-Sasaki equation,

$$f'' + \left(k^2 - \frac{a''}{a}\right) f = 0, \quad (2.215)$$

which resembles the equation for an harmonic oscillator. Indeed, in the subhorizon

limit where $k \gg \mathcal{H}$, we have exactly the harmonic oscillator equation,

$$f'' + k^2 f = 0. \quad (2.216)$$

Viewing the inflaton as a quantum field, we may calculate its vacuum expectation value. We promote the field perturbation $f(\mathbf{r}, \tau)$ to an operator $\hat{f}(\mathbf{r}, \tau)$. The momentum conjugate to f is given by $\pi = f'$, which is also promoted to a quantum operator, $\hat{\pi}(\mathbf{r}, \tau)$. These two operators must obey the equal-time canonical commutation relation,

$$[\hat{f}(\mathbf{r}, \tau), \hat{\pi}(\mathbf{r}', \tau)] = i\hbar\delta^3(\mathbf{r} - \mathbf{r}'). \quad (2.217)$$

Expanding the operators in Fourier space, finding an equivalent commutation relation,

$$[\hat{f}(\mathbf{k}, \tau), \hat{\pi}(\mathbf{k}', \tau)] = i\hbar\delta^3(\mathbf{k} + \mathbf{k}'). \quad (2.218)$$

We may also expand the field operator in terms of the creation and annihilation operators, $\hat{a}_k$ and $\hat{a}_k^\dagger$, as

$$\hat{f}(\mathbf{k}, \tau) = f(\mathbf{k}, \tau)\hat{a}_k + f^*(\mathbf{k}, \tau)\hat{a}_k^\dagger, \quad (2.219)$$

where $f(\mathbf{k}, \tau)$ is a solution of the classical field equation 2.215 and $f^*(\mathbf{k}, \tau)$ is its complex conjugate. Inserting this operator expansion in the Fourier-space commutation relation, we obtain

$$(ff'^* - f'f^*)[\hat{a}, \hat{a}^\dagger] = i\hbar\delta^3(\mathbf{k} + \mathbf{k}'). \quad (2.220)$$

Using the Mukhanov-Sasaki equation, one can notice that the term $(ff'^* - f'f^*)$ is constant,

$$(ff'^* - f'f^*)' = ff^{*''} - f''f^* = f(-\omega_k^2 f^*) - (-\omega_k^2 f)f^* = 0, \quad (2.221)$$

where $\omega_k^2 = k^2 - a''/a$. Therefore, we can always normalize the classical solutions f such that

$$(ff'^* - f'f^*) = i\hbar, \quad (2.222)$$

implying that

$$[\hat{a}, \hat{a}^\dagger] = \delta^3(\mathbf{k} + \mathbf{k}'). \quad (2.223)$$

Thus, we can define a vacuum quantum state $|0\rangle$ such that

$$\hat{a}_k |0\rangle = 0, \quad (2.224)$$

and every quantum state of the field can be constructed using creation operators

in vacuum state,

$$(a_{k_1}^\dagger)^{n_1}(a_{k_2}^\dagger)^{n_2}\dots(a_{k_N}^\dagger)^{n_N}|0\rangle = |n_{1,k_1}n_{2,k_2}\dots n_{N,k_N}\rangle. \quad (2.225)$$

The vacuum of our inflation theory can be defined in the infinite past, $\tau \rightarrow -\infty$. At this point, all Fourier modes were deep inside the horizon, so all of them obey the simple harmonic oscillator equation,

$$f_k'' + k^2 f_k = 0. \quad (2.226)$$

This equation has two linearly independent solutions,

$$f_k \propto e^{\pm ik\tau}. \quad (2.227)$$

To properly define the vacuum, we must choose one of the functions, and we choose the positive frequency one,

$$\lim_{\tau \rightarrow -\infty} f_k \propto e^{-ik\tau}. \quad (2.228)$$

Finally, let us solve the Mukhanov-Sasaki equation. Using the de Sitter approximation, in which the inflaton is completely frozen, we have

$$\begin{aligned} H^2 &= \frac{8\pi G\rho}{3} = C^2, \\ \mathcal{H}^2 &= \frac{8\pi G\rho}{3} a^2 = C^2 a^2, \\ \mathcal{H} &= Ca, \\ a' &= Ca^2, \\ a &= -\frac{1}{C\tau}, \\ a' &= \frac{1}{C\tau^2}, \\ a'' &= -\frac{2}{C\tau^3}, \\ \frac{a''}{a} &= \frac{2}{\tau^2}. \end{aligned}$$

Therefore, the Mukhanov-Sasaki equation becomes

$$f_k'' + \left(k^2 - \frac{2}{\tau^2}\right) f_k = 0. \quad (2.229)$$

This equation has the solution

$$f_k = A_k e^{-ik\tau} \left(1 - \frac{i}{k\tau}\right) + B_k e^{ik\tau} \left(1 + \frac{i}{k\tau}\right). \quad (2.230)$$

By our choice of vacuum, we must impose that $B_k = 0$, and by the normalization condition, $A_k = 1/\sqrt{2k}$. Therefore, the modes used to expand the quantum operator are

$$f_k = \frac{1}{\sqrt{2k}} e^{-ik\tau} \left(1 - \frac{i}{k\tau}\right). \quad (2.231)$$

Having completely defined the quantum operators, we may now turn to the vacuum fluctuations. We are interested in calculating expectation values involving the operator $\hat{f}(\mathbf{r}, \tau)$. Since f is already a first order perturbation, we may assume statistical homogeneity, so it's sufficient to calculate the expectation values at any point in space, and we can choose the origin $\mathbf{r} = 0$. The expectation value of the fluctuations themselves is zero,

$$\langle 0 | \hat{f}(\tau) | 0 \rangle = 0. \quad (2.232)$$

However, the variance of the fluctuations is not zero,

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} \langle 0 | \hat{f}_k(\tau) \hat{f}_{k'}(\tau) | 0 \rangle, \quad (2.233)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} \langle 0 | (f_k \hat{a}_k + f_k^* \hat{a}_k^\dagger) (f_{k'} \hat{a}_{k'} + f_{k'}^* \hat{a}_{k'}^\dagger) | 0 \rangle, \quad (2.234)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} f_k f_{k'}^* \langle 0 | \hat{a}_k \hat{a}_{k'}^\dagger | 0 \rangle, \quad (2.235)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} f_k f_{k'}^* \langle 0 | \hat{a}_{k'}^\dagger \hat{a}_k + \delta^3(\mathbf{k} + \mathbf{k}') | 0 \rangle, \quad (2.236)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k'}{(2\pi)^{3/2}} f_k f_{k'}^* \delta^3(\mathbf{k} + \mathbf{k}'), \quad (2.237)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^3} f_k f_{-k}^*, \quad (2.238)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{d^3k}{(2\pi)^3} |f_k|^2, \quad (2.239)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int \frac{dk}{2\pi^2} k^2 |f_k|^2, \quad (2.240)$$

$$\langle 0 | \hat{f}(\tau)^2 | 0 \rangle = \int d \ln k \frac{k^3 |f_k|^2}{2\pi^2}. \quad (2.241)$$

$$(2.242)$$

Therefore, the variance of the inflaton fluctuations receives contributions from all Fourier modes. We define the dimensionless power spectrum as

$$\Delta_f^2 = \frac{d \langle \hat{f}^2 \rangle}{d \ln k} = \frac{k^3 |f_k|^2}{2\pi^2}. \quad (2.243)$$

Going back to $\delta\phi = f/a$, we have a power spectrum for the inflaton fluctuations,

$$\Delta_{\delta\phi}^2 = \frac{k^3 |\delta\phi_k|^2}{2\pi^2} = \frac{k^3}{2\pi^2} \frac{1}{a^2} \frac{1}{2k} \left| 1 - \frac{i}{k\tau} \right|^2 = \frac{k^2}{4\pi^2 a^2} \left(1 + \frac{1}{k^2 \tau^2} \right) = \frac{k^2}{4\pi^2 a^2} + \frac{1}{4\pi^2 a^2 \tau^2}. \quad (2.244)$$

From our de Sitter approximation, we know that $a\tau = -H^{-1}$. Considering superhorizon modes where $k \ll aH$, we may neglect the first term in the power spectrum. We can then compute the power spectrum for each Fourier mode at horizon crossing, $k = \mathcal{H} = aH$, and we get

$$\Delta_{\delta\phi}^2 = \frac{H^2}{4\pi^2}. \quad (2.245)$$

In the spatially flat gauge, the inflaton perturbation $\delta\phi$ is related to the comoving curvature perturbation $\mathcal{R}$ via

$$\mathcal{R} = -\frac{\mathcal{H}}{\phi'} \delta\phi. \quad (2.246)$$

Therefore, quantum fluctuations of the inflaton field produce comoving curvature perturbations. Their power spectra are related via

$$\Delta_{\mathcal{R}}^2 = \frac{\mathcal{H}^2}{\phi'^2} \Delta_{\delta\phi}^2. \quad (2.247)$$

Defining the inflation slow roll parameter ε as

$$\varepsilon = \frac{\phi'^2}{2\mathcal{H}^2 M_{\text{pl}}^2}, \quad (2.248)$$

we can then calculate the comoving curvature perturbation power spectrum,

$$\Delta_{\mathcal{R}}^2 = \frac{1}{8\pi^2 \varepsilon} \frac{H^2}{M_{\text{pl}}^2}. \quad (2.249)$$

Since the power spectrum is evaluated at the moment when the perturbation exits the horizon, this may depend implicitly on the scale k . We parametrize this

dependence as

$$\Delta_{\mathcal{R}}^2 = A_s \left(\frac{k}{k_p} \right)^{n_s-1}, \quad (2.250)$$

where A_s is the amplitude of the initial scalar power spectrum, k_p is a pivot scale chosen as $k_p = 0.05 \text{Mpc}^{-1}$ and n_s is the scalar spectral index.

Inflaton perturbations generate all perturbations in the metric and matter. In particular, the initial comoving curvature perturbations follow the primordial dimensionless power spectrum in Equation 2.250. Relating $\mathcal{R}$ to other variables, we can obtain the initial dimensionless power spectrum for all other perturbations. By solving the Einstein-Boltzmann equations, we can find the transfer functions for some perturbation variable X , defined as

$$T_X(k, a) = \frac{X(k, a)}{X(k, a_{\text{ini}})}. \quad (2.251)$$

We can use the transfer functions to relate current perturbations to initial perturbations and then use the initial power spectrum. For instance, the variance of curvature perturbations $\mathcal{R}$ today is given by

$$\Delta_{\mathcal{R}}^2(a=1) = \langle \mathcal{R}(k, a=1) \mathcal{R}(k, a=1) \rangle = T^2(k, a=1) \Delta_{\mathcal{R}}^2(a=a_{\text{ini}}). \quad (2.252)$$

Therefore, we cannot predict matter perturbations, we can predict matter perturbation variances, which are also measurable via correlation functions.

2.3.9 Matter Power Spectrum

One observable of interest is the matter distribution, which forms the so-called large-scale structure of the Universe. Matter inhomogeneities are the basin for the formation of galaxy clusters, which we can observe. We define the matter transfer function as

$$T_m(k, a) = \frac{\delta_m(k, a)}{\delta_m(k, a_{\text{ini}})}, \quad (2.253)$$

where

$$\delta_m = \frac{\delta\rho_c + \delta\rho_b}{\rho_c + \rho_b}. \quad (2.254)$$

Massive neutrinos are also taken into account, but for simplicity let us use only CDM and baryons. After solving the perturbation equations numerically, we obtain the transfer functions. We can then relate primordial and current (dimensionful) matter power spectra via

$$P_m(k, a) = \frac{2\pi^2}{k^3} \Delta_{\mathcal{R}}^2(k) T_m^2(k, a). \quad (2.255)$$

The 2-point correlation function of matter perturbations, $\xi(\mathbf{r})$, is defined as

$$\xi(\mathbf{r}) = \frac{1}{V} \int d^3\mathbf{r}' \delta_m(\mathbf{r}') \delta_m(\mathbf{r}' + \mathbf{r}). \quad (2.256)$$

Due to statistical isotropy, the correlation is only a function of the distance r . The matter power spectrum is the Fourier transform of the correlation function,

$$P_m(k) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k} \cdot \mathbf{r}} \xi(\mathbf{r}). \quad (2.257)$$

The matter power spectrum therefore encodes the 2-point statistics of the matter fluids. It is one of the main cosmological quantities, used to calculate weak lensing and galaxy clustering correlations.

Unfortunately, the matter power spectrum prediction from linear perturbation theory stops being valid in small scales. Due to the gravitational attraction and lack of pressure support, matter overdensities tend to grow. In small scales and late times, these overdensities grow past the validity limit of linear perturbation theory [30]. Accurate predictions of the matter power spectrum at small scales are one of the biggest challenges in current cosmology, requiring expensive N-body simulations which do not assume small matter fluctuations. This is the subject of my work "Modeling nonlinear scales with the comoving Lagrangian acceleration method: Preparing for LSST Y1" [25], which tackles this problem using the Comoving Lagrangian Acceleration algorithm.

2.3.10 Cosmic Shear

Cosmic shear is the weak gravitational lensing of galaxies' emitted photons in the large-scale structure of the Universe. In principle, galaxy shapes are randomly distributed across the sky¹⁰. When the photons travel until reaching our telescopes, they travel across the large-scale structure and "feel" the effects of matter and metric perturbations. The complex distribution of matter deflects the photon in its path. When light reaches us, the images of galaxies are slightly distorted. The cosmic shear effect cannot be seen by naked eye. However, since all galaxies' photons travel across the same large-scale structure, cosmic shear imposes correlations in the galaxy shapes.

To briefly study this effect, we may assume the Newtonian gauge,

$$ds^2 = -(1 - 2\Psi)dt^2 + a^2(t)(1 - 2\Phi)dl^2. \quad (2.258)$$

Furthermore, since cosmic shear is measured from galaxies at redshifts $z \leq 3$, we

¹⁰Actually, tidal gravitational fields can correlate galaxy shapes, an effect called intrinsic alignment.

can assume negligible anisotropic stress,

$$k^2(\Phi + \Psi) = 0 \implies \Phi = -\Psi, \quad (2.259)$$

and, at small scales (large k), the Poisson equation,

$$k^2\Phi = 4\pi G a^2 \rho \delta. \quad (2.260)$$

The photon geodesics are given by $ds = 0$, and thus

$$(1 - 2\Psi)dt^2 = (1 - 2\Phi)dr^2 \implies \frac{dt}{dr} = (1 + 2\Psi), \quad (2.261)$$

where $dr = adl$. Therefore, the time taken by a photon in its trajectory is given by

$$t = \int dt = \int (1 + 2\Psi)dr. \quad (2.262)$$

Now, it is important to define some geometry. Let us define the z -axis as the line of sight, i.e. the direction we are looking. We are interested in deviations in the photon trajectory in the xy -plane. In the xy -plane, we can define the 2-vector θ as the position of the photon at that specific z coordinate. We then define the position of the source of light (i.e. a galaxy) as

$$\mathbf{x}_s = (\chi\theta_s, \chi). \quad (2.263)$$

Due to the effect of lensing, the source has an apparent position

$$\mathbf{x}_a = (\chi\theta_a, \chi). \quad (2.264)$$

Our goal is to obtain the source position θ_s in terms of the apparent position θ_a . These two are related by the lens equation,

$$\theta_s = \theta_a - \Delta\theta(\theta_a), \quad (2.265)$$

where $\Delta\theta$ is the angular deflection, which is a function of the apparent position. The lens equation is a general framework that applies for various lensing problems.

The photons feel the gravitational deflection through transverse gradient of the gravitational potential. At zeroth order in perturbations, $dt = -ad\chi$ ¹¹, where χ is the comoving distance. The deflection in the directions perpendicular to the

¹¹From our perspective, as we trace the distance from us to the source, we are going back on time.

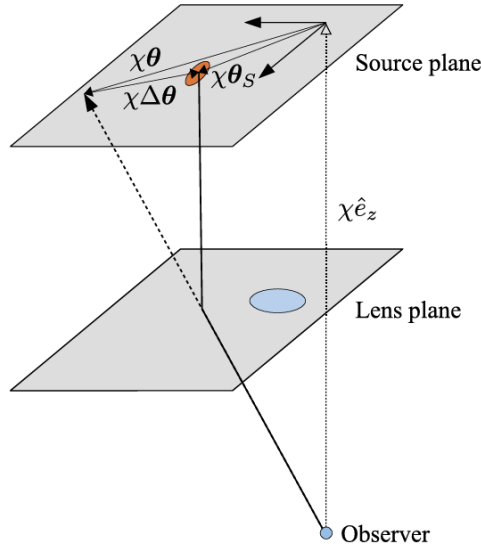


Figura 2.2: Schematic representation of the lensing problem.

line of sight, per comoving distance, is

$$\frac{dx^i}{d\chi} = -a \frac{dx^i}{dt} = -\hat{p}^i, \quad (2.266)$$

where $\hat{p}^i$ is the normalized photon momentum. Therefore,

$$\Delta x^i = - \int d\chi \hat{p}^i. \quad (2.267)$$

By calculating the geodesic equation for massless particles, we have

$$\frac{dp_i}{dt} = \frac{p}{a} \partial_i (\Phi - \Psi) = 2 \frac{p}{a} \partial_i \Phi. \quad (2.268)$$

Therefore, we obtain

$$\frac{d\hat{p}^i}{dt} = \frac{2}{a} \partial_i \Phi. \quad (2.269)$$

Transforming to comoving distance, we have

$$\frac{d\hat{p}^i}{d\chi} = -2\partial_i \Phi \implies \Delta \hat{p}^i = -2 \int_0^\chi d\chi' \partial_i \Phi(\chi' \theta^1, \chi' \theta^2, \chi', \tau_0 - \chi'). \quad (2.270)$$

Inserting the momentum variation in the deviation equation, we get

$$\Delta x^i = 2 \int_0^\chi d\chi' \int_0^{\chi'} d\chi'' \partial_i \Phi(\chi'' \theta^1, \chi'' \theta^2, \chi'', \tau_0 - \chi''). \quad (2.271)$$

Since $\theta = \mathbf{x}/\chi$, we obtain

$$\Delta \theta^i = \frac{2}{\chi} \int_0^\chi d\chi' \int_0^{\chi'} d\chi'' \partial_i \Phi(\chi'' \theta^1, \chi'' \theta^2, \chi'', \tau_0 - \chi''). \quad (2.272)$$

The double integral can be performed by changing the order of the integration as

$$\int_0^z dx \int_0^x dy = \int_0^z dy \int_y^z dx. \quad (2.273)$$

Therefore,

$$\Delta \theta^i = \frac{2}{\chi} \int_0^\chi d\chi'' \int_{\chi''}^\chi d\chi' \partial_i \Phi(\chi'' \theta^1, \chi'' \theta^2, \chi'', \tau_0 - \chi'') \quad (2.274)$$

$$\Delta \theta^i = 2 \int_0^\chi d\chi'' \frac{\chi - \chi''}{\chi} \partial_i \Phi(\chi'' \theta^1, \chi'' \theta^2, \chi'', \tau_0 - \chi''). \quad (2.275)$$

Therefore, we obtain the source angular position

$$\theta_s^i = \theta_a^i + 2 \int_0^\chi d\chi' \frac{\chi - \chi'}{\chi} \partial_i \Phi(\chi' \theta_a^1, \chi' \theta_a^2, \chi', \tau_0 - \chi'). \quad (2.276)$$

Noticing that $\partial/\partial x^i = (1/\chi)\partial/\partial \theta^i$, we can write the lensing deflection as a gradient of the **lensing potential** ψ ,

$$\Delta \theta^i = \frac{\partial}{\partial \theta^i} \left(2 \int_0^\chi \frac{d\chi'}{\chi'} \frac{\chi - \chi'}{\chi} \Phi(\chi' \theta_a^1, \chi' \theta_a^2, \chi', \tau_0 - \chi') \right) = \frac{\partial}{\partial \theta^i} \psi(\theta_a). \quad (2.277)$$

Since the deflections are small, we may linearize the lens equation,

$$\theta_s^i = A_{ij} \theta_a^j, \quad (2.278)$$

where

$$A_{ij} = \frac{\partial \theta_s^i}{\partial \theta^j} = \delta_{ij} + \frac{\partial^2}{\partial \theta^i \partial \theta^j} \psi = \delta_{ij} + \psi_{ij}. \quad (2.279)$$

The matrix A_{ij} is the distortion matrix, which maps apparent coordinates to source

coordinates. We define its components as

$$A_{ij} = \begin{pmatrix} 1 - \kappa - \gamma_1 & \gamma_2 \\ \gamma_2 & 1 - \kappa + \gamma_1 \end{pmatrix}. \quad (2.280)$$

The quantity κ is the convergence,

$$\kappa = -\frac{1}{2} \left(\frac{\partial^2}{\partial \theta_1^2} + \frac{\partial^2}{\partial \theta_2^2} \right) \psi, \quad (2.281)$$

and it accounts for isotropic enhancement or shrinkage of the image. The other two components are the shear,

$$\gamma_1 = -\frac{1}{2} \left(\frac{\partial^2}{\partial \theta_1^2} - \frac{\partial^2}{\partial \theta_2^2} \right) \psi, \quad (2.282)$$

$$\gamma_2 = \frac{\partial^2}{\partial \theta_1 \partial \theta_2} \psi, \quad (2.283)$$

and the object $\gamma = (\gamma_1, \gamma_2)$ transforms as a spin-2 quantity. The inverse determinant of A_{ij} is the magnification,

$$\mu = |A_{ij}|^{-1} = \frac{1}{(1 - \kappa)^2 - \gamma_1^2 - \gamma_2^2}. \quad (2.284)$$

Transforming Equation 2.279 in Fourier space, we obtain

$$\tilde{\psi}_{ij} = -l_i l_j \tilde{\psi}, \quad (2.285)$$

where tildes denote Fourier transforms and $\mathbf{l}$ is the 2-dimensional wavevector. It is common to separate the Fourier-space distortion matrix into two components, the so-called E and B modes. The E mode comes from the transverse part of the tensor $\tilde{\psi}_{ij}$, and is given by

$$E(\mathbf{l}) = \left(\frac{l_i l_j}{l^2} - \frac{1}{2} \delta_{ij} \right) (-\tilde{\psi}_{ij}) = \frac{1}{2} l^2 \tilde{\psi} = \tilde{\kappa}. \quad (2.286)$$

Therefore, the E-mode of the distortion is sourced by the convergence field, a function of the gravitational potential. The remaining part is the B-mode, given by

$$B_{ij}(\mathbf{l}) = \tilde{\psi}_{ij} - 2 \frac{l_i l_j}{l^2} E = 0. \quad (2.287)$$

Since the lensing matrix $\tilde{\psi}_{ij}$ is purely transverse, the B-mode vanishes. Therefore, the power spectrum of the E-modes in Fourier space is the power spectrum of the convergence field, given by

$$\langle \tilde{\kappa}(\mathbf{l}) \tilde{\kappa}^*(\mathbf{l}') \rangle = (2\pi)^2 \delta^2(\mathbf{l} - \mathbf{l}') C_{\kappa\kappa}(l). \quad (2.288)$$

The power spectrum of κ is related to that of the lensing potential,

$$\frac{1}{2} l^2 \tilde{\psi} = \tilde{\kappa} \implies C_{\kappa\kappa}(l) = \frac{1}{4} l^4 C_{\psi\psi}(l). \quad (2.289)$$

In order to advance further, let us go back to the expression of the lensing potential ψ . So far, we have only seen the lensing of a single galaxy. We actually observe an ensemble of source galaxies. Suppose that their density is $n_s(z)$, normalized such that $\int_0^\infty n_s(\chi) d\chi = 1$. The lensing potential for the observed galaxies is a sum over all galaxies,

$$\psi = 2 \int_0^\infty d\chi n_s(\chi) \int_0^\chi d\chi' \left(\frac{\chi - \chi'}{\chi'} \right) \Phi(\theta^1 \chi', \theta^2 \chi', \chi', \tau_0 - \chi'). \quad (2.290)$$

Once again, changing the order of integration, we obtain

$$\psi = 2 \int_0^\infty \frac{d\chi'}{\chi'} q_\kappa(\chi') \Phi(\theta^1 \chi', \theta^2 \chi', \chi', \tau_0 - \chi'), \quad (2.291)$$

where $q_\kappa(\chi)$ is the lensing efficiency, given by

$$q_\kappa(\chi) = \int_\chi^\infty d\chi' \frac{\chi' - \chi}{\chi'} n_s(\chi'). \quad (2.292)$$

Therefore, we can now relate the correlation of the lensing potential with the correlation function of Φ ,

$$P_{\psi\psi}(\boldsymbol{\theta}) = 4 \int_0^\infty \int_0^\infty \frac{d\chi'}{\chi'} \frac{d\chi''}{\chi''} q_\kappa(\chi') q_\kappa(\chi'') \times \langle \Phi(\theta^1 \chi', \theta^2 \chi', \chi', \tau_0 - \chi') \Phi(\theta^1 \chi'', \theta^2 \chi'', \chi'', \tau_0 - \chi'') \rangle. \quad (2.293)$$

Instead of doing this integral, we notice that the results depend on the direction $\boldsymbol{\theta}$.

Let's perform the Fourier transform of the kernels,

$$\int_0^\infty \frac{d\chi}{\chi} q_\kappa(\chi) \Phi(\theta^1 \chi, \theta^2 \chi, \chi, \tau_0 - \chi) = \int_0^\infty \frac{d\chi}{\chi} \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{n} \chi} q_\kappa(\chi) \Phi(\mathbf{k}, \tau_0 - \chi), \quad (2.294)$$

$$= 4\pi \sum_{l,m} i^l \int_0^\infty \frac{d\chi}{\chi} \frac{d^3 k}{(2\pi)^3} j_l(k\chi) Y_{lm}(\mathbf{n}) Y_{lm}^*(\hat{\mathbf{k}}) q_\kappa(\chi) \Phi(\mathbf{k}, \tau_0 - \chi) \quad (2.295)$$

where in the last line I used the identity

$$e^{i\mathbf{k} \cdot \mathbf{x}} = 4\pi \sum_{l=0}^\infty i^l \sum_{m=-l}^l j_l(kx) Y_{lm}(\hat{\mathbf{k}}) Y_{lm}^*(\hat{\mathbf{x}}). \quad (2.296)$$

Let's then define the multipoles of our shear field as the coefficients of $Y_{lm}(\mathbf{n})$,

$$a_{lm} = 4\pi i^l \int_0^\infty \frac{d\chi}{\chi} \frac{d^3 k}{(2\pi)^3} j_l(k\chi) Y_{lm}^*(\hat{\mathbf{k}}) q_\kappa(\chi) \Phi(\mathbf{k}, \tau_0 - \chi). \quad (2.297)$$

The correlations between these coefficients are the so-called angular power spec-

trum,

$$\langle a_{lm} a_{l'm'}^* \rangle = \delta_{ll'} \delta_{mm'} C_{\psi\psi}(l) = (4\pi)^2 i^{l-l'} \int_0^\infty \frac{d\chi}{\chi} \int_0^\infty \frac{d\chi'}{\chi'} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \times \\ j_l(k\chi) j_{l'}(k'\chi') Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}') q_\kappa(\chi) q_\kappa(\chi') \langle \Phi(\mathbf{k}, \tau_0 - \chi) \Phi(\mathbf{k}', \tau_0 - \chi') \rangle, \quad (2.298a)$$

$$\langle a_{lm} a_{l'm'}^* \rangle = (4\pi)^2 i^{l-l'} \int_0^\infty \frac{d\chi}{\chi} \int_0^\infty \frac{d\chi'}{\chi'} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \times \\ j_l(k\chi) j_{l'}(k'\chi') Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}') q_\kappa(\chi) q_\kappa(\chi') (2\pi)^3 \delta^D(\mathbf{k} - \mathbf{k}') P_\Phi(k, \chi, \chi'), \quad (2.298b)$$

$$\langle a_{lm} a_{l'm'}^* \rangle = (4\pi)^2 i^{l-l'} \int_0^\infty \frac{d\chi}{\chi} \int_0^\infty \frac{d\chi'}{\chi'} \int \frac{k^2 dk \Omega}{(2\pi)^3} \times \\ j_l(k\chi) j_{l'}(k\chi') Y_{lm}^*(\hat{\mathbf{k}}) Y_{l'm'}(\hat{\mathbf{k}}') q_\kappa(\chi) q_\kappa(\chi') P_\Phi(k, \chi, \chi'), \quad (2.298c)$$

$$\langle a_{lm} a_{l'm'}^* \rangle = (4\pi)^2 i^{l-l'} \int_0^\infty \frac{d\chi}{\chi} \int_0^\infty \frac{d\chi'}{\chi'} \int \frac{k^2 dk}{(2\pi)^3} \times \\ j_l(k\chi) j_{l'}(k\chi') \delta_{ll'} \delta_{mm'} q_\kappa(\chi) q_\kappa(\chi') P_\Phi(k, \chi, \chi'). \quad (2.298d)$$

$$C_{\psi\psi}(l) = \frac{2}{\pi} \int_0^\infty \frac{d\chi}{\chi} \int_0^\infty \frac{d\chi'}{\chi'} \int k^2 dk \times j_l(k\chi) j_l(k\chi') q_\kappa(\chi) q_\kappa(\chi') P_\Phi(k, \chi, \chi'), \quad (2.298e)$$

where, to obtain the second to last line, I used the orthonormality of spherical harmonics.

This triple integral is cumbersome and computationally expensive to calculate. The **Limber approximation** [31] argues that, for sufficiently large l , the only contributions to this integral are those with $\chi' = \chi$. This argument is inspired by the fact that

$$\frac{2}{\pi} \int k^2 dk j_l(k\chi) j_l(k\chi') = \frac{1}{\chi^2} \delta^D(\chi - \chi'). \quad (2.299)$$

However, this integral has one extra term in $P_\Phi(k, \chi, \chi')$. The argument is that the product $j_l(k\chi) j_l(k\chi')$ is sharply peaked at $k\chi = k\chi' = l + 1/2$. Therefore, if $P_\Phi(k, \chi, \chi')$ does not vary significantly over the range of k where the product $j_l(k\chi) j_l(k\chi')$ is appreciable, we obtain we get

$$C_{\psi\psi}(l) = \int_0^\infty \frac{d\chi'}{\chi'^4} q_\kappa(\chi')^2 P_\Phi\left(k = \frac{l+1/2}{\chi'}, \tau(\chi')\right). \quad (2.300)$$

Now this is a single integral, much easier to compute than the full expression.

For low values of l , the product of spherical Bessel functions is not so sharp, and therefore the Limber approximation is worse. In practice, one needs to assess whether the Limber approximation biases the cosmological constraints. For current generation galaxy surveys such as the Dark Energy Survey, the Limber approximation has been validated for cosmic shear and galaxy-galaxy lensing calculations, but biases the results for galaxy clustering. As galaxy surveys get increasingly precise, the applicability of the Limber approximation needs to be assessed [32].

Finally, using the Poisson equation, we can relate the gravitational potential Φ to matter overdensities,

$$k^2\Phi = -4\pi G a^2 \rho_m \delta_m, \quad (2.301)$$

$$\rho_m = \rho_{cr} \Omega_m a^{-3} = \frac{3H_0^2}{8\pi G} \Omega_m a^{-3} \quad (2.302)$$

$$4\pi G a^2 \rho_m = \frac{3}{2} H_0^2 \Omega_m a^{-1} \quad (2.303)$$

$$k^2\Phi = -\frac{3}{2} H_0^2 \Omega_m a^{-1} \delta_m \quad (2.304)$$

$$P_\Phi(k) = \left(\frac{3\Omega_m H_0^2}{2ak^2} \right)^2 P_m(k). \quad (2.305)$$

We obtain the convergence power spectrum,

$$C_{\kappa\kappa}(l) = \left(\frac{3\Omega_m H_0^2}{2} \right)^2 \int_0^\infty \frac{d\chi'}{a^2(\chi')} q_\kappa(\chi')^2 P_m \left(k = \frac{l+1/2}{\chi'}, \tau(\chi') \right). \quad (2.306)$$

The shear field γ comes from the same lensing potential as the convergence field κ , and thus the shear correlations can also be written in terms of the convergence power spectrum. In particular, we define the shear correlation functions as

$$\xi_\pm(\theta) = \langle \gamma_1(0) \gamma_1(\theta^i) \rangle \pm \langle \gamma_2(0) \gamma_2(\theta^i) \rangle = \int \frac{ldl}{2\pi} J_{2\mp 2}(l\theta) C_{\kappa\kappa}(l), \quad (2.307)$$

where $\langle \rangle$ is an average over galaxies separated by angle θ and $J_n(x)$ are Bessel functions.

2.3.11 CMB Temperature Power Spectrum

The Cosmic Microwave Background is a bath of primordial photons created during reheating. These photons were tightly coupled to protons and electrons via Thomson scattering, forming a fluid known as the photon-baryon plasma. As the Universe expands, the plasma cools down. When the temperature reaches

the hydrogen binding energy, $T \approx 13.6\text{eV}$, protons and electrons start forming hydrogen atoms, which don't scatter photons. Thus, the mean free path of photons diverges, photons decouple from baryonic matter and free-stream throughout the Universe until reaching our radio telescopes.

The CMB radiation forms an almost perfect blackbody radiation spectrum with temperature $T_{\text{CMB}} \approx 2.7255\text{K}$, measured by the COBE satellite. As CMB measurements became more precise, anisotropies have been detected. The temperature of the CMB photons depends on the direction of the sky we are observing. These fluctuations are very small, of order $\Delta T/T \approx 10^{-5}$. However, the temperature measurements are so precise that these anisotropies are detected with great precision.

CMB anisotropies are expected for several different reasons. First, inflation has provided adiabatic quantum fluctuations which were imprinted in the photon-baryon plasma. These fluctuations are characterized by an almost scale-invariant power spectrum, $\Delta_{\mathcal{R}} = A_s(k/k_p)^{n_s-1}$. Observations of the CMB temperature and polarization power spectra agree with this power-law initial power spectrum, predicting an amplitude of $A_s \approx 2.1 \times 10^{-9}$ and a spectral index $n_s \approx 0.96$ [33]. Using the transfer functions, we can predict the power spectrum of photon fluctuations at any time in cosmological history. Besides, after recombination, these photons traveled throughout the Universe, traversing the gravitational potential generated by matter overdensities, causing the Sachs-Wolfe effect on the CMB power spectrum.

Telescopes and satellites, such as the ESA Planck or the Atacama Cosmology Telescope, measure the temperature of the CMB as a function of the direction, $T(\mathbf{n})$. The anisotropies are defined as

$$\Theta(\mathbf{n}) = \frac{T(\mathbf{n}) - T_{\text{CMB}}}{T_{\text{CMB}}}, \quad (2.308)$$

where T_{CMB} is the angular-averaged temperature. The temperature anisotropies can be expanded in spherical harmonics,

$$\Theta(\mathbf{n}) = \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_{\ell m}(\mathbf{n}). \quad (2.309)$$

Statistical isotropy requires that the different ℓ and m are uncorrelated, and then

$$\langle a_{\ell m} a_{\ell' m'}^* \rangle = \delta_{\ell \ell'} \delta_{m m'} C_{\ell}. \quad (2.310)$$

We can predict the correlations C_{ℓ} using the transfer functions of the photon

multipoles $T_\gamma(k, \ell)$,

$$\frac{\ell(\ell+1)C_\ell}{2\pi} = \int \frac{dk}{k} T_\gamma^2(k, \ell) \Delta_{\mathcal{R}}(k), \quad (2.311)$$

where $\Delta_{\mathcal{R}}(k)$ is the primordial power spectrum.

Chapter 3

Cosmological Observations and Tensions

This chapter explains cosmological observations and analyses throughout the history. I briefly present both historical and recent results, presenting multiple ways of probing cosmology. After reviewing cosmological probes, I explain cosmological tensions: disagreements between different experiments in the last years. Finding the cause of such tensions is one of the biggest challenges in current observational cosmology.

3.1 Observables

3.1.1 Luminosity Distances and Type-Ia Supernovae

Type Ia supernovae (SNIa) are star explosions in binary systems, where one of the stars is a white dwarf. White dwarfs are old stars, or remnants of a star's core, and are mainly composed of heavy elements such as carbon and oxygen, as the light elements have already fused. These stars are very dense, being supported from gravitational collapse by the electrons' degeneracy pressure. However, when they form a binary system with another star, they may accrete matter from the companion, and when they reach a certain mass - the Chandrasekhar mass - they collapse, either forming a neutron star or causing an explosion: the Type Ia supernova.

The intrinsic luminosity for all SNIa is the same because of the white dwarf mass limit [34]. Measuring their luminosity over time - the light curve -, one sees that the luminosity rapidly increases until a peak, and then slowly fade. We can only measure the apparent luminosity, which is affected by the distance to the SNIa and by dust, for instance. We say that SNIa are standardizable candles: we can use another standard candle such as Cepheid variable stars in the same galaxy that hosts the SNIa to calibrate the relation between intrinsic and apparent luminosities [35]. Without calibration, the intrinsic SN magnitude M is degenerate with the Hubble constant H_0 , but can still be used to infer the evolution of the Hubble factor and therefore cosmological parameters such as Ω_m and w , the dark

energy equation of state. Section 3.1.2 discusses one of the current methods to calibrate SNIa using the local distance ladder, obtaining precise measurements of H_0 .

SNIa luminosity distances are historically important cosmological observables, since they have revealed for the first time the accelerated expansion of the Universe. Departures from the linear Hubble law, $cz = H_0 D$, can only be measured for redshifts $z > 0.3$. In the 1990's, two collaborations, the High- z Supernovae Search Team, led by Adam Riess and Brian Schmidt, and the Supernovae Cosmology Project, led by Saul Perlmutter, aimed to measure SNIa at high redshifts in order to measure the deceleration of the Universe's expansion and infer the matter fractional density Ω_m [17, 18]. To their surprise, both teams have independently detected an accelerated expansion with high statistical significance, compatible with a flat Universe comprised of 30% ordinary matter and 70% dark energy.

The inference is performed via the relation between intrinsic magnitude m , apparent magnitude M and luminosity distance D_L (in units of megaparsec),

$$m - M = 5 \log(D_L) + 25. \quad (3.1)$$

The luminosity distance predicted in the Λ CDM model is

$$D_L(z) = \frac{c(1+z)}{H_0} S_k \left(\int_0^z \frac{dz}{\sqrt{\Omega_m(1+z)^3 + (1 - \Omega_m - \Omega_\Lambda)(1+z)^2 + \Omega_\Lambda}} \right) = \frac{c}{H_0} f(z), \quad (3.2)$$

and thus we can write

$$m - M = 5 \log \left(\frac{c}{H_0} \right) + 5 \log(f) + 25, \quad (3.3)$$

$$m - M - 5 \log \left(\frac{c}{H_0} \right) = 5 \log(f) + 25, \quad (3.4)$$

where the degeneracy between H_0 and magnitudes is made explicit.

At the time of writing, there are several state-of-the-art, public supernovae datasets. The PantheonPlus catalog [36], a continuity of the Pantheon catalog [36], is comprised of 1550 SNe; the Union3 catalog [37, 38] consists of 2087 SNe; the Dark Energy Survey Year 5 catalog [39, 40] contains 1650 SNe. These catalogues have multiple SN in common, but they all differ in the systematic error treatment.

3.1.2 Local Distance Ladder

The local distance ladder is a technique to measure the distance to different standard candles, using nearby objects to calibrate the distance to farther ones [34]. Notably, the Supernova H_0 for the Equation of State (SH0ES) collaboration has

developed the technique over the last two decades, obtaining very precise measurements of the H_0 parameter [41, 35, 21, 42].

One of the most precise ways to measure the distance of galactic objects is using parallaxes. By measuring the angular displacement of an astronomical body over half a year, we can use geometry to determine the distance from the Earth to said body. Intuitively, objects farther away will have less angular displacement. If p is the displacement angle in arcseconds, the parallax distance is defined as

$$D = \frac{1}{p} \text{ parsec}, \quad (3.5)$$

where parsec is a distance unit, $1\text{pc} \approx 3.09 \times 10^{16}\text{m}$.

Cepheid variable stars are astronomical objects that can be used as standard candles. In 1912, the astronomer Henrietta Swan Leavitt discovered a relation between the period and intrinsic luminosity of these stars [27]. This relation can be calibrated if we can also measure the parallax of some cepheids. This is one of the distance ladder steps. By measuring the parallax of nearby cepheids, we can calibrate the period-luminosity relation and determine the distance to farther cepheids whose parallax is too small.

Finally, all type Ia supernovae share an intrinsic magnitude. By measuring cepheid variable stars in the same galaxies that host type Ia supernovae, we can calibrate this intrinsic magnitude, which allows determining the distance to even farther supernovae, the final step of the distance ladder. With these distances, we can determine the late-time expansion of the Universe, specifically the H_0 parameter via the distance-redshift relation for nearby objects,

$$cz = H_0 D. \quad (3.6)$$

The state-of-the-art measurements of the cosmic distance ladder were conducted by the SH0ES collaboration using parallax data from the Gaia survey. The inferred value of H_0 is $H_0 = 73.15 \pm 0.97\text{kms}^{-1}\text{Mpc}^{-1}$ [21].

3.1.3 Cosmic Microwave Background Anisotropies

In 1965, physicists Arno Penzias and Robert Wilson accidentally discovered a low-temperature, isotropic radiation signal: the Cosmic Microwave Background [4]. At the time, cosmologists already predicted a radiation signal due to the photons created during the Big Bang, which matched exactly Penzias and Wilson's discovery. In the following decades, precise telescopes were developed to measure this radiation, determining its temperature across the sky.

In the 1990s, the Cosmic Background Explorer (COBE) satellite measured the CMB radiation with great precision [10]. The DMR experiment, led by G. Smoot, measured temperature anisotropies, while the FIRAS experiment, led by John

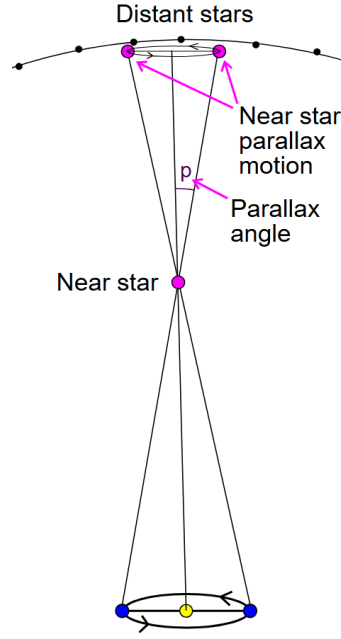


Figura 3.1: Geometric diagram of the parallax effect. Here, p represents the angular displacement of the distant object. Taken from [Wikipedia](#).

Mather, measured its absolute temperature [11]. Both scientists were awarded the 2006 Nobel Prize in Physics "for their discovery of the blackbody form and anisotropy of the cosmic microwave background radiation".

In the 2000s, the NASA's Wilkinson Microwave Anisotropy Probe (WMAP) experiment marked the beginning of the precision cosmology era. They have measured the CMB temperature and polarization anisotropies up until multipoles $\ell = 1200$ and were able to determine the Λ CDM cosmological parameters with unprecedented precision to that day [43].

In the 2010s, the Planck experiment, from the European Space Agency (ESA) began its measurements. In 2018, they released one of their final datasets, dubbed

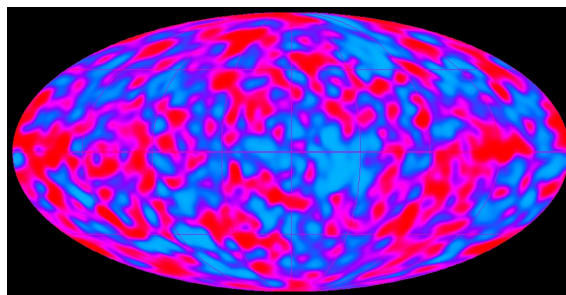


Figura 3.2: CMB temperature anisotropies measured by the COBE satellite. Taken from <https://www.nasa.gov/wp-content/uploads/2013/06/403322main-cobeallsky-full.jpg>.

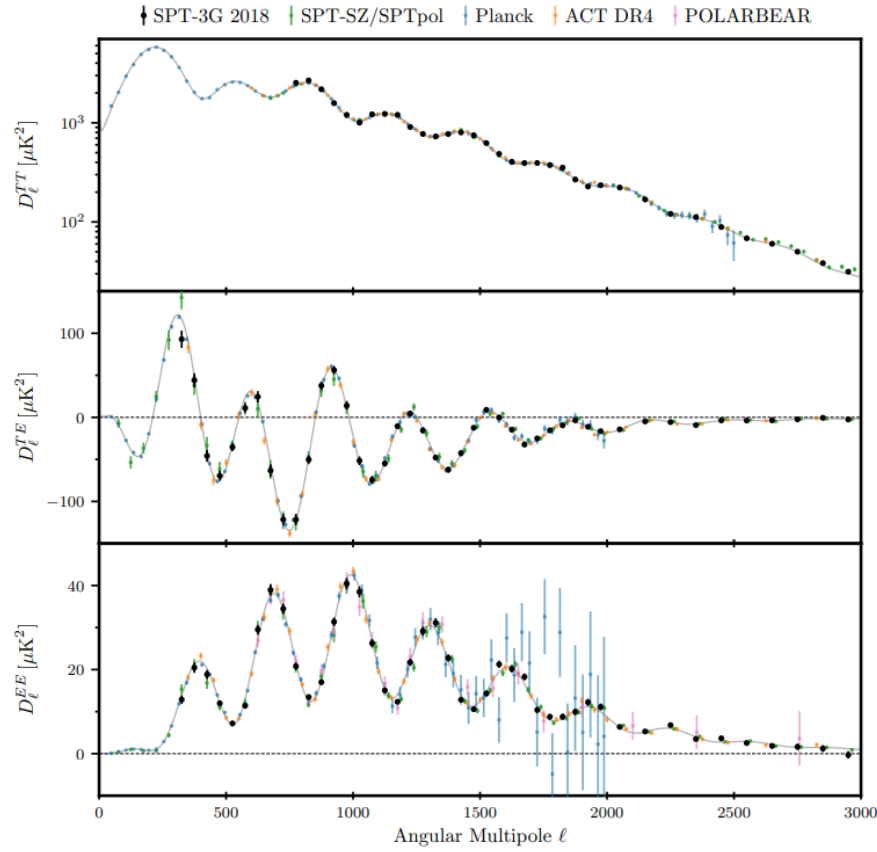


Figure 3.3: CMB temperature and polarization angular power spectra from multiple CMB surveys: SPT (black and green dots), Planck 2018 (blue dots), ACT (orange dots) and POLARBEAR (pink dots). Taken from [48].

Planck 2018, measuring the CMB anisotropies up to multipoles $\ell = 2508$, surpassing the WMAP precision. To this day, the Planck 2018 dataset continues to be one of the state-of-the-art CMB measurements [44, 5, 33].

Newer measurements have taken place since Planck. Most notably, the Atacama Cosmology Telescope (ACT) could measure the CMB anisotropies until $\ell = 4000$ [45]. However, since it is a ground-based experiment, it could not measure the large-scale CMB anisotropies at $\ell < 600$. Many analyses combine ACT and Planck data to obtain precise constraints on cosmological parameters [46, 47]. Finally, the South Pole Telescope (SPT) has measured the CMB anisotropies up to $\ell = 3000$ [48].

3.1.4 CMB Lensing

CMB photons are scattered in the large-scale structure of the Universe, being deflected on their path. This lensing effect leaves imprints in the CMB temperature and polarization power spectra: these imprints depend on large-scale structure

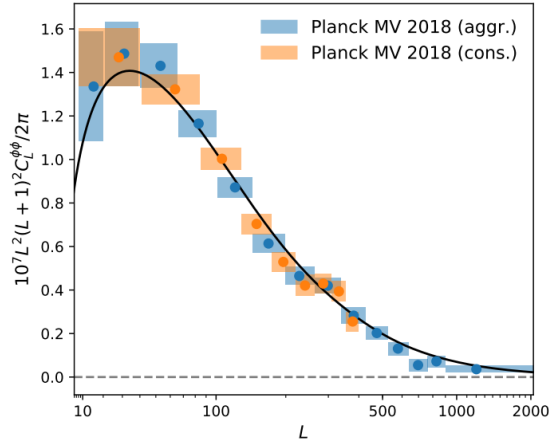


Figure 3.4: Lensing power spectrum $C_{\ell}^{\phi\phi}$ reconstructed from Planck 2018 data. Taken from [49].

properties. From the temperature and polarization power spectra, one can reconstruct the lensing potential power spectrum, which is related to the matter power spectrum.

The three state-of-the-art CMB anisotropy datasets, Planck, ACT and SPT, have also reconstructed the lensing power spectrum from their data. Besides Planck 2018 lensing, we also have the lensing reconstruction from SPT-3G and ACT DR6.

3.1.5 Cosmic Shear, Galaxy Clustering and Cross-Correlations

One of the cosmological predictions concerns the distribution of matter throughout the Universe. In particular, the two-point correlation of matter densities are encoded in the matter power spectrum, $P(k)$. Much of the matter correlations are driven by dark matter, which has not been detected yet. However, we can measure **tracers of matter**: observables whose distribution is determined by the matter distribution. Galaxies are one prime example of such tracers: where there is more matter, there will be more galaxies. Therefore, studying the distribution of galaxies, we can infer properties of the matter distribution, which can be confronted with theoretical predictions. In the last years, galaxy surveys such as the Dark Energy Survey (DES), the Kilo-Degree Survey (KiDS) and the Hyper Suprime Cam (HSC) have mapped tens of millions of galaxies, providing cosmological constraints matching the CMB precision.

When galaxies are observed, we can measure their angular position and redshift. To produce meaningful statistics, millions of galaxies are mapped. Photometric redshift measurement is a more efficient method to quantify the redshift of millions of galaxies. However, today, the Dark Energy Spectroscopic Instrument (DESI) uses spectroscopic redshift to measure tens of millions of galaxies, improving the precision of galaxy catalogues over photometric redshift ones [50].

The distance to the measured galaxies, however, is not known. Without distance information, we can only perform angular statistics, which essentially integrates the 3D statistics over the line of sight.

Galaxy clustering is the study of galaxy position correlations. As tracers of matter, galaxy densities can be related to matter densities using a **galaxy bias** model. The simplest one is the linear bias, which assumes a linear relation between the galaxy density contrast δ_g and the matter density contrast δ_m ,

$$\delta_g = b_1 \delta_m, \quad (3.7)$$

where b_1 is the linear galaxy bias. In principle, b_1 can be a function of k and a , but the most simplistic assumption is a constant bias. A redshift-dependence of the galaxy bias is considered in a simplistic way, where the galaxies in the catalog are divided in tomographic redshift bins, and the linear galaxy bias is assumed constant within each bin.

Each tomographic bin has a number density of galaxies $n^i(z)$, where i denotes the bin and $n^i(z)dz$ is the number of galaxies between redshifts z and $z + dz$. We can turn this galaxy number density into a matter radial density as

$$q^i = b_1 n^i \frac{dz}{d\chi}, \quad (3.8)$$

where $\chi(z)$ is given by Equation 2.56. We can then calculate the angular correlations using the Limber approximation,

$$C_{\delta_g \delta_g}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q^i q^j P\left(k = \frac{\ell + 1/2}{\chi}, z(\chi)\right). \quad (3.9)$$

Finally, we can sum the multipoles to obtain the real-space galaxy clustering angular correlation $w^{ij}(\theta)$

$$w^{ij}(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} P_{\ell}(\cos \theta) C_{\delta_g \delta_g}^{ij}(\ell), \quad (3.10)$$

where $P_{\ell}(x)$ are Legendre polynomials. Since we are dealing with binned correlations, it is common to swap P_{ℓ} with its angular average,

$$\bar{P}_{\ell} = \int_{\theta_{\min}}^{\theta_{\max}} P_{\ell}(\cos \theta) \sin \theta d\theta. \quad (3.11)$$

Cosmic shear is a visual distortion of galaxies' shapes, as their emitted light is weakly lensed when travelling across the large-scale structure of the Universe. This lensing effect is very weak, and it cannot be seen by naked eye. However,

when measuring the shapes of millions of galaxies, this weak lensing induces spatial correlations in their (otherwise uncorrelated) shapes.

The angular shape correlations can be predicted as follows. Defining the lensing efficiency q_κ^i as

$$q_\kappa^i = \frac{3H_0^2\Omega_m}{2} \int d\chi' \frac{\chi' - \chi}{\chi'} n^i \frac{dz}{d\chi'}, \quad (3.12)$$

the Fourier-space correlations are given by

$$C_{\kappa\kappa}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q_\kappa^i q_\kappa^j P\left(k = \frac{\ell + 1/2}{\chi}, z(\chi)\right), \quad (3.13)$$

and we sum the multipoles to obtain the cosmic shear angular correlation function

$$\xi_\pm^{ij}(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \frac{G_{\ell,2}^+(\cos\theta) \pm G_{\ell,2}^-(\cos\theta)}{\ell^2(\ell+1)^2} C_{\kappa\kappa}^{ij}(\ell), \quad (3.14)$$

where $G_{\ell,2}^\pm$ are analytic functions and their sum and subtraction are given by [51, 52]

$$G_{\ell,2}^+(x) \pm G_{\ell,2}^-(x) = P_\ell^2(x) \left[\frac{4 - \ell + 2x(\ell - 1)}{1 + x^2} - \frac{\ell(\ell + 1)}{2} \right] + P_{\ell-1}^2(x) \frac{(\ell + 2)(x \mp 2)}{1 - x^2}, \quad (3.15)$$

where $P_\ell^2(x)$ is the associated Legendre polynomial P_ℓ^m with $m = 2$.

Finally, if we have two separate catalogues, one measuring galaxy positions (the **lenses**) and another measuring galaxy shapes (the **sources**), we can cross-correlate the positions in the first catalog and the shapes in the second. This correlation function is called **galaxy-galaxy lensing**, denoted by $\gamma_t(\theta)$. Its Fourier-space correlations are given by

$$C_{\kappa\delta_g}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q_\kappa^i q^j P\left(k = \frac{\ell + 1/2}{\chi}, z(\chi)\right), \quad (3.16)$$

where q_κ^i is the lensing efficiency of the galaxy shape catalog and q^j is the radial galaxy density of the galaxy position catalog. The angular correlation function $\gamma_t(\theta)$ is given by

$$\gamma_t(\theta) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} P_\ell^2(\cos\theta) C_{\kappa\delta_g}^{ij}(\ell), \quad (3.17)$$

where $P_\ell^2(x)$ is the associated Legendre polynomial P_ℓ^m with $m = 2$.

The three 2-point correlation functions $w(\theta)$, $\gamma_t(\theta)$ and $\xi_\pm(\theta)$ form the so-called **3x2pt analysis**. These datasets can constrain with great precision the large-scale

structure of matter, more specifically the matter density Ω_m and σ_8 , a parameter which measures the mean amplitude of matter fluctuations inside a sphere of radius $R = 8\text{Mpc}/h$, given by

$$\sigma_8^2 = \langle \delta_m^2 \rangle = \int_0^\infty \frac{dk}{k} \frac{k^3 P(k)}{2\pi^2} W(k, R = 8\text{Mpc}), \quad (3.18)$$

where $W(k, R) = 3 \sin(kR)/kR$. Since dark energy affects structure formation, the 3x2pt analysis is also used to constrain dark energy properties such as its equation of state.

The state-of-the-art photometric galaxy surveys are the Dark Energy Survey, the Kilo-Degree Survey and the Hyper Suprime Cam survey. Each survey has a different strategy, balancing survey area, depth and photometry. DES has produced three galaxy catalogues: the Metacalibration catalog maps the shapes of 100 million source galaxies, the MagLim (or Magnitude Limited) sample, which contains 10.7 million lens galaxies, and the redMaGiC sample, containing 2.6 million Luminous Red Galaxies as lenses [53, 8, 52]. The full result of their 6 years of observations is going to be released in the first semester of 2025.

KiDS has measured around 1 million source galaxies with high redshift precision due to a 9-band photometry. Besides using the two-point correlation functions, their analysis also test other summary statistics: Complete Orthogonal Set of E/B Integrals (COSEBIs) and band powers, finding consistent results across the three analysis choices [54, 55]. HSC is a japanese-led survey whose source galaxy catalog contains around 25 million galaxies [56, 57].

Spectroscopic galaxy surveys focus on measuring the clustering of nearby galaxies. Notable surveys are CfT, 2dFGS, SDSS and its extensions, which culminated in the BOSS and eBOSS surveys. These spectroscopic galaxy catalogues can be used in conjunction with cosmic shear data from photometric surveys [58, 59, 9, 60].

DES, HSC and KiDS form the so-called Stage-III cosmic shear surveys, whose measurements began in the 2010s and finished in the 2020s. As of 2024, the scientific community is preparing for the beginning of Stage-IV cosmological surveys. The two most prominent future surveys are Euclid, by the European Space Agency, and the Vera C. Rubin Observatory's Legacy Survey of Space and Time (LSST). Both surveys will begin observations in the next years [61, 62].

3.1.6 Baryonic Acoustic Oscillations

Figure 3.6 shows the matter 2-point correlation function, $\xi(r)$. We can notice a pronounced peak at $r \approx 100\text{Mpc}/h$, corresponding to the sound horizon at baryon drag epoch, r_d . This scale is imprinted in the distributions of tracers of matter, such as galaxies. As distances to tracers are unknown, the r_d scale can be used as a ruler, so we can determine the distance to the tracers relative r_D , namely D_L/r_d . This effect is known as Baryonic Acoustic Oscillations (BAOs), and were

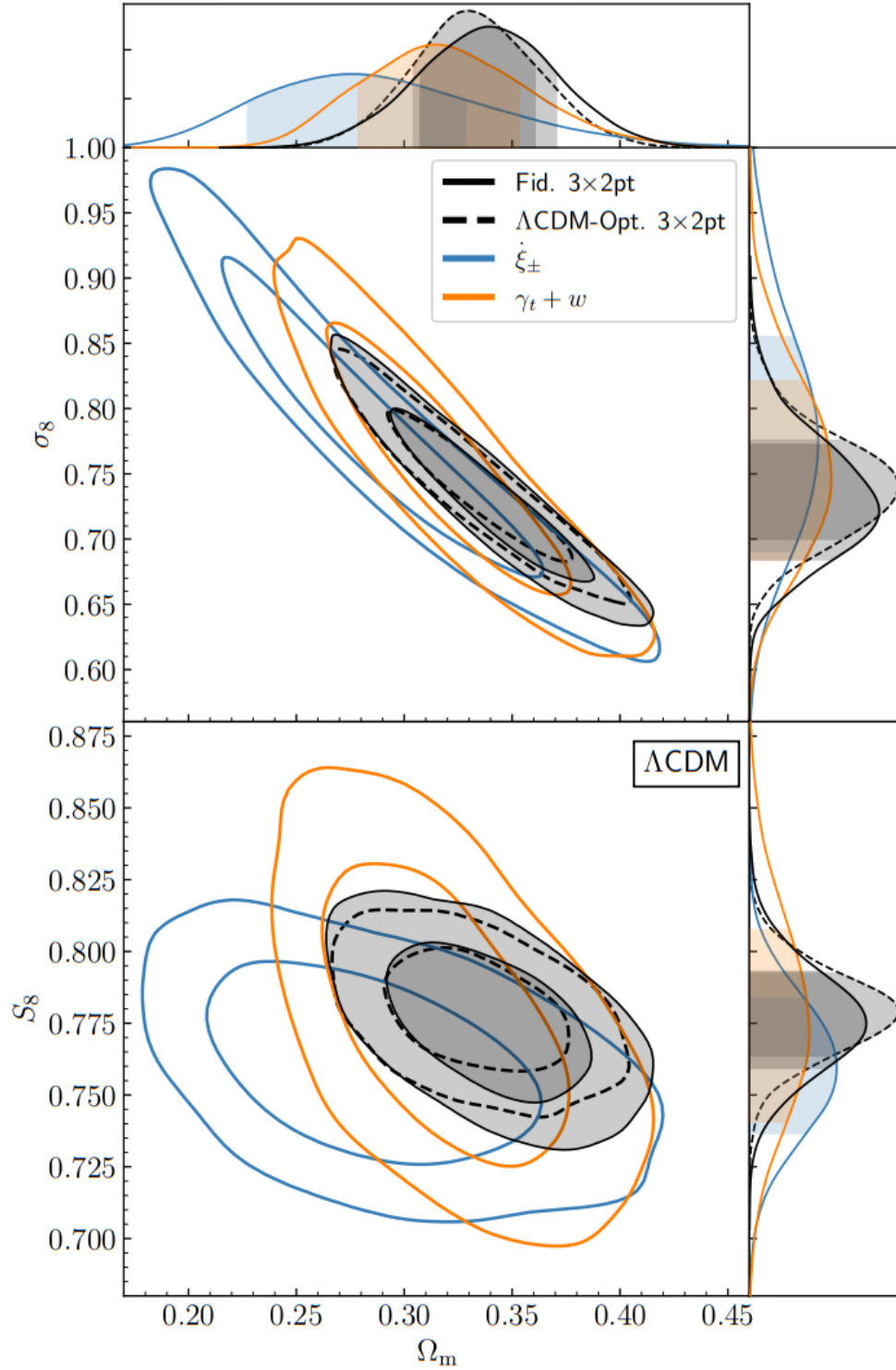


Figura 3.5: Constraints from the Dark Energy Survey 3-year analysis on the cosmological parameters Ω_m , σ_8 and S_8 . The black thick line shows the constraints from their fiducial analysis, the black dashed line shows constraints from a Λ CDM optimized analysis with less conservative scale cuts, the blue line shows constraints from cosmic shear only and the orange line shows constraints from joint galaxy clustering and galaxy-galaxy lensing. Taken from <https://arxiv.org/pdf/2105.13549>.

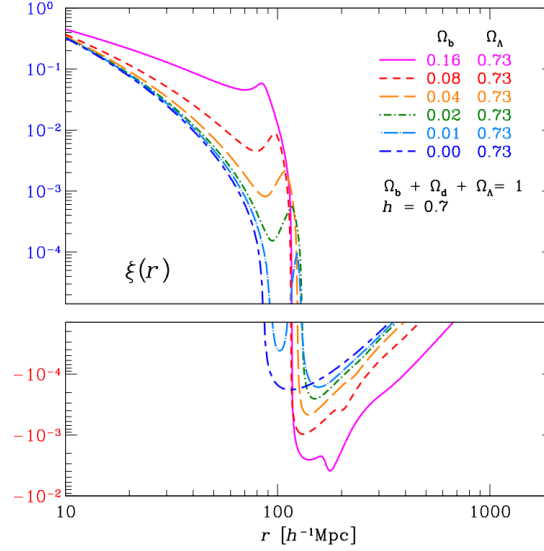


Figure 3.6: Matter correlation function $\xi(r)$ for various values of Ω_b . Taken from [63].

first measured in 2005 by the Sloan Digital Sky Survey (SDSS) and the 2-degree Field Galaxy Survey (2dFGS).

The methodology for measuring distances with BAO scales is as follows. Take a sample of matter tracers, such as galaxies, within a given redshift bin of width Δz . By analyzing the 2-point correlations, one can find a preferred angular separation $\Delta\theta$ and a preferred redshift separation Δz . These are related to the sound horizon scale at baryon drag epoch, r_d , via the comoving distance to the ensemble $D(z)$

$$D(z) = \frac{r_d}{\Delta\theta}, \quad (3.19)$$

and to the Hubble parameter at the ensemble redshift, $H(z)$

$$D_H(z) = \frac{c}{H(z)} = \frac{r_d}{\Delta z}. \quad (3.20)$$

Following the methodology from the Dark Energy Spectroscopic Instrument (DESI), if the BAO feature is detected with low signal-to-noise ratio (SNR), one can increase the SNR by measuring the volume-averaged distance

$$D_V = (zD(z)^2 D_H(z))^{1/3}. \quad (3.21)$$

This way, a BAO dataset consists in a series of distance measurements in terms of the baryon drag epoch, either the pair $D(z)/r_d$, D_H/r_d or the single measurement of D_V/r_d .

The success of SDSS and 2dFGS motivated other galaxy surveys to measure

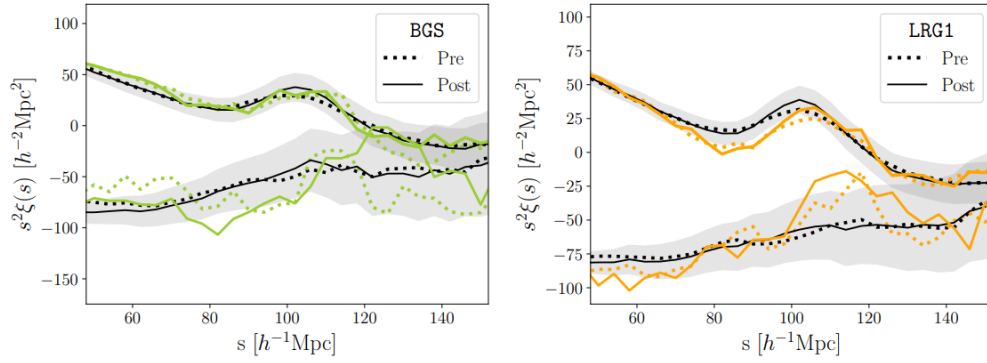


Figure 3.7: Correlation function for different tracers of matter: bright galaxies (left panel) and luminous red galaxies (right panel), measured by the DESI collaboration. Taken from [64].

the BAO feature, such as the 6-degree Field Galaxy Survey (6dFGS) and the SDSS extensions, SDSS-II, SDSS-III and SDSS-IV, leading to the Baryon Oscillation Spectroscopic Survey (BOSS). At the time of writing, the current state-of-the-art is the DESI survey, which maps several tracers of matter including galaxies, quasars and the Lyman- α forest. Although BAO distance-redshift measurements are binned, resulting in less data points than SN measurements, BAO surveys can reach higher redshifts: the DESI survey measures distances up to redshift $z = 2.33$. It is important to remark that BAO is not the only science goal of spectroscopic galaxy surveys, as they can be used to measure the full shape of the clustering 2-point correlation function.

3.1.7 Redshift Space Distortions

When observing galaxies, we can obtain information about their angular position in the sky and their redshift, which can be used as a third dimension instead of their distance. The measured redshift is a combination of the cosmological redshift but also of the peculiar velocity of the galaxy with respect to the observer. Therefore, when mapping the 3D distribution of galaxies using redshifts, this distribution may appear stretched or squashed due to peculiar velocities. On small scales, random motions within a cluster of galaxies will cause galaxies at the same distance to have slightly different redshifts. This distortion effect elongates structures, causing the so-called "fingers of God". On large scales, objects tend to fall in towards overdense regions, such as galactic nuclei. This makes nearby galaxies move away from us, and farther galaxies move towards us, effectively squashing structures, an effect known as "pancakes of God". These and other effects caused by peculiar velocities are referred to as **redshift space distortions** (RSDs).

While the matter power spectrum describes the variance of the matter fluctu-

ations in real space, redshift surveys have access to an analogous quantity, the redshift-space power spectrum, where once again the radial coordinate is given by the redshift instead of the distance. A simple model relating real-space matter power spectrum and redshift-space power spectrum of a matter tracer is given by [65]

$$P_{\text{obs}}(k, \mu) = (b_1 + f\mu^2)^2 P_m(k), \quad (3.22)$$

where P_{obs} is the redshift-space power spectrum of the tracer, b_1 is the linear bias of the tracer, $f = d \ln D / d \ln a$ is the derivative of the growth rate and μ is the angle between $\mathbf{k}$ and the line-of-sight. In Λ CDM, $f \approx \Omega_m^{0.6}$. By measuring the redshift-space power spectrum, one can constrain the quantity $f(z)\sigma_8(z)$. Since the measurement of RSDs necessitate precise redshift measurements, they are measured by spectroscopic galaxy surveys such as 2dFGS [66], SDSS [67] and BOSS [68].

3.1.8 Big Bang Nucleosynthesis

Big Bang Nucleosynthesis (BBN) is the formation of atomic elements throughout cosmic history, starting from a hot plasma of protons, electrons and neutrons. One of its biggest successes is the prediction of the helium-to-hydrogen mass ratio of

$$\frac{m_{\text{He}}}{m_{\text{H}}} \approx \frac{1}{4}, \quad (3.23)$$

confirmed in stellar measurements. The mass fractions of each element depend on one particular quantity: the baryon-to-photon ratio η , defined as

$$\eta = \frac{n_b}{n_\gamma} \approx 5.5 \times 10^{-10} \left(\frac{\Omega_b h^2}{0.02} \right), \quad (3.24)$$

where n_b and n_γ are the baryon and photon number densities, respectively. Nowadays, there are several BBN calculator codes such as `PArthENoPE` [69] and `PRyMordial` [70]. By measuring helium and deuterium abundances in low-metallicity stars, one can constrain η . Using Particle Data Group recommended light element abundances, the constraints on baryon density are $\Omega_b h^2 = 0.02218 \pm 0.00055$ [7].

3.1.9 Standard Sirens

Gravitational waves (GWs) are small perturbations in the metric, specifically in the transverse-traceless degrees of freedom, caused by the motion of massive bodies. In particular, rotating binary systems produce gravitational waves with a well-predicted waveform, and may be detected in large interferometers such

as the Laser Interferometer Gravitational-Wave Observatory (LIGO) [71], the Laser Interferometer Space Antenna (LISA) [72] and the Kamioka Gravitational Wave Detector (KAGRA) [73]. The measured waveform depends, among other parameters, on the luminosity distance D_L to the binary system.

One of the ways to extract cosmological information from detected gravitational waves is through its redshift z , which is, in principal, inaccessible. During the binary system's orbit, part of the system's energy is radiated in form of GWs, and the individual bodies start infalling towards one another until they coalesce. For a few lucky events, we may observe the electromagnetic counterpart of the GW, the kilonova and afterglow caused by the merger of the binary system. GW events that we can measure the electromagnetic counterpart are called **bright sirens**, and directly provide cosmological information via $D_L(z)$. At the time of writing, out of the detected GWs, only a single bright siren has been detected, named GW170817 [74].

Without electromagnetic counterparts, we may still infer the redshift of a GW event using galaxy catalogues. The method has been proposed in [75]. We assign a probability that the GW was emitted by a binary system in a certain galaxy, and we use the galaxy redshift as the GW redshift. In the end, the GW redshift is a random variable with wide distribution, and with the number of GW events we have detected thus far, the constraints on H_0 are still much larger than constraints from cosmic distance ladder and CMB. However, in the future years, with the new GW detectors from the Einstein Telescope and Cosmic Explorer, the cosmological information provided by standard sirens can match the precision of CMB and cosmic distance ladder, providing useful information about the current standing Hubble tension.

3.1.10 Cosmic Chronometers

In galaxy clusters, one can measure a vast and diverse population of galaxies. Some galaxies are old and passively evolving. Suppose we measure a pair of such galaxies with similar ages, t_1 and t_2 , and redshifts, z_1 and z_2 . We can approximate the redshift derivative as

$$\frac{dz}{dt} \approx \frac{z_2 - z_1}{t_2 - t_1}. \quad (3.25)$$

This derivative is related to the Hubble factor

$$\frac{dz}{dt} = \frac{dz}{da} \dot{a} = -\frac{1}{a} H = -(1+z)H(z). \quad (3.26)$$

Therefore, pairs of evolving galaxies can be used to measure the Hubble factor $H(z)$, and are called **cosmic chronometers**. The technique has been used on the beginning of the 2000s [76], and more chronometers are added to this day [77].

3.2 Cosmological Tensions

The Λ CDM cosmological model provides a remarkably good fit to all of the datasets discussed in this section. This success has motivated increasingly ambitious and precise surveys to pinpoint the Λ CDM parameters. The increased precision has revealed inconsistencies, or **tensions**, in the inferred parameter values from independent surveys. These discrepancies, might be caused by unaccounted-for systematic effects in any experiment, but can also be a sign of the incompleteness of the Λ CDM model. In this Section, I review the most relevant cosmological tensions.

3.2.1 Quantifying Tensions

The simplest technique to quantify tensions between two marginalized posterior distributions of a variable X is the 1D tension metric [78]

$$T = \frac{|\langle X \rangle_1 - \langle X \rangle_2|}{\sqrt{\sigma_1^2(X) + \sigma_2^2(X)}}, \quad (3.27)$$

where $\langle X \rangle_i$ are the posterior means and $\sigma_i(X)$ are the posterior standard deviations. The quantity T measures how many standard deviations separate the two means, and is usually denoted in terms of σ (i.e. "a tension of $T\sigma$ between the experiments"). If the posterior is Gaussian, $X \sim \mathcal{N}(\langle X \rangle, \sigma)$, then $e^{-T^2/2}$ is the probability of one experiment obtaining its results given that the other experiment is correct.

While Equation 3.27 can be used to quantitatively measure tensions, it does not capture the full, multidimensional posterior distributions. We can generalize this metric to many dimensions by computing the **figure of bias**, given by

$$\text{FOB} = [\Delta \langle \theta \rangle^T (C_1 + C_2)^{-1} \Delta \langle \theta \rangle]^{1/2}, \quad (3.28)$$

where $\Delta \langle \theta \rangle = \langle \theta \rangle_2 - \langle \theta \rangle_1$ is a column vector containing the differences in the parameter means of each experiment and C_1 and C_2 are the covariance matrices of the parameters θ . While this generalizes to multiple dimensions, its interpretation as a statistical significance still relies on the assumption that the posteriors are Gaussian. While more advanced techniques exist to assess tensions [78], the figure of bias can still be used as a simple way to quantify tensions between two experiments.

3.2.2 The Hubble Tension

The Hubble tension is a discrepancy in the parameter H_0 , the current expansion rate of the Universe. On one hand, we have the cosmic distance ladder measurements, which do not depend on the cosmological model, but are sensitive to the calibration of the ladder rungs. The state-of-the-art measurements come from the SH0ES collaboration using SN from the Hubble Space Telescope calibrated by precise parallax measurements of Cepheid variable stars from the Gaia spacecraft's Early Data Release 3, obtaining a value of $H_0 = 73.04 \pm 1.04 \text{ km s}^{-1} \text{ Mpc}^{-1}$ [42].

On the other hand, CMB measurements can constrain H_0 by measuring the angular scale of the sound horizon at recombination, θ_* , well-determined by the location of the peaks in the CMB power spectra. To obtain H_0 from θ_* , a cosmological model must be assumed. The angular scale θ_* is given by

$$\theta_* = \frac{r_s(z_*)}{D_A(z_*)} = \frac{\int_{z_*}^{\infty} \frac{c_s(z) dz}{H(z)}}{\int_0^{z_*} \frac{dz}{H(z)}}, \quad (3.29)$$

where $z_* \approx 1100$ is the recombination redshift and $c_s(z)$ is the photon-baryon fluid sound speed,

$$c_s = \frac{1}{\sqrt{3}} \sqrt{\frac{1}{1 + \frac{3\rho_b}{4\rho_\gamma}}}. \quad (3.30)$$

Assuming the Λ CDM model, the Planck collaboration reported a value of $H_0 = 67.36 \pm 0.54 \text{ km s}^{-1} \text{ Mpc}^{-1}$. Using the 1D tension metric of Equation 3.27, we find $T = 4.8$. Interpreting T as an actual statistical significance, we would obtain a p-value of approximately 8×10^{-6} : this means the probability of statistical fluctuations being the cause of this discrepancy is extremely low, and there must be some underlying systematic or theoretical modelling incompleteness causing the tension.

Both experiments are sensitive to different systematic errors. The cosmic distance ladder relies on the progressive calibration of standard candles, and the measured magnitude can be affected by dust or other extinction factors. CMB measurements can be affected, for instance, by foregrounds, interference, instrumental systematics, among other effects. Failing to account for systematic effects can bias the cosmological parameter inference, and much effort is put to make sure the results are robust under systematic errors. Even though the experiments pass stringent tests, we cannot rule out unknown systematics as a cause of cosmological tensions.

The cause of cosmological tensions could be an incompleteness of the theoretical model, rather than the statistical model. The Hubble tension has motivated an exploration of many cosmological models beyond Λ CDM, assessing whether the extension can alleviate the tension. Some of the models will be reviewed in

Chapter 4.

3.2.3 The S_8 Tension

The σ_8 parameter, defined in Equation 3.18, describes the "clumpiness" of the Universe, or the ability to form small-scale structures. Cosmic shear measurements are particularly sensitive to σ_8 , or more specifically to a combination of σ_8 and Ω_m called the S_8 parameter,

$$S_8 = \sigma_8 \sqrt{\frac{\Omega_m}{0.3}}. \quad (3.31)$$

CMB measurements probe the initial power spectrum amplitude A_s , which controls σ_8 by rescaling the matter power spectrum $P(k)$. The Planck 2018 results reported a value of $S_8 = 0.832 \pm 0.013$ [33]. Other CMB datasets such as those from the Atacama Cosmology Telescope and the South Pole Telescope confirm the higher S_8 value from Planck 2018 [46, 48]. On the other hand, cosmic shear measurements are sensitive to integrals of $P(k)$ and can determine S_8 with great precision. The Dark Energy Survey collaboration released the data analysis of 3 years of data, reporting $S_8 = 0.776 \pm 0.017$. Using the tension metric of Equation 3.27, we find $T = 2.6$. The significance of this tension varies with the dataset considered and the systematic error treatment. The Kilo Degree Survey (KiDS), for instance, has reported a 3σ tension with Planck 2018 [79], and the Hyper Suprime Cam (HSC) survey has reported a 2.5σ tension with Planck 2018 [80]. While the S_8 tension is less statistically significant than the Hubble tension, at the time of writing, we are on the verge of Stage-IV cosmological surveys, which will increase the precision and reduce the error bars on the cosmological parameters. If the trend persists, the S_8 tension can reach more significant levels.

Chapter 4

Beyond Λ CDM Models

This chapter discusses possible avenues to extend the Λ CDM model and presents a non-exhaustive list of theoretical modifications to the Λ CDM model proposed in the literature.

4.1 Remarks about Λ CDM

Before presenting modifications to the Λ CDM model, I make a non-exhaustive list of some Λ CDM model assumptions and properties. These predictions are aspects of the Λ CDM model that can be broken within extended cosmological models. Challenging these predictions is a method of testing the consistency of the Λ CDM model and exploring the effect of new physics in the cosmological tensions.

4.1.1 General Relativity

Λ CDM assumes General Relativity as the fundamental gravity model. The Einstein equations can be obtained from the Einstein-Hilbert action

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2 R}{2} + \mathcal{L}_m \right], \quad (4.1)$$

where $M_{\text{Pl}}^2 = \hbar c / 8\pi G$ is the (reduced) Planck mass and $\mathcal{L}_m$ is the matter lagrangian. This action leads to the Einstein field equations

$$G_{\mu\nu} = 8\pi G T_{\mu\nu}, \quad (4.2)$$

which ultimately dictate how the Universe expands and how matter clusters. **Modified theories of gravity** introduce new terms in the gravitational action, altering the expansion of the Universe and the clustering of matter.

4.1.2 Constant Dark Energy Density

In Λ CDM, dark energy has a constant energy density. One may challenge this assumption by considering models in which dark energy is described by a fluid with dynamical density $\rho(t)$ and equation of state $w(t) = P(t)/\rho(t)$. A dynamical dark energy behavior would alter the late-time expansion, affecting predicted distances. A common strategy is to parametrize $\rho(t)$ or $w(t)$. Another possibility is to consider dark energy as a scalar field ϕ , solve the equation of motion for ϕ , and then derive its energy density ρ . This is a more fundamental approach than creating phenomenological parametrizations, and some scalar field models have inspirations in string theory [81]. Canonical scalar fields in the FLRW spacetime are defined via the action

$$S_\phi = \int d^4x \sqrt{-g} \left[-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - V(\phi) \right]. \quad (4.3)$$

Knowing the field ϕ as a function of time, we can derive its energy density and equation of state,

$$\rho_\phi = \frac{\dot{\phi}^2}{2} + V(\phi), \quad (4.4)$$

$$w_\phi = \frac{\frac{\dot{\phi}^2}{2} - V(\phi)}{\rho_\phi}. \quad (4.5)$$

Notice that, if the potential energy is much greater than the kinetic energy in absolute value, $V \gg \dot{\phi}^2$, then $w_\phi \approx -1$: a cosmological constant can be realized by a scalar field with negligible kinetic energy.

In scalar field models, the extra degrees of freedom are in the potential $V(\phi)$ and the scalar field initial conditions $\phi(z = z_{\text{ini}})$ and $\dot{\phi}(z = z_{\text{ini}})$ at high enough redshifts, $z_{\text{ini}} \gg z_*$. To solve for the scalar field evolution, the Klein-Gordon equation must be integrated numerically.

4.1.3 Negligible Dark Energy at Early Times

In Λ CDM, dark energy is only relevant to the background energy density at low redshifts $z \leq 2$. In recent literature, Early Dark Energy (EDE) models have gained attention as a candidate solution for the Hubble tension [82]. EDE models assume that dark energy has a significant contribution to the total energy density near recombination. It is common to separate EDE from late-time dark energy, the latter controlling the late-time expansion acceleration. If at $z \approx z_* \approx 1100$, around 10% of the total energy budget of the Universe, the sound horizon r_s would decrease, and the value of H_0 inferred from CMB would increase, relaxing the Hubble tension. This early dark energy contribution must quickly dissipate after

recombination to restore the Λ CDM expansion history at late times.

4.1.4 No Interactions in the Dark Sector

In Λ CDM, dark matter and dark energy only interact through gravity. Dark sector interactions have been first considered to solve the so-called coincidence problem [83]: the fact that current observations imply that dark matter and dark energy currently have energy densities of the same order of magnitude. Assuming the Λ CDM model, dark matter dominated the energy budget in the past, and in the far future dark energy will dominate. Therefore, we are living in a special time, the transition from a matter-dominated era into a dark energy-dominated era. This coincidence could be explained by interactions between dark matter and dark energy. Nowadays, these interactions were revisited in the context of cosmological tensions [84, 85].

4.1.5 Smooth Dark Energy

In Λ CDM, dark energy has no perturbations. Even when assuming phenomenological parametrizations or quintessence, it is common to assume a comoving sound speed of $c_s^2 = 1$, which damps subhorizon dark energy perturbations. Non-canonical scalar fields can have $c_s^2 \approx 0$ [86, 87, 88], which means that dark energy has no pressure support against gravitational collapse and may have appreciable perturbations.

4.1.6 Pressureless Dark Matter

In Λ CDM, dark matter is a pressureless fluid. While this model works, one could assume that dark matter has an equation of state w_{DM} and, using the synchronous gauge fluid equations 2.138 and 2.144, one could assume nonzero sound speed c_s^2 and viscosity c_v^2 , altering structure formation.

4.2 Testing Λ CDM Assumptions

All cosmological models must provide predictions to the observables mentioned in Chapter 3, and through statistical methods which will be described in Chapter 5, these observations provide constraints on the values of cosmological parameters. In Λ CDM, the fundamental parameters are: H_0 , Ω_m , Ω_b , A_s , n_s , and when analyzing CMB, the reionization optical depth τ . One way to challenge the Λ CDM model is using statistical null tests: introducing additional physical assumptions that are parameterized by some parameter p in such a way that, when

$p = 0$, the model reduces to Λ CDM. If data prefers values $p \neq 0$, then the data is inconsistent with the null hypothesis, Λ CDM, at some statistical significance.

I now present in more detail several cosmological models that challenge the assumptions discussed above.

4.2.1 Late-Time Dynamical Dark Energy

Late-time dynamical dark energy is a class of models consisting in time-varying dark energy densities. We can divide them into two subclasses:

- Phenomenological parametrizations: *ad-hoc* parametrizations of either the dark energy density ρ or its equation of state w as a function of redshift or scale factor, targetting specific behaviors;
- Scalar field models: *ad-hoc* parametrizations of the dark energy action as a scalar field ϕ .

Phenomenological Parametrizations

To solve the perturbation equations 2.95a, 2.95b, 2.96a-2.96d, one must find $a(\tau)$ by integrating the Friedmann equation in conformal time, Equation 2.32. To perform this integration, one must know the total energy density ρ as a function of the scale factor a . For radiation, matter, and massive neutrinos, the density as a function of scale factor is known a priori. For the cosmological constant model, the energy density is simply a constant, $\rho_\Lambda = \Omega_\Lambda \rho_{\text{cr}}$. However, one can provide an alternative parametrization of the dark energy density $\rho_{\text{DE}}(a)$, which would also allow for the numerical integration of the Friedmann equation. From $\rho_{\text{DE}}(a)$, one can find the dark energy equation of state $w_{\text{DE}}(a)$ using the continuity equation,

$$\dot{\rho}_{\text{DE}} + 3H(1 + w_{\text{DE}})\rho_{\text{DE}} = 0, \quad (4.6)$$

$$w = -1 - \frac{1}{3} \frac{d \ln \rho_{\text{DE}}}{d \ln a}. \quad (4.7)$$

Alternatively, one can parametrize the dark energy equation of state $w_{\text{DE}}(a)$ as a function of the scale factor a . To obtain $\rho_{\text{DE}}(a)$, one must integrate the continuity equation,

$$\rho_{\text{DE}}(z) = \rho_{\text{cr}} \Omega_{\text{DE}} \exp \left(\int_0^z \frac{1 + w_{\text{DE}}(z')}{1 + z'} dz' \right). \quad (4.8)$$

Due to the Λ CDM success in fitting multiple cosmological datasets, the expansion history must not deviate from Λ CDM much radically. Viable dynamical dark energy models must have $\rho_{\text{DE}}(a = 1)/\rho_{\text{cr}} \approx 0.7$ and $w_{\text{DE}}(a = 1) < -1/3$, a requirement for cosmic acceleration.

If we only consider the expansion of the Universe, nothing prevents dark energy of having $w_{\text{DE}} < -1$, a behavior named **phantom dark energy**. Phantom dark energy cannot be realized by canonical scalar fields, as we will see ahead. Furthermore, the fluid perturbation equations 2.138 and 2.144 are unstable when $w = -1$, and having a negative adiabatic sound speed makes the perturbations unstable. Despite these theoretical issues regarding phantom dark energy, phenomenological models may realize these exotic fluids.

The simplest, most widely used dynamical dark energy model is the $w_0 w_a$ parametrization [89], also known as the Chevallier-Polaski-Linder parametrization, a phenomenological ansatz for the dark energy equation of state as a linear expansion in the scale factor,

$$w(a) = w_0 + w_a(1 - a). \quad (4.9)$$

The parameter w_0 is the current equation of state of dark energy, and w_a is (minus) the current derivative of w with respect to the scale factor. The CPL parametrization is used to probe departures from Λ CDM: any indication of $w_0 \neq -1$ or $w_a \neq 0$ would put the cosmological constant model in check.

Other examples of phenomenological parametrizations are: the generalized emergent dark energy [90], parametrized by

$$\rho_{\text{DE}} = \rho_{\text{DE},0} \frac{1 - \tanh\left(\Delta \times \log\left(\frac{1+z}{1+z_t}\right)\right)}{1 + \tanh\left(\Delta \times \log\left(\frac{1+z}{1+z_t}\right)\right)}, \quad (4.10)$$

the Barboza-Alcaniz parametrization [91], given by

$$w(z) = w_0 + w_1 \frac{z(1+z)}{1+z^2}, \quad (4.11)$$

oscillating parametrizations [92], such as

$$w(a) = w_0 + A \sin(B \ln a + C), \quad (4.12)$$

a transition parametrization [93],

$$w(z) = w_0 + \frac{w_1 - w_0}{2} \left(1 + \tanh\left(\frac{z - z_c}{\sigma}\right) \right), \quad (4.13)$$

a general binned parametrization [93] of the form

$$w(z) = \begin{cases} w_0, & \text{if } z < z_1, \\ w_1, & \text{if } z_1 < z < z_2, \\ w_2, & \text{if } z_2 < z < z_3, \\ \dots & \\ w_{N-1}, & \text{if } z_{N-1} < z < z_N, \\ w_N, & \text{if } z > z_N. \end{cases} \quad (4.14)$$

among many others. These parametrizations are phenomenological: they are only *ansatze* made to target specific dark energy behaviors.

To model the dark energy perturbations, we can employ the synchronous gauge fluid equations 2.138 and 2.144. These equations, however, cannot be integrated if the equation of state crosses $w_{\text{DE}} = -1$ at some point. The Parametrized Post-Friedmann framework is an approach to dark energy perturbations that is stable even when the equation of state crosses $w_{\text{DE}} = -1$ [94].

Quintessence

Quintessence models use a scalar field to describe late-time ($z < 3$) dark energy and the Universe's expansion acceleration. The action of a scalar field ϕ is given by Equation 4.3. The term $X = -\partial_\mu \phi \partial^\mu \phi / 2$ is the kinetic energy of the field. Assuming homogeneity, the kinetic term evaluates to

$$X = -\frac{1}{2} \partial_0 \phi \partial^0 \phi = -\frac{1}{2} g^{00} \dot{\phi}^2 = \frac{\dot{\phi}^2}{2}. \quad (4.15)$$

The field potential $V(\phi)$ determines the evolution of the scalar field. By using the Euler-Lagrange equations, we obtain the classical equation of motion for the field ϕ in the FLRW spacetime (a derivation is shown in Appendix A.4),

$$\ddot{\phi} + 3H\dot{\phi} + V'(\phi) = 0. \quad (4.16)$$

Equation 4.16 is the **Klein-Gordon equation** for a homogeneous scalar field in the FLRW spacetime. The energy-momentum tensor of the scalar field is given by

$$T^{\mu\nu} = \frac{2}{\sqrt{-g}} \frac{\delta \mathcal{L}}{\delta g_{\mu\nu}} = \frac{2}{a^3} \left(\sqrt{-g} \frac{\delta(X - V)}{\delta g_{\mu\nu}} + (X - V) \frac{\delta \sqrt{-g}}{\delta g_{\mu\nu}} \right). \quad (4.17)$$

Since $X = -g_{\mu\nu}\partial^\mu\phi\partial^\nu\phi/2$, then

$$\frac{\delta(X - V)}{\delta g_{\mu\nu}} = -\frac{1}{2}\partial^\mu\phi\partial^\nu\phi. \quad (4.18)$$

The variation of the metric determinant is given by

$$\frac{\delta\sqrt{-g}}{\delta g_{\mu\nu}} = \frac{1}{2}\sqrt{-g}g^{\mu\nu}. \quad (4.19)$$

Therefore, the energy-momentum tensor is

$$T^{\mu\nu} = \frac{2}{a^3} \left(-\frac{a^3}{2}\partial^\mu\phi\partial^\nu\phi + \frac{1}{2}a^3(X - V)g^{\mu\nu} \right) = -\partial^\mu\phi\partial^\nu\phi + g^{\mu\nu}(X - V). \quad (4.20)$$

Its energy density is given by

$$T_{00} = -\rho = -\dot{\phi}^2 + \left(\frac{\dot{\phi}^2}{2} - V \right) = -\frac{\dot{\phi}^2}{2} - V(\phi). \quad (4.21)$$

Its pressure is given by

$$T_{ii} = P = X - V = \frac{\dot{\phi}^2}{2} - V(\phi). \quad (4.22)$$

Therefore, the quintessence equation of state is given by

$$w_\phi = \frac{\dot{\phi}^2 - 2V(\phi)}{\dot{\phi}^2 + 2V(\phi)}. \quad (4.23)$$

In the limit where the kinetic energy is much greater than the potential energy, $w_\phi \approx 1$; conversely, if the potential energy is much greater than the kinetic energy, then $w_\phi \approx -1$. Since the kinetic energy X is positive, the quintessence equation of state is always $1 \geq w_\phi \geq -1$.

To solve the Friedmann equation, one must know the quintessence energy density as a function of scale factor. This can be achieved by integrating the Klein-Gordon equation in terms of the scale factor a as

$$\frac{d}{dt} = aH \frac{d}{da}, \quad (4.24)$$

$$\frac{d\phi}{da} = \frac{\dot{\phi}}{aH}, \quad (4.25)$$

$$\frac{d\dot{\phi}}{da} = -3\frac{\dot{\phi}}{a} - \frac{V'(\phi)}{aH}. \quad (4.26)$$

This system must be integrated from a high redshift before recombination, $z_i \approx 10^6$. The initial conditions for the scalar field, $\phi(a_i)$ and $\dot{\phi}(a_i)$, are free parameters of the quintessence model.

The Klein-Gordon equation 4.16 is analogous to the Newtonian equation of motion for a particle with position $x(t)$ subject to a potential $V(x)$ and a time-dependent dissipating force $F_d = b(t)\dot{x}$, related to the term $3H\dot{\phi}$: the **Hubble friction**. In the initial conditions, the Hubble friction term is usually much greater than the potential term $V'(\phi)$, and the field remains in a regime called **slow roll**, where the kinetic energy is greatly suppressed. For this reason, it is common to assume $\dot{\phi}(a_i) = 0$.

Given an arbitrary choice of $V(\phi)$ and initial conditions, it is not guaranteed that the scalar field will obey the energy density condition

$$\rho_\phi(a = 1) = \rho_{cr}(1 - \Omega_m - \Omega_r). \quad (4.27)$$

Since $\rho_\phi(a = 1)$ is a function of the potential parameters and initial conditions, it is common to choose one of the available parameters to perform numerical root-finding algorithms, finding the value of the parameter that satisfies the energy density condition.

The scalar field potential determines the evolution of the scalar field and its dynamical properties. Depending on the potential, scalar fields can model dark matter, dark energy, dark radiation, or other behaviors. Usual potential functions that can model late-time cosmic acceleration are exponentials and power laws,

$$V(\phi) = V_0 e^{\beta\phi}, \quad (4.28)$$

$$V(\phi) = V_0 \left(\frac{\phi}{\phi_r} \right)^\alpha. \quad (4.29)$$

Depending on the choice of the potential function, quintessence may exhibit a **tracking behavior** [95], when the scalar field evolution is largely insensitive to the initial conditions.

The quintessence dynamics is usually classified into two types depending on their behavior after the slow roll phase ends:

- Thawing behavior: when $w_\phi \approx -1$ in the past, and the field eventually becomes dynamic with $w_\phi > -1$. Power law potentials with $\alpha > 0$ fall into this category.
- Freezing behavior: when $w_\phi > -1$ in the past, but asymptotically approaches $w_\phi = -1$. Exponential and inverse power law potentials fall into this category.

We may also introduce position-dependent perturbations in the scalar field,

$$\phi = \bar{\phi}(t) + \delta\phi(\mathbf{r}, t). \quad (4.30)$$

For conciseness, the bar will be omitted from the homogeneous term. Assuming an arbitrary gauge (i.e. the metric is given by Equation 2.93), the perturbed Klein-Gordon equation in Fourier space becomes [29]

$$\delta\phi'' + 2\mathcal{H}\delta\phi' + (k^2 + a^2V''(\phi))\delta\phi = -2a^2V'(\phi)A + \phi'(A' + 3H'_L - kB + H'_T). \quad (4.31)$$

The quintessence perturbed energy-momentum components are

$$\delta\rho_\phi = \frac{1}{a^2}(\phi'\delta\phi' - \phi'^2(3H'_L - H'_T)) + V'(\phi)\delta\phi, \quad (4.32)$$

$$\delta P_\phi = \frac{1}{a^2}(\phi'\delta\phi' - \phi'^2(3H'_L - H'_T)) - V'(\phi)\delta\phi, \quad (4.33)$$

$$(\rho_\phi + P_\phi)v_\phi = \frac{1}{a^2}k\phi'\delta\phi, \quad (4.34)$$

$$\Pi_\phi = 0. \quad (4.35)$$

K-Essence

Even though quintessence can have many different behaviors, its equation of state is restricted to the interval $w_\phi \in [-1, 1]$. One may construct a different scalar field action from the field ϕ and the kinetic term X ,

$$S_\phi = \int d^4x \sqrt{-g}P(X, \phi), \quad (4.36)$$

where $P(X, \phi)$ is an analytic function of both variables. For quintessence, $P(X, \phi) = X - V(\phi)$. Scalar fields with non-canonical lagrangians are called **k-essence**. One of the simplest non-canonical scalar fields is the **phantom scalar field**, whose action is given by

$$P(X, \phi) = -X - V(\phi). \quad (4.37)$$

This phantom scalar field is interesting for having an equation of state possibly below -1 . The **quintom** models [96] are characterized by two scalar fields: one phantom and one quintessence. The effective equation of state of both fields can cross $w_{\text{eff}} = -1$ even if the individual equations of state cannot.

The kinetically-driven scalar field [86] models impose a second-order Taylor expansion of P in X . By suitable field redefinitions, the function P becomes

$$P(X, \phi) = V(\phi)(-X + X^2). \quad (4.38)$$

For general $P(X, \phi)$, the energy density and equation of state of the field are given by

$$\rho_K = 2X \frac{\partial P}{\partial X} - P, \quad (4.39a)$$

$$w_K = \frac{P(X, \phi)}{\rho_K}. \quad (4.39b)$$

Finally, to find the field evolution in time, one must solve a generalized form of the Klein-Gordon equation,

$$\left(\frac{\partial P}{\partial X} + \phi^2 \frac{\partial^2 P}{\partial X^2} \right) \ddot{\phi} + 3H \frac{\partial P}{\partial X} \dot{\phi} + \frac{\partial^2 P}{\partial X \partial \phi} \dot{\phi}^2 - \frac{\partial P}{\partial \phi} = 0. \quad (4.40)$$

Non-canonical scalar field perturbations are characterized by its effective sound speed

$$c_s^2 = \frac{\delta P}{\delta \rho} = \frac{\frac{\partial P}{\partial X}}{\frac{\partial P}{\partial X} + 2X \frac{\partial^2 P}{\partial X^2}}. \quad (4.41)$$

If $c_s^2 < 0$, perturbations are unstable and grow exponentially [96, 97].

4.2.2 Early Dark Energy

Early Dark Energy (EDE) models postulate a past epoch in which a dark energy component had significant energy density,

$$\frac{\rho_{\text{EDE}}}{\rho_{\text{tot}}} \approx 10\%. \quad (4.42)$$

While this hypothesis can be applied at any point in the cosmological history, recent studies show that an EDE component right before recombination, at $z \approx 3000$, can solve the Hubble tension [82].

CMB can measure the sound horizon angular scale at recombination, given by

$$\theta_* = \frac{r_s(z_*)}{D_A(z_*)} = \frac{\int_{z_*}^{\infty} \frac{c_s(z) dz}{H(z)}}{\int_0^{z_*} \frac{dz}{H(z)}}. \quad (4.43)$$

If we add another fluid with significant contribution to the total energy density just before recombination, the sound horizon decreases, as $H \sqrt{\rho}$. To keep θ_* fixed, the angular distance to the last scattering surface $D_A(z_*)$ must also decrease by increasing the value of H_0 .

The general recipe for early dark energy is to have a fast transition in the EDE

equation of state between two values,

$$w_{\text{EDE}} = \begin{cases} -1, & \text{if } z \gg z_c, \\ w_n > 0, & \text{if } z \ll z_c, \end{cases} \quad (4.44)$$

Since EDE is constant before z_c , its relative contribution to the total energy density increases, because matter and radiation energy densities are decreasing. After z_c , if $w_n > 1/3$, then the EDE density decays faster than radiation, and EDE quickly becomes negligible. The EDE model was created to change the expansion rate near recombination without spoiling the good fit to late-time observables such as BAO and Supernovae distances. The general idea of EDE can be realized in several ways described in the following.

Fluid EDE

A first model for EDE is a fluid whose energy density is given by [98]

$$\rho_{\text{EDE}}(a) = \frac{2\rho_{\text{EDE}}(a_c)}{1 + \left(\frac{a}{a_c}\right)^{3(1+w_n)}}. \quad (4.45)$$

Using the continuity equation, its equation of state is given by

$$w_{\text{EDE}}(a) = \frac{1 + w_n}{1 + \left(\frac{a}{a_c}\right)^{3(1+w_n)}} - 1. \quad (4.46)$$

Its perturbations are given by the fluid equations in synchronous gauge, Equations 2.138 and 2.138. Therefore, the model has four parameters: $\rho_{\text{EDE}}(a_c)$, a_c , w_n and a fourth parameter Θ_i which controls the effective sound speed [98]. The two former parameters can be redefined as

$$z_c = \frac{1}{a_c} - 1, f_{\text{EDE}}(z_c) = \frac{\rho_{\text{EDE}}(z_c)}{\rho_{\text{tot}}(z_c)}. \quad (4.47)$$

Axion-like EDE

This is a canonical scalar field model inspired by axion potentials arising from string theory [99]. The potential is given by

$$V(\phi) = m^2 f^2 \left[1 - \cos\left(\frac{\phi}{f}\right) \right]^n. \quad (4.48)$$

At early times, the Hubble friction dominates and $w_\phi \approx -1$. As the Universe expands, the Hubble friction decreases and the field starts oscillating around the potential minimum with an average equation of state

$$\langle w_\phi \rangle = \frac{n-1}{n+1}. \quad (4.49)$$

For $n > 1$, the scalar field energy density decays faster than matter.

In practice, one would like to control the parameters z_c and $f_{\text{EDE}}(z_c)$ instead of the potential parameters m and f . Implementations of scalar field EDE models perform a two-dimensional **shooting** to map given z_c and $f_{\text{EDE}}(z_c)$ into potential parameters m and f .

Rock 'n' Roll EDE

For values $\phi \ll f$, the axion-like potential in Equation 4.48 can be expanded as

$$V(\phi) = V_0 \left(\frac{\phi}{1M_{\text{Pl}}} \right)^{2n}. \quad (4.50)$$

This simple power law is the so-called Rock 'n' Roll EDE model [100]. It exhibits the same behavior as the axion-like EDE model, but with one less parameter. In this case, the parameter V_0 and the initial field value ϕ_i are adjusted to give the desired z_c and $f_{\text{EDE}}(z_c)$.

4.2.3 Modified Gravity

Modified gravity theories generalize the Einstein-Hilbert action introducing new terms. For instance, $f(R)$ theories use a generalized action of the form

$$S = \int d^4x \sqrt{-g} \left[\frac{M_{\text{Pl}}^2 (R + f(R))}{2} \right]. \quad (4.51)$$

Among $f(R)$ theories, an interesting example is the Starobinsky model [19] given by

$$f(R) = \frac{R^2}{6M^2}, \quad (4.52)$$

where M is a constant controlling the deviation from General Relativity. Another $f(R)$ gravity model is the Hu-Sawicki model [101], which evades Solar system

constraints on modified gravity, given by

$$f(R) = -m^2 \frac{c_1(R/m^2)^n}{c_2(R/m^2)^n + 1}. \quad (4.53)$$

In 1974, Gregory Horndeski developed a very general gravitational theory described by the metric tensor $g_{\mu\nu}$ and a scalar field ϕ , assuming only second-order equations of motion [102]. The Horndeski action is given by

$$S = \int d^4x \sqrt{-g} \left[\sum_{i=2}^5 M_{\text{Pl}}^2 \mathcal{L}_i \right], \quad (4.54)$$

where we have five different terms

$$\mathcal{L}_2 = G_2(\phi, X), \quad (4.55)$$

$$\mathcal{L}_3 = G_3(\phi, X) g^{\mu\nu} \nabla_\mu \nabla_\nu \phi, \quad (4.56)$$

$$\mathcal{L}_4 = G_4(\phi, X) R + \frac{\partial G_4(\phi, X)}{\partial X} \left[(\nabla^\mu \nabla_\mu \phi)^2 + \nabla_\mu \nabla_\nu \phi \nabla^\mu \nabla^\nu \phi \right], \quad (4.57)$$

$$\mathcal{L}_5 = G_5(\phi, X) G^{\mu\nu} \nabla_\mu \nabla_\nu \phi - \frac{1}{6} \frac{\partial G_5(\phi, X)}{\partial X} \left[(\nabla^\mu \nabla_\mu \phi)^3 + 2 \nabla_\mu \nabla^\nu \phi \nabla_\nu \nabla^\alpha \phi \nabla_\alpha \nabla^\mu \phi - 3 \nabla_\mu \nabla_\nu \phi \nabla^\mu \nabla^\nu \phi \nabla^\alpha \nabla_\alpha \phi \right], \quad (4.58)$$

where R is the Ricci scalar and $X = -\partial_\mu \phi \partial^\mu \phi / 2$ is the kinetic term of the scalar field. In Horndeski theory, we need to specify four functions G_i of two arguments: the scalar field ϕ and the scalar field kinetic term X . Horndeski theory is a very general framework, encompassing many modified gravity models, such as Brans-Dicke gravity [103], and scalar-tensor models, such as quintessence and k-essence.

Finally, one can also introduce phenomenological modifications of gravity, such as the $\mu - \Sigma$ model [104]. Assuming negligible anisotropic stress, the Newtonian gauge metric equations are

$$k^2 \Phi = -4\pi G a^2 \delta\rho_c, \quad (4.59)$$

$$k^2 (\Phi - \Psi) = -8\pi G a^2 \delta\rho_c, \quad (4.60)$$

$$(4.61)$$

where $\delta\rho_c = \delta\rho + 3\mathcal{H}(\rho + P)v/k$ is the comoving gauge density perturbation. The

$\mu - \Sigma$ parametrization modifies these equations as

$$k^2\Phi = -4\pi Ga^2\mu(k, a)\delta\rho_c, \quad (4.62)$$

$$k^2(\Phi - \Psi) = -8\pi Ga^2\Sigma(k, a)\delta\rho_c. \quad (4.63)$$

$$(4.64)$$

Since μ and Σ are free functions of both scale factor and k , parametrizations of these functions are often assumed.

4.2.4 Dark Sector Interactions

The energy-momentum conservation equations imply

$$\nabla_\mu T^{\mu\nu} = 0 \implies \dot{\rho} + 3H(1+w)\rho = 0, \quad \text{for all non-interacting fluids.} \quad (4.65)$$

The conservation equation is a statement that the energy and momentum of the fluid are conserved. However, when there are interactions among two fluids, each fluid's energy and momentum are not individually conserved anymore due to exchanges among them. Their joint energy and momentum are still conserved. In the case of interacting dark matter and dark energy, we have

$$\nabla_\mu (T_{\text{CDM}}^{\mu\nu} + T_{\text{DE}}^{\mu\nu}) = 0 \implies \nabla_\mu T_{\text{CDM}}^{\mu\nu} = -\nabla_\mu T_{\text{DE}}^{\mu\nu} = Q^\nu, \quad (4.66)$$

where we defined Q^ν as the energy-momentum flux between DE and CDM. With this definition, a positive Q^ν implies a transfer of energy and momentum from DE to CDM.

From a field theoretical standpoint, Q^ν is a function of the interacting fields. Its form can be calculated at action level by introducing an interaction term in the Lagrangian. Suppose that DE is modelled by a real scalar field ϕ and CDM by a fermionic field ψ . A Yukawa interaction between them is modeled with the following lagrangian

$$\mathcal{L} = \sqrt{-g} \left\{ \frac{1}{2} \nabla_\mu \phi \nabla^\mu \phi - V(\phi) + \bar{\psi}(\not{\partial} - m)\psi + \alpha \phi \bar{\psi} \psi \right\}, \quad (4.67)$$

where m is the dark matter rest mass, $\not{\partial} = i\gamma^\mu \partial_\mu$, γ^μ are the Dirac matrices and α is a coupling constant. This Lagrangian which can be rewritten as

$$\mathcal{L} = \frac{1}{2} \nabla_\mu \phi \nabla^\mu \phi - V(\phi) + \bar{\psi}(\not{\partial} - m(\phi))\psi, \quad (4.68)$$

where $m(\phi) = m - \alpha\phi$. This interaction can be generalized by letting $m(\phi)$ be any

function of ϕ . Another example would be one of a quartic interaction among two scalar fields ϕ and χ , representing dark energy and dark matter, respectively. An example of such lagrangian is [105]

$$\mathcal{L} = \sqrt{-g} \left\{ -\frac{1}{2}\partial\phi^2 - \frac{1}{2}\partial\chi^2 - V(\phi, \chi) \right\}, \quad (4.69)$$

with

$$V(\phi, \chi) = \frac{\lambda}{4}(M^2 - \chi^2)^2 + \frac{1}{2}g^2\phi^2\chi^2 + \frac{1}{2}\mu^2\phi^2, \quad (4.70)$$

where M is the symmetry-broken dark matter mass, μ is the dark energy mass, λ and g are coupling constants. We can obtain the explicit form of Q^ν by defining the individual energy-momentum tensor of any species and verifying the absence of conservation.

However, dark matter and dark energy are usually not modeled as fields, instead, they are commonly modeled as fluids. One approach to interacting dark matter and dark energy models is to propose phenomenological parametrizations of Q^ν as a function of the fluid variables $\rho, w, \delta\rho, \delta P, v^i, \Pi^{ij}$ and the cosmological expansion rate H . Assuming CDM as a pressureless fluid, DE as a fluid with constant w , one example of interaction parametrization is

$$Q^\nu = \xi H \rho_{\text{DE}} u_{\text{CDM}}^\nu, \quad (4.71)$$

where u_{CDM}^ν is the CDM bulk 4-velocity and ξ is a coupling constant. This interaction is one particular choice of a more general prescription $Q^\nu = \xi_{XY} H \rho_X u_Y^\nu$, where X and Y can be either DE or CDM. This particular choice avoids early-time instabilities and previous studies have shown this model can help alleviate the Hubble tension [85, 22]. A positive constant ξ would indicate energy transfer from DE to CDM and vice-versa.

At the background level, the Einstein equations are not altered by the interactions: the only fluid quantities involved in the Friedmann equation are their densities. However, the evolution of those densities will be affected by the interaction, and the continuity equation will change according to equation 4.66. The CDM velocity components are $u^\nu = (1, 0, 0, 0)$. Thus, we get the following conservation equations

$$\dot{\rho}_c + 3\mathcal{H}\rho_c = \xi\mathcal{H}\rho_x, \quad (4.72)$$

$$\dot{\rho}_x + 3\mathcal{H}(1+w)\rho_x = -\xi\mathcal{H}\rho_x. \quad (4.73)$$

The DE equation can be readily integrated,

$$\dot{\rho}_x + 3\mathcal{H} \left(1 + w + \frac{\xi}{3} \right) \rho_x \implies \rho_x = \rho_{x,0} a^{-3 \left(1 + w + \frac{\xi}{3} \right)}. \quad (4.74)$$

Notice that this would be equivalent if DE was non-interacting with $w = w_{\text{eff}} = w + \xi/3$. We can now substitute and solve for the CDM density

$$\dot{\rho}_c + 3\mathcal{H}\rho_c = \xi\mathcal{H}\rho_{x,0}a^{-3(1+w_{\text{eff}})} \quad (4.75)$$

First, we change the derivative from τ to a ,

$$\begin{aligned} \frac{d\rho_c}{da}\dot{a} + 3\mathcal{H}\rho_c &= \xi\mathcal{H}\rho_{x,0}a^{-3(1+w_{\text{eff}})} \\ \frac{d\rho_c}{da} + 3\frac{\rho_c}{a} &= \xi\rho_{x,0}a^{-1-3(1+w_{\text{eff}})}. \end{aligned}$$

Second, to help the integration, we define $\tilde{\rho}_c = \rho_c a^3$. A simple chain rule can show that

$$\frac{d\rho_c}{da} + 3\frac{\rho_c}{a} = \frac{1}{a^3} \frac{d\tilde{\rho}_c}{da}. \quad (4.76)$$

Inserting into the continuity equation, we get

$$\begin{aligned} \frac{1}{a^3} \frac{d\tilde{\rho}_c}{da} &= \xi\rho_{x,0}a^{-1-3(1+w_{\text{eff}})} \\ \frac{d\tilde{\rho}_c}{da} &= \xi\rho_{x,0}a^{2-3(1+w_{\text{eff}})} \end{aligned}$$

and this can be readily integrated,

$$\begin{aligned} \tilde{\rho}_c &= -\frac{\xi\rho_{x,0}}{3w_{\text{eff}}}a^{-3w_{\text{eff}}} + C \\ \rho_c &= -\frac{\xi\rho_{x,0}}{3w_{\text{eff}}}a^{-3}a^{-3w_{\text{eff}}} + Ca^{-3}. \end{aligned}$$

The constant can be related to the CDM energy density today,

$$\begin{aligned} a = 1 : \quad \rho_{c,0} &= -\frac{\xi\rho_{x,0}}{3w_{\text{eff}}} + C \\ C &= \rho_{c,0} + \frac{\xi\rho_{x,0}}{3w_{\text{eff}}}, \end{aligned}$$

and we can finally write the CDM energy density as a function of a , after rearranging terms,

$$\rho_c = \rho_{c,0}a^{-3} + \frac{\xi\rho_{x,0}}{3w_{\text{eff}}}a^{-3} \left(1 - a^{-3w_{\text{eff}}}\right). \quad (4.77)$$

Within this parametrization, the perturbation equations are

$$\delta'_x = -(1 + w_x) \left(\theta_x + \frac{h'}{2} \right) - 3\mathcal{H}(c_s^2 - c_a^2) \left[\delta_x + \mathcal{H}[3(1 + w_x) + \xi] \frac{\theta_x}{k^2} \right], \quad (4.78)$$

$$v'_x = 2\mathcal{H} \left(1 + \frac{\xi}{1 + w_x} \right) v_x - \mathcal{H}\xi \frac{v_c}{1 + w_x} + k \frac{\delta_x}{1 + w_x}, \quad (4.79)$$

$$\delta'_c = +\xi \mathcal{H} \frac{\rho_x}{\rho_c} (\delta_x - \delta_c) - \rho_c \left(k v_c + \frac{h'}{2} \right), \quad (4.80)$$

$$v'_c = -\mathcal{H} v_c. \quad (4.81)$$

Out of all the models presented in this Chapter, only a few have been analyzed during my PhD. An analysis of early dark energy models is presented in Chapter 6, and late-time dynamical dark energy, including phenomenological parametrizations and an oscillating k-essence model, are analyzed in Chapter 7. Additionally, I am conducting an analysis of interacting dark energy models within the DES collaboration, to be published in the next months.

Chapter 5

Cosmological Data Analysis

This chapter explains the methods employed to analyze data and extract information about the cosmological model. I will present concepts from Bayesian statistics, explain how observational data is modelled and how to infer cosmological model parameters from data. In the end, I explain the computational structure necessary for performing such analysis and the costs involved.

5.1 The Bayesian Interpretation of Probability

Probability is a fundamental mathematical concept, useful for modelling stochastic processes such as a coin toss or quantum measurements. The field of statistics relies heavily on probability to describe properties of populations and data. Probability can be defined by the **frequentist** point of view. Consider a repeatable experiment with outcomes $x \in X$. After repeating the experiment N times, each outcome x will have a frequency $f_N(x)$. The probability of x is defined as:

$$p(x) = \lim_{N \rightarrow \infty} \frac{f_N(x)}{N}. \quad (5.1)$$

However, there are questions such as "what is the probability that a given candidate wins the presidential elections?" in which frequentist probability cannot be used, as the experiment in question is not repeatable. **Bayesian statistics** is a branch of statistics with another interpretation of probability, but still based on the same mathematical tools. The Bayesian perspective can be stated as follows: given a random variable X with possible outcomes x , the probability of a given outcome, $p(x)$, is the degree of confidence in that outcome. This degree of confidence assumes perfect knowledge and impartiality of whoever is attributing the probability. As we will see later, the confidence in a certain outcome is affected by experiments and by prior knowledge. Bayesian probability is a more general concept than frequentist probability, since more quantities can be interpreted as random variables even if the experiments are not repeatable. Bayesian probability is widely used in science, as one can calculate the probability of model parameters given experimental data, obtaining constraints on the model parameters starting from zero prior knowledge.

In the Bayesian interpretation, every quantity that can have uncertainties is

modelled as a random variable. The measurement of some observable (i.e. the data) is a random variable, because there are uncertainties related to the measurement process; the underlying model $\mathcal{M}$ used to describe the measurements is also a random variable, usually fixed throughout the analysis, since we don't know the exact model; within a model, model parameters θ are random variables. In the context of cosmology, we can think of measurements of observables described in Chapter 3, models such as Λ CDM and those described in Chapter 4, and model parameters include standard cosmological parameters H_0 , Ω_m , Ω_b , A_s , n_s , τ and other parameters describing more complex behavior.

5.2 The Bayes' Theorem: likelihood, prior and posterior distributions

In the context of data analysis, where some data is observed and a theoretical model $\mathcal{M}$ with parameters θ is assumed to describe the data, we can specialize Bayes' theorem as

$$p(\theta|\text{data}, \mathcal{M}) = \frac{p(\text{data}|\theta, \mathcal{M})p(\theta|\mathcal{M})}{p(\text{data}|\mathcal{M})}. \quad (5.2)$$

In Bayesian statistics, we interpret each term as:

- $p(\theta|\text{data}, \mathcal{M})$ is the **posterior distribution**, the confidence we have on model parameters after taking the data into account;
- $p(\theta|\mathcal{M})$ is the **prior distribution**, the amount of confidence we have on model parameters before taking the data into account;
- $p(\text{data}|\theta, \mathcal{M})$ is the **likelihood**, also denoted as $\mathcal{L}$, which assumes the model and the parameters as true and quantify how likely it is to measure the observed data under that model;
- $p(\text{data}|\mathcal{M})$ is the **Bayesian evidence** of the model.

The prior distribution is usually very large, a reflex of our complete uncertainty about the model parameters before data is taken into account. The Bayesian interpretation of 5.2 is that using the likelihood function, we can update our prior distribution, obtaining a posterior distribution that is much more constrained than the prior. In Bayesian statistics, **observations serve to update our prior beliefs**. The goal of a cosmological analysis is to obtain the posterior distribution of the cosmological parameters H_0 , Ω_m , Ω_b , A_s , n_s , τ , Ω_k , among others, from multiple probes described in Chapter 3.

A fundamental ingredient in this process is the likelihood: a function that incorporates all measurement uncertainties and systematic errors that affect the observations. Each cosmological probe must take into account different systematic effects in the likelihood. In general, an experiment measures quantities that can be put together in a column vector $\mathbf{d}$, the data vector. Given a model $\mathcal{M}$ and its parameters θ , we obtain a theoretical prediction for the measured quantities, which we also put together in a column vector $\mathbf{d}^{\text{th}}(\theta)$. The likelihood usually depends on how different the theoretical predictions are from the actual measured observables, $\mathbf{d} - \mathbf{d}^{\text{th}}(\theta)$. A gaussian form for the likelihood is usually assumed,

$$\mathcal{L} = \frac{1}{\sqrt{2\pi \det(C)}} \exp \left(-\frac{1}{2} (\mathbf{d} - \mathbf{d}^{\text{th}}(\theta))^T \cdot C^{-1} \cdot (\mathbf{d} - \mathbf{d}^{\text{th}}(\theta)) \right), \quad (5.3)$$

where $\cdot$ denotes matrix multiplication, T denotes matrix transposition and C is the data covariance matrix, which encodes all systematic and theoretical uncertainties in the analysis. Each different survey estimates uncertainties in a different way, and each covariance matrix is unique; the form of likelihood, Equation 5.3, remains the same. It's common for collaborations to publish their data vectors and covariance matrices, as well as other important data, so independent science groups can implement the likelihood and perform different analyses.

One example of simple covariance is that of the 1998 High- z Supernovae Search Team analysis [17]. Their data vector consisted of distance moduli, a proxy of the luminosity distance given by $\mu = 5 \log(d_L / 1\text{Mpc}) + 25$, of Type Ia supernovae as a function of their redshifts. They assume that each supernova is measured independently, so the data points are independently distributed, and the covariance matrix is diagonal. The diagonal elements of the covariance represent the variance in the estimation of the data vector elements. They directly measure the distance moduli with errors σ_i at each measurement, whose values are listed in the article. Another contribution to the uncertainty comes from the velocity dispersion of the galaxy, which affects the redshift measurement of the galaxy; assuming a velocity dispersion of $\Delta v = 200\text{km/s}$, they compute the uncertainty in distance moduli due to the redshift uncertainty, which can be approximated by

$$\sigma_v = \frac{5}{\ln(10)} \frac{\Delta v}{cz}. \quad (5.4)$$

Summing the contributions from measurement errors and velocity dispersion uncertainty, their covariance is given by

$$C = \text{diag}(\sigma_i + \sigma_{v,i}). \quad (5.5)$$

Other datasets may have more complicated covariance matrices. This is the case of the 3x2-point analysis of galaxy surveys, where the covariance matrices are

not diagonal and include a myriad of statistical uncertainty sources, for instance: cosmic variance is the intrinsic stochasticity of the matter fields, shot noise or Poisson noise comes from the finite sample of galaxies, super-sample covariance is the error due to fluctuations in long-wavelength modes bigger than the survey footprint, among other sources [52].

5.3 Markov Chain Monte Carlo and the Metropolis-Hastings algorithm

In possession of a likelihood $\mathcal{L}$, one wants to assess in region of the model parameter space the posterior distribution is concentrated, unknown a priori. One way to do this is to make a rectangular grid in the parameter space, covering each dimension with N points, calculating the posterior at each grid point and finding those points with higher posterior. The total amount of sampled points is N^D , where D is the dimension of the parameter space. Rectangular grid sampling scales exponentially with the dimension of the space. Unfortunately, the cosmological parameter space is already large: with three parameters controlling the background H_0, Ω_m, Ω_b , two controlling the perturbation power spectra A_s, n_s , one controlling the optical depth to reionization τ , the Λ CDM model has six parameters. In addition, each survey treats systematic effects with nuisance parameters, increasing the parameter space dimensionality drastically. This makes grid sampling - or other methods like random sampling - unpractical for cosmological analyses.

This impracticality has to do with the fact that, out of the N^D rectangular grid samples, only a very small amount of them will have appreciable posterior value. For high-dimensional parameter spaces, the posterior distribution is concentrated in a very small volume. Sampling would be optimized if the sampled points would be spread where the posterior is concentrated, neglecting other regions. This is the idea behind the Metropolis-Hastings algorithm, a central tool of cosmological analyses.

Out of the full posterior distribution, we are interested in statistical properties such as the posterior average for a model parameter θ_i

$$\bar{\theta}_i = \int d^D \theta p(\theta | \text{data}, \mathcal{M}) \theta_i, \quad (5.6)$$

where the integral is performed over the full parameter space. If we have a sample of points in the parameter space $\{\theta_n\}_{n=1}^N$ drawn from the posterior distribution

$p(\boldsymbol{\theta}|\text{data}, \mathcal{M})$, we could approximate $\bar{\theta}_i$ by

$$\bar{\theta}_i \approx \frac{1}{N} \sum_{n=1}^N (\theta_n)_i. \quad (5.7)$$

In general, in order to extract statistical properties of the posterior distribution, one needs samples of points drawn from that distribution. Unfortunately, we don't know the explicit form of $p(\boldsymbol{\theta}|\text{data}, \mathcal{M})$ as a function of the model parameters.

The Metropolis-Hastings algorithm draws points from a distribution whose explicit form is unknown, such as the posterior. The algorithm goes as follows:

- Step 1: Start from a random point $\boldsymbol{\theta}_{\text{curr}}$, the current point, drawn from the prior distribution. Calculate the posterior of this point using Bayes' theorem.
- Step 2: Consider a proposal distribution $p(\Delta\boldsymbol{\theta})$, which can be uniform or gaussian, whose only requirement is to be centered at zero and have a significantly smaller width than the prior distribution $p(\boldsymbol{\theta}|\mathcal{M})$.
- Step 3: Draw a step $\Delta\boldsymbol{\theta}$ from the proposal distribution. Use it to go to a new point in the parameter space, $\boldsymbol{\theta}_{\text{new}} = \boldsymbol{\theta}_{\text{curr}} + \Delta\boldsymbol{\theta}$.
- Step 4: Calculate the posterior at the new point.
- Step 5: Take the ratio of posteriors between the new and current points, $r = p(\boldsymbol{\theta}_{\text{new}}|\text{data}, \mathcal{M}) / p(\boldsymbol{\theta}_{\text{curr}}|\text{data}, \mathcal{M})$.
- Step 6: If $r > 1$, include the new point in the sample and go to Step 3, now considering the new point as the current point.
- Step 7: If $r < 1$, draw a number s from an uniform distribution $\mathcal{U}[0, 1]$.
- Step 8: If $s > r$, discard the new point and go to Step 3.
- Step 9: If $s < r$, include the new point in the sample and go to Step 3, now considering the new point as the current point.

It can be shown that, as the number of samples approaches infinity, the samples follow the posterior distribution. Notice that it's more likely to draw samples that have a higher posterior value, and thus this sampling process does not explore regions of the parameter space with negligible posterior. The Metropolis-Hastings algorithm is an example of a Markov Chain Monte Carlo (MCMC) method, a way of sampling points where the probability of the next point being drawn only depends on the current point. The algorithm is implemented for cosmological purposes in the programs `Cobaya` [106], `CosmoMC` [107] and `CosmoSIS` [108], and it's widely used in most cosmological data analyses.

5.3.1 The Gelman-Rubin Convergence Criterion

How many samples should we draw using the MCMC? The Metropolis-Hastings algorithm is proven to reproduce the target distribution as the number of samples tends to infinity, but we cannot affirm the same for a finite number of samples: we only know that the distribution of sampled points converge to the target distribution as more and more points are sampled. In 1992, Gelman and Rubin [109] proposed a method to assess the convergence of an MCMC. Suppose that N_c chains are performed, each one with N_s samples. I denote by $\theta_j^{(i)}$ the j -th sample of the i -th chain. Let

$$\bar{\theta}^{(i)} = \frac{1}{N_s} \sum_{j=1}^{N_s} \theta_j^{(i)} \quad (5.8)$$

be the average of chain i ,

$$\bar{\theta}_c = \frac{1}{N_c} \sum_{i=1}^{N_c} \bar{\theta}^{(i)} \quad (5.9)$$

be the average of the averages of the chains,

$$\sigma(\bar{\theta})_c = \frac{1}{N_c - 1} \sum_{i=1}^{N_c} (\bar{\theta}^{(i)} - \bar{\theta}_c)^2 \quad (5.10)$$

be the variance of the averages of the chains, and

$$\bar{\sigma}(\theta)_c = \frac{1}{N_c} \sum_{i=1}^{N_c} \left(\frac{1}{N_s - 1} \sum_{j=1}^{N_s} (\theta_j^{(i)} - \bar{\theta}^{(i)})^2 \right) \quad (5.11)$$

be the average of the chain variances. As N_s goes towards infinity, all $\bar{\theta}^{(i)}$ approaches the average of the posterior distribution, and $\bar{\sigma}(\theta)_c$ approaches the variance of the posterior distribution. $\sigma(\bar{\theta})_c$ represents the scatter of the chain averages, since each chain is a stochastic process. The Gelman-Rubin statistic measures the scatter of the chain averages relative to the true variance of the target distribution. Ideally, $\sigma(\bar{\theta})_c$ must be much smaller than $\bar{\sigma}(\theta)_c$: this is a way of measuring how the chains have converged. The Gelman-Rubin statistic is defined as

$$R - 1 = \frac{\sigma(\bar{\theta})_c}{\bar{\sigma}(\theta)_c}. \quad (5.12)$$

During the sampling process, $R - 1$ may be checked periodically. If $|R - 1|$ is below a chosen threshold, the chain is considered converged and stops. It's usual to set this threshold to 0.01, but more costly analyses may relax this threshold.

5.3.2 Confidence Contours and Marginalized Statistics

With a good sample of the posterior distribution, we may now obtain relevant statistical properties of the cosmological parameters. The easiest quantity is the mean, which would be the average of all samples

$$\langle \theta \rangle = \frac{1}{N_{\text{samples}}} \sum_{i=1}^{N_{\text{samples}}} \theta_i. \quad (5.13)$$

We may also obtain the distribution of a given parameter $\theta^{(j)}$ by making a histogram of the samples. This way, we obtain the 1D marginalized posterior distribution of the parameter $\theta^{(j)}$. Often, this marginalized posterior distribution is Gaussian with mean μ and standard deviation σ , and so results are usually reported as

$$\theta^{(j)} = \mu \pm \sigma. \quad (5.14)$$

The 1D marginalized distribution for all parameters, however, disregards correlations between pairs of parameters. One common visualization method is the **triangle plot**, which shows 2D marginalized constraints for all pairs of parameters. An example of triangle plot is shown in Figure 5.1 The 2D marginalized constraints are shown as a 2D contour plot. Usually, two contours are shown, corresponding to 68% and 95% confidence levels. To obtain the 2D marginalized distribution, it's common to use the Kernel Density Estimation (KDE) algorithm, which transforms a multidimensional set of samples into a continuous distribution by smoothing each sample. This algorithm is implemented in the Python package `GetDist` [110], widely used by the cosmological community.

5.3.3 Optimizing MCMCs

MCMCs are computationally expensive simulations, often requiring dozens of CPUs and taking several days to converge. Each project usually requires dozens of MCMCs, and so this is usually a bottleneck. There are several techniques to optimize the convergence time of MCMCs:

- **Reference points:** The MCMC starts from a random point drawn from the prior. This usually is a point with negligible posterior, and it takes a few thousand steps until the chain actually samples the high-posterior region. If this region is known a priori, one can fine-tune the initial point to be around that region, saving valuable time.
- **Proposal:** If the proposal distribution is too large, steps may overshoot the high-posterior region; if the proposal distribution is small, the steps would take long to sample a good volume of the parameter space. A gaussian step

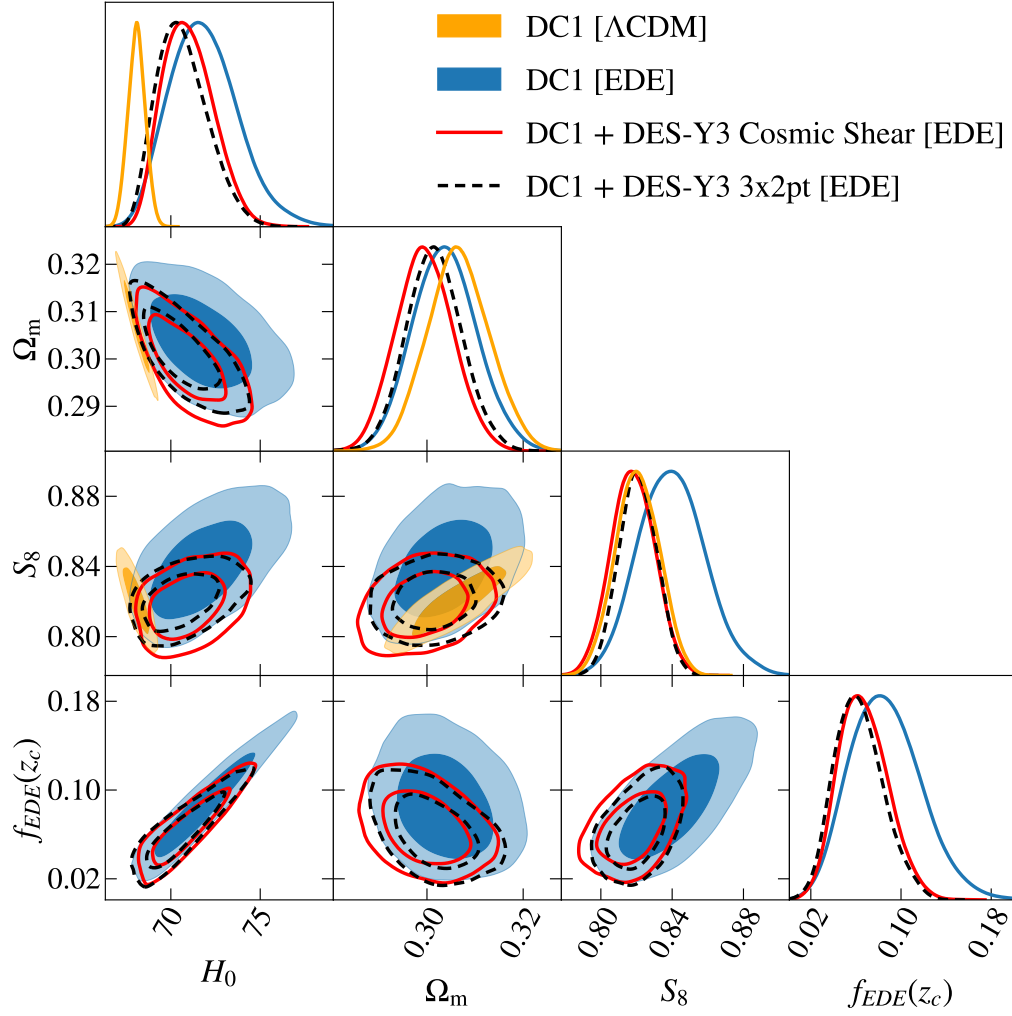


Figure 5.1: An example of triangle plot showing 2D marginalized posterior of four parameters: H_0 , S_8 and the early dark energy parameters z_c and $f_{EDE}(z_c)$ (see Chapter 4 for an introduction to early dark energy).

distribution with covariance 2.4 times larger than the posterior covariance is an optimal choice [111, 112], balancing acceptance rate and step length. The posterior covariance is usually output by MCMC codes, and can be used as the proposal step distribution for future chains.

- **Speed hierarchy:** Changing one of the cosmological parameters, such as Ω_m , requires recomputation of the Einstein-Boltzmann equations, usually the most expensive computation during the MCMC. However, if only A_s or n_s is changed, the transfer functions don't change, just the initial power spectrum. Therefore, by taking more steps in the A_s and n_s directions, one can explore more of the parameter space in less time, since the transfer function calculation doesn't need to be repeated. This fast-slow parameter hierarchy was first explored in [113] and used to optimize cosmological analyses.
- **Choice of sampling parameters:** If a certain experiment is sensitive to a particular parameter combination, it might be optimal to sample in this combination rather than in the original parameters. One example is when analyzing CMB data, which places very stringent constraints on the parameter $\theta_* = r_s(z_*)/D_A(z_*)$. Sampling on θ_* instead of H_0 optimizes the acceptance rate.
- **Parallelization:** MCMC codes often mix two parallelization techniques. MPI parallelization launches multiple processes each with their own memory, while OpenMP parallelization employs multiple CPUs to a single process. In *Cobaya*, each MPI process corresponds to a random walker performing the Metropolis-Hastings algorithm. Each walker must call *CAMB*, which uses the OpenMP parallelization to solve the Einstein-Boltzmann equations. Finding an optimal configuration of MPI processes and number of CPUs per process is difficult and requires a lot of testing, but can definitely save time in the long run. Also, each cluster might benefit from specific settings, and the support staff might help optimizing the simulations.

5.3.4 Importance Sampling

Importance sampling is the process of inferring properties from one statistical distribution using samples from another statistical distribution. This technique uses the samples from an MCMC simulation as a basis to perform other statistical analysis modifying the data vector or the modelling.

One of the examples that importance sampling can help is when the precision settings make MCMC sampling too expensive. Current CMB datasets, such as those from the Atacama Cosmology Telescope, require the calculation of high multipoles in the photon Boltzmann hierarchy, which can make Einstein-Boltzmann codes slower. One technique is to run MCMCs with lower accuracy settings,

take the resulting samples and recalculate the posterior distribution with higher accuracy settings. This process avoids rejecting points that were too expensive to calculate.

Another example of importance sampling application comes in model robustness analyses. Theoretical and systematic modelling in galaxy surveys can have a big impact on the inferred values of cosmological parameters. Model robustness is a process where MCMC samples are taken using a fiducial data vector, and then the posteriors of the samples are recalculated swapping the data vector by a contaminated data vector which includes systematic effects that have not been taken into account, i.e. nonlinear modelling differences, magnification offsets, reduced shear instead of just the shear, among other effects. If any contamination shifts the parameter posteriors by over some threshold, this indicates that the cosmological parameter can mimic the effect of this contamination.

5.4 Model Selection

As a function of the cosmological parameters, the likelihood can be maximized using numerical algorithms, finding the minimum value of χ^2 that a cosmological model can achieve, as well as the **best-fit** model. The minimum χ^2 is a measure of goodness-of-fit and can be used to choose between models. However, in the context of cosmological models, the models described in Chapter 4 that extend Λ CDM are likely to achieve a better fit than Λ CDM due to their increased generality. Therefore, statistical methods have been proposed to penalize models with extra parameters. One of them is the **Akaike Information Criterion** (AIC) [114]: if a model has N_p parameters and its minimum χ^2 is $\chi^2_{\min}$, then we define

$$\text{AIC}(\text{Model}) = \chi^2_{\min} + 2N_p. \quad (5.15)$$

The preferred model is the one that has the lowest AIC.

Another model selection metric is the **Bayesian Information Criterion** (BIC) [115], defined similarly as AIC. If n is the length of the data vector, then

$$\text{BIC}(\text{Model}) = \chi^2_{\min} + N_p \ln(n). \quad (5.16)$$

Once again, the preferred model is the one with the lowest BIC.

The **probability to exceed** (PTE) is based on the fact that if the likelihood is Gaussian, then χ^2 follows a χ^2 -distribution with $n - N_p$ degrees-of-freedom. Therefore, if we have two models with $N_p^{(1)}$ and $N_p^{(2)}$ parameters, then $\Delta\chi^2 = \chi^2_{(1)} - \chi^2_{(2)}$ also follows a χ^2 distribution with $N_p^{(2)} - N_p^{(1)}$ degrees-of-freedom. Let $\Delta\chi^2_{\min} = \chi^2_{(1),\min} - \chi^2_{(2),\min}$ be the difference in the minimum χ^2 of the two models.

Then, the PTE is defined as the probability that $\Delta\chi^2$ exceeds $\Delta\chi_{\min}^2$,

$$\text{PTE} = P(\Delta\chi^2 > \Delta\chi_{\min}^2). \quad (5.17)$$

This probability to exceed is usually related to a z-score. Let Z be a random variable following a standard Gaussian distribution. We define the z-score as the value z such that

$$P(-z < Z < z) = 1 - \text{PTE}. \quad (5.18)$$

The PTE, or equivalently the z-score, is a measure of how much model 2 can improve the fit upon model 1. In a cosmological context, model 1 is Λ CDM and model 2 is any extended model.

Finally, the **Bayes factor** requires the computation of the Bayesian evidence, the denominator of Equation 5.2, which in turn requires integrating the posterior distribution over the parameter space. This is usually not done when performing the Metropolis-Hastings algorithm, but more sophisticated sampling techniques such as nested sampling [116] can obtain the Bayesian evidence. If two models $\mathcal{M}_1$ and $\mathcal{M}_2$ have evidences $E_1 = p(\text{data}|\mathcal{M}_1)$ and $E_2 = p(\text{data}|\mathcal{M}_2)$, the Bayes factor is

$$B_{12} = \frac{E_1}{E_2}. \quad (5.19)$$

A common interpretation of the Bayes factor is usually done using the Jeffreys' scale (see e.g. [117]):

- $|\ln(B_{12})| < 1$: Inconclusive;
- $1 < |\ln(B_{12})| < 2.5$: Weak evidence;
- $2.5 < |\ln(B_{12})| < 5$: Moderate evidence;
- $|\ln(B_{12})| > 5$: Strong evidence.

The sign of $\ln(B_{12})$ determined to which model the evidence points towards: a positive sign points towards $\mathcal{M}_1$ and a negative sign points towards $\mathcal{M}_2$.

5.5 Cosmological Analysis Pipeline

Using concepts from previous sections, I can now describe the full process of obtaining information about cosmological model parameters from observational data.

First of all, the homogeneous background description and linear perturbation equations for a given cosmological model must be implemented. Two public codes perform the numerical integration of the Einstein-Boltzmann equations in the Λ CDM theory: `CAMB` [118] and `CLASS` [119]. To study a specific extended model,

one must derive the background and linear perturbation equations, implement the modified equations in the Einstein-Boltzmann solver, and recompile the codes, effectively implementing the specific extension.

After integrating the Einstein-Boltzmann system of differential equations, the model vector must be calculated in order to be compared with the data vector. `CAMB` and `CLASS` were created to perform CMB anisotropy analysis, and thus the codes can already perform the necessary projection integrals to calculate the temperature and polarization angular power spectra C_ℓ . In the case of galaxy surveys, where the data vector consists of angular correlations between galaxy positions and shapes, codes such as `Cosmolike` [120] and `CosmoSIS` [108] can take the matter power spectrum prediction from the Einstein-Boltzmann solver and calculate the correlation functions. Supernovae, BAO, and Cosmic Chronometers data only require distance predictions, so they don't require perturbation theory predictions; however, Einstein-Boltzmann codes can also output distances.

The likelihood of the model is given by Equation 5.3, and the posterior can be obtained by simply multiplying the likelihood by the prior distribution. When multiple datasets are considered and their cross-correlations are negligible, we can simply multiply the likelihoods.

One can use the MCMC algorithm to sample the parameter space consisting of cosmological parameters and nuisance parameters. Even though the posterior is not normalized from the prescription, MCMC algorithms don't require a normalized likelihood, and we can still obtain constraints for the model parameters. Examples of software that perform posterior sampling are `Cobaya` and `CosmoSIS`.

With the MCMC samples, one can obtain 1D and 2D marginalized posteriors using `GetDist`, which performs Kernel Density Estimation to transform the samples into continuous distributions. With the MCMC samples, one can also perform **importance sampling**, where some of the samples can be chosen to be recalculated after changing minor settings such as accuracy or data vector contamination.

Another statistical technique is to perform **likelihood maximization**, finding the minimum value of χ^2 that the model can achieve and the **best-fit** model. The minimum χ^2 is a measure of goodness-of-fit, and can be used to choose between models using, for instance, the Akaike Information Criterion.

A typical MCMC requires $O(10^5 - 10^6)$ computations of the Einstein-Boltzmann system of equations until it converges. Furthermore, numerical Einstein-Boltzmann solvers take $O(1)$ seconds to complete. While the precise time varies, an MCMC using Planck CMB data to analyze the Λ CDM model takes around one day to converge using 4 MCMC walkers, each with 8 CPUs. A complete statistical analysis of an extended cosmological model considering multiple probes requires dozens of chains to test different theoretical models, priors, dataset combinations, and choices within a dataset (i.e. scale cuts, systematic error modelling, precision para-

meters, etc). Therefore, a single project might require thousands of CPU-hours¹. Such computations are performed in High-Performance Computers (HPCs), or cluster computers, which share resources among hundreds of scientists. It is paramount to optimize the MCMC simulations in order to obtain the desired results in a practical time frame, given that bugs might be present, mistakes may happen and preliminary results may motivate new explorations and new rounds of MCMCs. UNESP provides access to the GridUnesp cluster², which enabled many science applications during my PhD. Through the Laboratório Interinstitucional de e-Astronomia (LIneA), I have also obtained access to the the Santos Dumont³ national cluster.

¹CPU-hour is a measure of computational expense, defined by the usage of a single CPU for one hour.

²<https://www.ncc.unesp.br/gridunesp/docs/v2/>

³<https://sdumont.lncc.br/>

Chapter 6

Early Dark Energy Constraints with Late-Time Expansion Marginalization

This chapter presents Early Dark Energy (EDE), a model under great debate at the time of writing this thesis. I present the theoretical model, an overview of the literature discussion regarding the model, and an original analysis of EDE combined with late-time modifications. This analysis culminated in the article *Early dark energy constraints with late-time expansion marginalization* [23], which is reproduced below with permission from the Journal of Cosmology and Astroparticle Physics.

6.1 Introduction

A viable cosmological model must be able to consistently explain the myriad of observational data stemming from a large span of the history of the Universe, from the formation of light nuclei in its first minutes to the distribution of galaxies formed in the past couple billion years. The spatially flat Λ CDM model has emerged as the standard cosmological model over the past decades: it is the simplest and most viable cosmological model (see e.g. [121]). It is based on a cosmological constant Λ to account for the current acceleration of the Universe [17], cold dark matter (CDM) necessary for structure formation and the existence of an early phase of inflation responsible for generating primordial perturbations with a power spectrum characterized by its amplitude and slope.

New physics beyond Λ CDM would manifest itself through tensions in the derived parameters from different observations as a consequence of the model incompleteness. Potentially, we are starting to see the first hints of such incompleteness from the recent tensions in measuring the Hubble constant H_0 . Although this tension appears in several measurements of early-time and late-time observables (for a review, see [122, 123]), it is most acute in the comparison between an indirect determination from the Cosmic Microwave Background (CMB) obtained by the Planck collaboration [33] and local measurements using the cosmic distance ladder [124, 42, 125], where a tension of the order of 5σ is reported.

In addition to the discrepancy in H_0 , a less severe tension has also been reported in a quantity related to the amplitude of matter fluctuations, the so-called S_8

parameter, with $S_8 = \sigma_8 \sqrt{\Omega_m}/0.3$, where σ_8 is the RMS amplitude of matter fluctuations at the scale $8h^{-1}\text{Mpc}$ and Ω_m is the current matter density fraction [126]. Measurements of two-point correlation functions in galaxy surveys such as the Dark Energy Survey [127, 128, 129, 130, 131, 132, 133, 134], the Kilo-Degree Survey [135, 136, 79, 55] and the Hyper Suprime-Cam Subaru Strategic Program [137, 57, 56], report a significantly smaller value for S_8 than the Planck 2018 result. For instance, this difference is at a 2.3σ level with the cosmic shear analysis from DES in harmonic space [132], while the recent analysis from KiDS reports a 3σ difference [55].

While these differences could be explained by unaccounted-for systematic errors in any of the experiments (see e.g. [138, 139, 140]), cosmological tensions could also be an indication that the standard ΛCDM model is unable to explain all data simultaneously, calling for new physics effects beyond this model. There has been a large body of research exploring different possibilities of extending the ΛCDM model in order to alleviate these tensions (see e.g. [141, 142, 22, 143]).

Among these possibilities, the presence of an early dark energy (EDE) component, proposed before the rise of the Hubble tension [144, 145], has been actively studied in this context (see e.g. [146, 98, 100, 82]). A non-negligible amount of dark energy around the recombination era that quickly dissipates afterwards would decrease the sound horizon relevant for CMB while leaving the diameter distance to the last scattering surface unchanged and hence could in principle ameliorate the Hubble tension [147].

EDE has been the subject of discussion in the recent literature, with ups and downs [148]. For instance, in [82] a 2σ detection of EDE was reported in combined Planck 2018, SH0ES and Pantheon data, reducing the Hubble tension to 1.7σ . Recent CMB data from the Atacama Cosmology Telescope (ACT) favors significantly the presence of EDE. ACT reports a 3σ preference for EDE in comparison with ΛCDM [47], whereas [149] reports a 2.6σ evidence when combining ACT and SPT-3G and [150] reports a 3.3σ evidence for EDE when combining ACT, SPT-3G and Planck 2018 data, even without the SH0ES late-time priors on H_0 [151]. However, recent studies have shown that large-scale structure (LSS) data disfavors EDE because the model causes an increase in the S_8 posterior mean, aggravating the S_8 tension [152, 153, 154]. In such works, LSS data limits the amount of EDE during recombination to values insufficient to solve the Hubble tension. While this is a strong argument against the EDE model, the discussion is not yet settled [155, 156, 157, 158].

Moreover, modifications in the late-time expansion history can affect the growth of structure, such as dynamical, smooth dark energy models¹ [159, 160, 161, 162, 163, 164]. Several models combining EDE with other modifications were studied in order to tackle both H_0 and S_8 tensions, such as decaying dark matter

¹Smooth in the sense that these dark energy fluids have negligible perturbations inside the horizon.

[165], interacting dark energy [85, 166], models with spatial curvature [167] and constant w [168], models with a (w_0, w_a) parameterization for the equation of state [169], models with massive neutrinos [170] and models with massive neutrinos coupled to dark energy [171], models with an anti-de Sitter vacuum phase [172] and axionic dark matter [173], to mention a few. For a recent review see [174].

The main goal of this work is to test new EDE models with modifications in the late-time expansion history of the Universe using recent LSS data and how they affect S_8 and the EDE constraints. We will model late dark energy as a fluid with negligible perturbations inside the horizon, also known as smooth dark energy. Also, we choose to employ a general parametrization for the late-time equation-of-state $w(z)$ as a piecewise constant function over several redshift bins. The redshift bins are chosen for $z < 3$, when dark energy starts becoming relevant to the background expansion. This model goes beyond the usual (w_0, w_a) parametrization, allowing for a more general study that is more suited for our goal. By marginalizing EDE constraints over the parameters describing $w(z)$, we obtain predictions that are independent of late-time expansion behaviour. We use different combinations of available cosmological datasets to assess the EDE parameter posteriors in these modified models. We primarily use CMB data from ACT which favors EDE models, and therefore allow us to better quantify the shifts in the posterior distributions of the EDE parameters. In addition, we use the recent DES-Y3 data on LSS in our analysis.

This Chapter is organized as follows: section 6.2 describes the dark energy models used in our analysis; section 6.3 describes the data used in our work and analysis methods; section 6.4 display the results of the analysis; we present our conclusions in section 6.5.

6.2 Dark Energy Models

In this section we describe the models we adopt to describe early and late dark energy.

6.2.1 Early Dark Energy (EDE)

There are two approaches to model EDE: using a microscopic scalar field description or using an effective fluid description. In the first case, EDE can be realized by a minimally-coupled scalar field and is fully described by its potential and initial conditions. It is usually assumed a generalized “axion-like” potential of the form

$$V(\phi) = m^2 f^2 \left[1 - \cos \left(\frac{\phi}{f} \right) \right]^n. \quad (6.1)$$

The usual axion potential is obtained for $n = 1$, where in this case m is the axion mass and f is the scale of spontaneous symmetry breaking that gives rise to the axion as a pseudo-Nambu-Goldstone boson. Initially, the field is frozen at its initial value by the large Hubble friction, with an equation of state $w_\phi \approx -1$. As the Universe expands, the Hubble friction decreases and at a critical redshift denoted by z_c the field starts to oscillate around the minimum of the potential, with an average equation of state $w_n = (n - 1)/(n + 1)$ [175]. For values of $n \geq 2$, the energy density in this field decays faster than matter and quickly becomes negligible with respect to the matter density. Although lacking a well-motivated fundamental origin, there are recent attempts to derive these models (for $n > 1$) from an ultraviolet theory [176]. The axion-like potential is used by most EDE analyses in the literature (e.g. [152, 47, 146, 153, 151]). A similar scalar field model is the so-called ‘‘Rock ‘n’ Roll’’ EDE [100], where a power-law potential is adopted:

$$V(\phi) = V_0 \left(\frac{\phi}{M_{\text{pl}}} \right)^{2n}, \quad (6.2)$$

where M_{pl} is the reduced Planck mass. We have also analysed this class of scalar field EDE models in this work. In order to do so we used the implementation of the scalar field perturbations in CAMB with different potentials.

Although exact, the scalar field description may suffer from numerical issues arising from the rapid oscillations around the minimum of the potential. The corresponding equation of state also experience fast variation and in this case one may use an effective fluid description with time-averaged quantities. In the case of axion-inspired models of EDE an effective fluid description was developed in [98] and it is characterized by the critical redshift z_c mentioned above and the energy density fraction of EDE at z_c , $f_{\text{EDE}}(z_c) = \rho_{\text{EDE}}(z_c)/\rho_{\text{tot}}(z_c)$. We parameterize the background quantities as:

$$\rho_{\text{EDE}}(z) = \frac{2\rho_{\text{EDE}}(z_c)}{1 + \left(\frac{1+z}{1+z_c} \right)^{3(1+w_n)}}, \quad (6.3)$$

where z_c and w_n are defined as above. The corresponding EDE equation of state w_{EDE} is given by:

$$w_{\text{EDE}}(z) = \frac{1 + w_n}{1 + \left(\frac{1+z}{1+z_c} \right)^{3(1+w_n)}} - 1. \quad (6.4)$$

At early times ($z \gg z_c$), the EDE energy density is approximately constant with $w_{\text{EDE}} \rightarrow -1$ since the field is frozen and behaves as a cosmological constant, while for $z \ll z_c$, the energy density scales as $\rho_{\text{EDE}} \propto (1+z)^{3(1+w_n)}$. We will assume $n = 3$ in this work, since this is the preferred value determined in previous

analyses [82], [177].

In order to study perturbations in the EDE fluid one also needs to specify the effective sound speed c_s (the adiabatic sound speed c_a is fixed by the background quantities). For a slow-rolling canonically normalized scalar field $c_a^2 = w$ and $c_s^2 = 1$ [29]. However, this is not valid anymore when the scalar field is rapidly oscillating. In this case, the adiabatic sound speed takes into account variations of the equation of state:

$$c_a^2 = w_{\text{EDE}} - \frac{\dot{w}_{\text{EDE}}}{3(1 + w_{\text{EDE}})\mathcal{H}}, \quad (6.5)$$

where the overdot denotes derivative with respect to conformal time, and the effective sound speed is given by (see [98]):

$$c_s^2(k, a) = \frac{2a^2(n-1)\bar{\omega}_0^2 a^{-6w_n} + k^2}{2a^2(n+1)\bar{\omega}_0^2 a^{-6w_n} + k^2}, \quad (6.6)$$

which follows from averaging both background and perturbations of the scalar field over its fast oscillations around the minimum of the potential.

The function $\bar{\omega}_0$ depends on an parameter Θ_i , which is related to the scalar field initial value by $\Theta_i = \phi_i/f$. Although this is a fluid model, it reproduces the oscillation-averaged behavior of the axion-like scalar field and therefore both models have the same number of parameters [98].

In summary, the effective fluid description of EDE is characterized by three parameters: z_c , $f_{\text{EDE}}(z_c)$ (which, for brevity, we will refer to as f_{EDE}) and Θ_i , which fixes the effective sound speed c_s . In the following we will mostly use the effective fluid description of EDE and we will briefly compare our results with a field theoretical description of EDE using both the axion-inspired and the "Rock 'n' Roll" models.

The background and linear perturbation equations for the EDE models have been incorporated in the Einstein-Boltzmann code CAMB². For the scalar field evolution, we set the initial value of the field, ϕ_i at $a = 10^{-7}$, when the field is still frozen. When comparing results from the scalar field with the effective fluid description of EDE we use a shooting method implemented in CAMB to transform the potential parameters m and f (or V_0 and ϕ_i in the Rock 'n' Roll model) into the effective fluid parameters z_c and f_{EDE} .

6.2.2 Late Dark Energy

Late dark energy has a significant impact on the growth of perturbations and hence it affects the cosmological parameter S_8 . In this work we want to assess if a general model for late dark energy can ameliorate the S_8 tension found in EDE models. Models with a canonically normalized, slow-rolling scalar field have an

²github.com/cmbant/CAMB

effective sound speed $c_s = 1$ and hence behave as smooth dark energy since in this case perturbations are suppressed inside the horizon.

Smooth dark energy models only affect the growth of structure through its contribution to the background expansion, determined by its equation of state $w(z)$. In order to be agnostic about the behavior of dark energy at late times, we consider a piecewise equation of state for different redshift bins:

$$w(z) = \begin{cases} w_0 & \text{if } 0 \leq z < z_1, \\ \dots & \\ w_{n-1} & \text{if } z_{n-1} \leq z < z_n, \\ w_n = -1 & \text{if } z \geq z_n. \end{cases} \quad (6.7)$$

This parameterization can approximate any dynamical dark energy model that does not vary rapidly within the redshift bins.

In this work we test three different bin choices such that have a significant number of redshift bins inside the Pantheon supernovae range of $z \in [0.01, 2.3]$, when late dark energy becomes relevant to the background energy density. The choices are:

- $z_i = \{0.7, 1.4, 2.1\}$,
- $z_i = \{0.5, 1.0, 1.5, 2.0, 3.0\}$,
- $z_i = \{0.3, 0.6, 0.9, 1.2, 1.5, 1.8, 2.1, 2.4, 2.7, 3.0\}$.

We show that these three cases are sufficient to test the impact of a general late dark energy model on S_8 . Adding extra parameters slows down the convergence of Monte Carlo Markov Chains (MCMCs), and thus we limit our investigation to 10 bins.

We implement both early and late dark energy models in a modified version of CAMB, which allows the combination of multiple dark energy fluids. The late dark energy perturbations are calculated using the parametrized post-Friedmann approach [178]. In this approach there are no instabilities in the perturbations from either phantom crossing ($w = -1$ crossing) or from discontinuities in the $w(z)$ which arise in our parametrization.

6.3 Datasets and Analysis

In this work we assess posteriors for EDE parameters marginalized over the behaviour of late dark energy using different datasets from CMB, SNe Ia, LSS and strong lensing measurements. We detail below these datasets and present our analysis strategy.

6.3.1 CMB data

We choose to use ACT data as our primary CMB dataset because the strongest claim of EDE detection comes from its analysis³ [47]. With ACT data, we can more clearly quantify the effects of late-time DE marginalization on the EDE constraints, the main focus of this work. We use the ACT CMB TT, TE and EE power spectra included in the ACTPOL DR4 likelihood [46] and implemented in PYACTLIKE⁴. The spectra are measured in the multipole range $\ell \in [600, 4500]$ for TT and $\ell \in [350, 4500]$ for TE and EE. We restrict ourselves to the multipole range $\ell \leq 3000$ in order to avoid biases due to baryonic feedback processes, as explained in [180]. The only nuisance parameter in the likelihood is the polarization efficiency y_p .

We complement ACT data with a subset of the Planck 2018 CMB data [33]. Following [47], we combine the ACT power spectra with the Planck 2018 TT power spectrum for $\ell < 650$, where Planck has more precise data compared to ACT. ACT data by itself cannot constrain the reionization optical depth τ . Instead of imposing a Gaussian prior on τ as in the ACT official analyses [46, 47], we choose to include Planck 2018 large-scale polarization spectrum ($\ell < 30$) data in order to constrain τ . The combination of ACT spectra up to $\ell = 3000$, Planck 2018 TT spectrum cut at $\ell = 650$ and low- ℓ EE will be henceforth referred to simply as CMB. We also study the inclusion of CMB Lensing from Planck 2018, and we refer to this dataset as CMBL.

6.3.2 SNe Ia data

We use the Pantheon sample of 1048 SNe Ia in the redshift range $0.01 < z < 2.3$ [181] to test the recent expansion history in our models⁵. We refer to this dataset as SNe.

³While this paper was in the referral process, a preprint appeared in the arXives reporting improved constraints on a similar axion-like early dark energy model using a new temperature and polarization Planck likelihood, finding $f_{\text{EDE}} < 0.061$ [179], without including DES data. We expect our results that smooth dark energy cannot be used to alleviate the S_8 tension to be valid in such a scenario as well. We left a detailed comparison between Planck and ACT data on EDE models fitted simultaneously with generalized late-time physics for future work. We thank the referee for bringing this reference to our attention.

⁴<https://github.com/ACTCollaboration/pyactlike>

⁵We use Pantheon rather than the very recent dataset Pantheon+ [36]. Pantheon is a subset of Pantheon+ with 1048 (of the 1550 in Pantheon+) spectroscopically confirmed Type-Ia supernovae. The cosmological constraints from both datasets are compatible within 1σ . In addition, the SNIa data does not constrain S_8 , one of the major purposes in our work. Thus, we do not expect significant changes in our results by using Pantheon+.

6.3.3 Large-Scale Structure data

We use Baryonic Acoustic Oscillation (BAO) data from multiple sources: the Six-degree Field Galaxy Survey (6dFGS) [59], the SDSS DR7 main galaxy sample [182] and from SDSS BOSS DR12 consensus sample [68]. We refer to this combination simply as BAO. The galaxies included in these surveys range from $z = 0.1$ to $z = 0.6$. Thus, the evolution of the BAO feature can provide information about the low redshift expansion history.

In addition, we use Dark Energy Survey (DES) measurements of two-point correlation functions of galaxy shear, galaxy clustering and their cross-correlations (the so-called 3x2pt analysis). DES data provides detailed information about the clustering of matter at low redshifts, strongly constraining S_8 and Ω_m and complementing other geometrical probes of the Universe. Since the most stringent constraints on S_8 comes from cosmic shear we also perform analyses with cosmic shear data only. All data was obtained from the DES-Y1⁶ and DES-Y3⁷ data release repositories.

We use the results from two galaxy catalogs: the source METACALIBRATION shape catalog and the REDMAGIC lens galaxy sample. The source shape catalog [183] contains the ellipticities and photometric redshifts of over 100 million galaxies and it is divided in 4 redshift bins, each bin with limits at $z = [0, 0.36, 0.63, 0.87, 2.0]$. The REDMAGIC lens sample [130] contains 2.5 million galaxies whose positions are used to measure clustering correlations and galaxy-galaxy lensing. This lens sample is divided in 5 redshift bins with limits at $z = [0.15, 0.35, 0.50, 0.65, 0.80, 0.90]$.

The galaxy clustering two-point angular correlation function in real space $w(\theta)$ is calculated in the following way [52]: the lens sample of galaxies is divided in redshift bins, each bin i with a galaxy number density $n_l^i(z)$. The source galaxy sample is also divided in redshift bins, with density $n_s^j(z)$. Let

$$q_l^i(\chi) = b_L^i \times n_l^i(z(\chi)) \frac{dz}{d\chi} \quad (6.8)$$

be the radial weight function, where b_L^i the linear galaxy bias, assumed constant on each redshift bin and scale independent, and χ is the comoving radial distance. We can calculate the two-point angular correlation function in real space by summing the correlations in Fourier space:

$$w^i(\theta) = \sum_{\ell} \frac{2\ell + 1}{4\pi} P_{\ell}(\cos \theta) C_{\delta_g \delta_g}^{ii}(\ell), \quad (6.9)$$

where $P_{\ell}(x)$ is the ℓ -th Legendre polynomial.

⁶<https://des.ncsa.illinois.edu/releases/y1a1/key-products>

⁷<https://des.ncsa.illinois.edu/releases/y3a2>

The Fourier space correlations could be calculated using the Limber approximation:

$$C_{\delta_g \delta_g}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q_1^i(\chi) q_1^j(\chi) P_{\text{NL}} \left(k = \frac{\ell + 1/2}{\chi}, z(\chi) \right), \quad (6.10)$$

where $P_{\text{NL}}(k, z)$ is the nonlinear matter power spectrum. However, for galaxy clustering, it has been shown that the Limber approximation leads to biases in cosmological constraints, and thus we use the FFTLog method proposed in [32]. For cosmic shear and galaxy-galaxy lensing, the Limber approximation is still used. The calculation of the shear auto-correlations is performed in a similar way. Defining the lensing efficiency as:

$$q_\kappa^i(\chi) = \frac{3\Omega_m H_0^2}{2} \times \int_\chi^{\chi_H} d\chi' \left(\frac{\chi' - \chi}{\chi} \right) n_s^i(z(\chi')) \frac{dz}{d\chi'}, \quad (6.11)$$

we calculate the correlations in real space as a sum in Fourier space:

$$\zeta_\pm^{ij}(\theta) = \sum_\ell \frac{2\ell + 1}{4\pi} \frac{2(G_{\ell,2}^+(x) \pm G_{\ell,2}^-(x))}{\ell^2(\ell + 1)^2} C_{\kappa\kappa}^{ij}(\ell), \quad (6.12)$$

where $x = \cos \theta$ and $G^\pm$ are analytic functions described in appendix A from [52]. The Fourier space correlations are given by:

$$C_{\kappa\kappa}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q_\kappa^i(\chi) q_\kappa^j(\chi) P_{\text{NL}} \left(k = \frac{\ell + 1/2}{\chi}, z(\chi) \right). \quad (6.13)$$

The correlation between galaxy shear and lens position is given by:

$$\gamma_t^{ij}(\theta) = \sum_\ell \frac{2\ell + 1}{4\pi} \frac{P_\ell^2(\cos \theta)}{\ell(\ell + 1)} C_{\delta_g \kappa}^{ij}(\ell), \quad (6.14)$$

where $P_\ell^2(x)$ is the associated Legendre polynomial $P_\ell^m(x)$ with $m = 2$ and:

$$C_{\delta_g \kappa}^{ij}(\ell) = \int \frac{d\chi}{\chi^2} q_1^i(\chi) q_\kappa^j(\chi) P_{\text{NL}} \left(k = \frac{\ell + 1/2}{\chi}, z(\chi) \right). \quad (6.15)$$

DES measures angular correlations averaged over a given angular bin. Therefore, one needs to modify the theory predictions to account for this procedure. In order to average over a finite angular bin $[\theta_{\min}, \theta_{\max}]$, one assumes that galaxies are uniformly distributed. It can be shown that for the galaxy clustering correlation

function $w(\theta)$ this leads to the modification in eq. (6.9):

$$P_\ell(\cos \theta) \rightarrow \bar{P}_\ell(\cos \theta) = \frac{[P_{\ell+1}(x) - P_{\ell-1}(x)]_{\cos \theta_{\min}}^{\cos \theta_{\max}}}{(2\ell + 1)(\cos \theta_{\min} - \cos \theta_{\max})}, \quad (6.16)$$

and the corresponding modifications for the galaxy-galaxy lensing correlation function $\gamma_t(\theta)$ and for the cosmic shear correlation functions $\zeta_\pm(\theta)$ can be found in [52].

The angular separations θ in the correlation functions are divided into 20 logarithmically spaced bins between 2.5 arcmin to 250 arcmin. After scale cuts to mitigate unaccounted for nonlinear effects such as baryonic feedback from active galactic nuclei (AGN), the final data vector for the Y3 3x2 analysis has 533 elements.

DES analyses assume several modelling choices that are described and tested in [184]. A simple linear, scale-independent model is used to describe galaxy bias for each redshift bin, $\delta_g = b_L^i \delta_m$. Intrinsic alignment is modelled using the Tidal Torquing and Tidal Alignment (TATT) model [185]. Photometric redshift uncertainties in both the lens and source galaxy samples are modelled as offsets in each bin $\Delta z_{l/s}^i$. Uncertainties in the shear measurements are modelled as multiplicative bias parameters m^i . Yet another correction factor called point-mass parameter B_i is introduced in the modelling of the galaxy-galaxy lensing correlation γ_t . The DES nuisance parameters that are sampled and marginalized over in our analysis are summarized in Table 6.2 [127].

We notice that the fiducial DES-Y3 3x2pt analysis uses an alternative lens galaxy sample, the so-called `MagLim` sample [131]. The main reason is that the 2x2pt analysis (i.e. without the shear correlation functions) revealed an unexplained internal tension which manifested itself in, among other places, the linear galaxy bias b_L derived from galaxy clustering and galaxy-galaxy lensing [130]. This result was further scrutinized in the final DES-Y3 3x2pt analysis, where an extra parameter denoted by X_{lens} was introduced to account for this tension in a phenomenological manner [127]. The inferred cosmological parameters from the fiducial analysis in Λ CDM are consistent with the ones obtained from the `REDMAGIC` lens sample with and without marginalizing over X_{lens} . We will corroborate these results in our case by showing consistency between a 3x2pt analysis with $X_{\text{lens}} = 1$ and a shear-only analysis, where the latter is insensitive to X_{lens} .

6.3.4 Strong Lensing

The H0LiCOW collaboration [186, 187, 188] measured time-delay distances from six quasar-lens systems, providing an H_0 constraint that agrees with local distance ladder measurements while being completely independent from those: $H_0 = 73.3_{-1.8}^{+1.7} \text{ km s}^{-1} \text{ Mpc}^{-1}$. We refrain from using SH0ES priors in our chains,

as their H_0 constraints are in severe tension with CMB constraints, which would lead to a degradation of the CMB fit and an artificial tightening of our constraints. Therefore we chose to use strong lensing measurements from H0LiCOW instead of local SH0ES measurements. We refer to using the H0LiCOW likelihood prior as SL.

6.3.5 Analysis

We perform our analysis using the COCOA⁸ pipeline [189], which combines the COBAYA⁹ sampler [106] with the COSMOLIKE¹⁰ code [120] for computing likelihoods for galaxy surveys using a halo-based theoretical covariance matrix [190] that was validated in DES-Y1 [191] and DES-Y3 [52] analyses. We use the Limber approximation to calculate cosmic shear and galaxy-galaxy lensing correlations, but not for galaxy clustering. The likelihoods from the other independent datasets are combined assuming no correlations.

We use our implementation of both early and late dark energy models in a modified version of CAMB with a Halofit model for the nonlinear matter power spectrum [192] supplemented by the Casarini prescription to account for the variable equation-of-state $w(z)$ model for late dark energy [193, 194]¹¹. Neutrinos are modelled using the default CAMB configuration, with an effective number of relativistic species at recombination $N_{\text{eff}} = 3.046$, and only one massive neutrino species with mass $m_\nu = 0.06$ eV. In order to validate our CAMB version, we have reproduced results from literature, specifically Fig. 2 from [100], Fig. 1 from [82] and Fig. 14 from [47].

We sample over the base cosmological parameters $\{\theta_*, \Omega_b h^2, \Omega_c h^2, \ln(10^{10} A_s), n_s, \tau\}$ with large, uninformative priors. We also sample over the EDE parameters $\{\log_{10}(z_c), f_{\text{EDE}}, \Theta_i\}$ ¹² instead of sampling over the potential parameters m and f . This choice is widely used in previous EDE analyses (for instance [47]) and we adopted it here since it allows for easy comparison with these works. The piecewise-constant equation of state in each redshift bin $\{w_i\}$ are also sampled with wide priors. The priors for base cosmological parameters and dark energy parameters are listed in Table 6.1. We also sample over nuisance parameters from ACT, DES-Y1 and DES-Y3. The priors for nuisance parameters follow the respective collaboration papers [46, 133, 127], and are shown in Table 6.2. Following the fiducial DES-Y3 analysis, we also analytically marginalize over a point-mass parameter describing small-scale effects in galaxy-galaxy lensing. We use the

⁸<https://github.com/CosmoLike/cocoa>

⁹<https://cobaya.readthedocs.io/en/latest/>

¹⁰<https://github.com/CosmoLike/>

¹¹Following [47], we increase the standard CAMB accuracy in order to calculate higher order multipoles. We use the increased accuracy settings `AccuracyBoost = 1.2` and `max_l = 10000`.

¹²We follow [82] and use $\Theta_i = \phi_i / f$ as a parameter instead of the effective speed of sound of the fluid.

Gelman-Rubin convergence criterion $|R - 1| < 0.05$ to stop the chains. We use GETDIST¹³ [110] to analyse the chains, obtain marginalized statistics and plot confidence contours. We emphasize that the main goal of this work is not to obtain state-of-the-art EDE constraints or compare the EDE model against Λ CDM. Rather, our main goal is to assess if general late-time dark energy models can affect EDE constraints, shifting f_{EDE} and S_8 posterior distributions, especially after including DES-Y3 LSS data. Thus, we refrain from performing model comparison analyses such as Bayesian evidence and Akaike Information Criterion (AIC): we simply compare the posterior distributions for different models and assess the changes in mean and variance.

In order to study the effects of different datasets on the estimation of cosmological parameters we run MCMC chains with five dataset combinations (DCs):

- DC1: CMB + BAO + SNe + CMBL;
- DC2: CMB + BAO + SNe;
- DC3: CMB + BAO + SNe + CMBL + SL;
- DC4: CMB + SNe + CMBL;
- DC5: CMB + SNe + SL.

We chose the combination DC1 as the baseline dataset. By comparing it with DC2 we assess the effect of including CMBL. In the same way, comparing DC1 with DC4 allows us to gauge the effect of including BAO in the analysis. DC3 includes SL, which tends to worsen the CMB fit, since the two datasets are somewhat in tension. Finally, DC5 also combines the datasets that are in tension, CMB on one side and SNe and SL on the other side of H_0 . In order to study the impact of DES data on the EDE constraints, we run chains with and without DES data, using cosmic shear only and full 3x2pt data, for each combination of the datasets above. We also compare results between Y1 and Y3 analysis, where we use the respective data vectors, covariances, scale cuts and prior choices.

For each dataset combination, we run chains with EDE+ Λ and the combined EDE+ $w(z)$ model with 3, 5, and 10 bins. Including tests and validation, we have run roughly 160 chains for this project. We describe our results in the next section.

6.4 Results and Discussion

6.4.1 Early Dark Energy

We start by discussing constraints on early dark energy models with the usual cosmological constant as late dark energy. The results in this subsection expand

¹³<https://getdist.readthedocs.io/en/latest/>

Parameter	Prior
Base Cosmological Parameters	
$\Omega_c h^2$	$\mathcal{U}[0.001, 0.99]$
$\Omega_b h^2$	$\mathcal{U}[0.005, 0.1]$
$100 \times \theta_*$	$\mathcal{U}[0.5, 10]$
$\ln(10^{10} A_s)$	$\mathcal{U}[1.61, 3.91]$
n_s	$\mathcal{U}[0.85, 1.1]$
τ	$\mathcal{U}[0.01, 0.8]$
Dark Energy Parameters	
$\log_{10}(z_c)$	$\mathcal{U}[3, 4.3]$
$f_{\text{EDE}}(z_c)$	$\mathcal{U}[0.001, 0.5]$
Θ_i	$\mathcal{U}[0.1, 3.1]$
w_0	$\mathcal{U}[-3, -0.1]$
$w_{n \geq 1}$	$\mathcal{U}[-3, 1]$

Tabela 6.1: Priors for cosmological and dark energy parameters sampled in our MCMCs. $\mathcal{U}[a, b]$ represents an uniform distribution with edges $[a, b]$.

on previous analyses with the inclusion of DES-Y3 data and the mitigation of baryonic effects on ACT data by considering multipoles $\ell < 3000$ in the TT, TE and EE power spectra.

One of the main arguments given by previous works in the literature in favor of the EDE model is its ability to improve the CMB fit with respect to the Λ CDM model. The EDE analysis from the ACT collaboration [47] has reported a 3σ evidence for EDE using full ACT spectra, Planck TT spectrum cut at $\ell = 650$, CMB lensing and BAO, finding $f_{\text{EDE}} = 0.091^{+0.020}_{-0.036}$. This is in agreement with our results using the DC1 dataset, which differs from [47] by the inclusion of SNe data and the cut in the multipoles in the ACT power spectra.

Figure 6.1 shows our results for the posterior distributions for the parameters H_0 , Ω_m , S_8 and f_{EDE} , using both the EDE model and a standard Λ CDM model for the base dataset DC1; we find $f_{\text{EDE}} = 0.088^{+0.028}_{-0.035}$. The figure shows that a preference for nonzero EDE has the desirable property of relaxing the Hubble tension by increasing the H_0 posterior mean. On the other hand, one notices that EDE also leads to a less dramatic increase in the S_8 posterior mean, from $S_8 = 0.820 \pm 0.012$ (DC1, Λ CDM) to $S_8 = 0.840^{+0.018}_{-0.020}$ (DC1, EDE). This effect further increases the disagreement with galaxy survey results, which prefer a significantly lower value in the Λ CDM scenario: the DES-Y3 fiducial analysis, for instance, reports $S_8 = 0.776 \pm 0.017$ [127]. In order to verify the effects of different implementations of EDE models, we show in Table 6.3 the consistency among the marginalized constraints for the parameters H_0 , S_8 and f_{EDE} obtained using dataset DC1 from the three different implementations of EDE models, namely an effective fluid description and the two scalar field models described in section 6.2.1. We

Parameter	Prior
ACT Nuisance Parameter	
y_p	$\mathcal{U}[0.9, 1.1]$
DES-Y3 Nuisance Parameters	
Photometric redshift offsets	
$\Delta z_{\text{source}}^1$	$\mathcal{N}[0, 0.018]$
$\Delta z_{\text{source}}^2$	$\mathcal{N}[0, 0.015]$
$\Delta z_{\text{source}}^3$	$\mathcal{N}[0, 0.011]$
$\Delta z_{\text{source}}^4$	$\mathcal{N}[0, 0.017]$
Δz_{lens}^1	$\mathcal{N}[0.006, 0.004]$
Δz_{lens}^2	$\mathcal{N}[0.001, 0.003]$
Δz_{lens}^3	$\mathcal{N}[0.004, 0.003]$
Δz_{lens}^4	$\mathcal{N}[-0.002, 0.005]$
Δz_{lens}^5	$\mathcal{N}[-0.007, 0.010]$
Intrinsic Alignment (TATT)	
$a^{1,2}$	$\mathcal{U}[-5, 5]$
$\eta^{1,2}$	$\mathcal{U}[-5, 5]$
b_{TA}^1	$\mathcal{U}[0, 2]$
Linear Galaxy Bias	
b_1^i	$\mathcal{U}[0.8, 3]$
Shear Calibration	
m^1	$\mathcal{N}[-0.006, 0.009]$
m^2	$\mathcal{N}[-0.020, 0.008]$
m^3	$\mathcal{N}[-0.024, 0.008]$
m^4	$\mathcal{N}[-0.037, 0.008]$
DES-Y1 Nuisance Parameters	
Photometric redshift offsets	
$\Delta z_{\text{source}}^1$	$\mathcal{N}[-0.001, 0.016]$
$\Delta z_{\text{source}}^2$	$\mathcal{N}[-0.019, 0.013]$
$\Delta z_{\text{source}}^3$	$\mathcal{N}[0.009, 0.011]$
$\Delta z_{\text{source}}^4$	$\mathcal{N}[-0.018, 0.022]$
Δz_{lens}^1	$\mathcal{N}[0.008, 0.007]$
Δz_{lens}^2	$\mathcal{N}[-0.005, 0.007]$
Δz_{lens}^3	$\mathcal{N}[0.006, 0.006]$
Δz_{lens}^4	$\mathcal{N}[0, 0.01]$
Δz_{lens}^5	$\mathcal{N}[0, 0.01]$
Intrinsic Alignment (NLA)	
a^1	$\mathcal{U}[-5, 5]$
η^1	$\mathcal{U}[-5, 5]$
Linear Galaxy Bias	
b_1^i	$\mathcal{U}[0.8, 3]$
Shear Calibration	
$m^i, i \in [1, 4]$	$\mathcal{N}[0.012, 0.023]$

Tabela 6.2: Priors for nuisance parameters sampled in the MCMC. $\mathcal{U}[a, b]$ represents an uniform distribution over the real interval $[a, b]$, while $\mathcal{N}[a, b]$ represents a Gaussian distribution with mean a and standard deviation b .

Model/Dataset	H_0 (km s ⁻¹ Mpc ⁻¹)	$10 \times S_8$	$100 \times f_{\text{EDE}}$
DC1			
Λ CDM	68.1 ± 0.50	8.20 ± 0.12	–
Axion-like	$71.6^{+1.3}_{-2.3}$	$8.35^{+0.17}_{-0.22}$	$10.6^{+2.7}_{-4.9}$
Rock 'n' Roll	$71.4^{+1.3}_{-2.0}$	$8.34^{+0.16}_{-0.19}$	$9.5^{+2.7}_{-3.6}$
Effective Fluid	$71.9^{+1.6}_{-2.1}$	$8.41^{+0.17}_{-0.20}$	$8.8^{+2.8}_{-3.5}$

Tabela 6.3: Marginalized constraints (mean and 68% limits) for the parameters H_0 , S_8 and f_{EDE} for three EDE models: Axion-like EDE, Rock 'n' Roll EDE and effective fluid EDE. We use the dataset combination CMB (ACT power spectra with $\ell_{\text{max}} = 3000$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ and EE spectrum with $\ell_{\text{max}} = 30$) + BAO (6dFGS, SDSS DR7 MGS and SDSS BOSS DR12 consensus sample) + SNe (Pantheon) + CMBLenS (Planck 2018 CMB Lensing potential).

verified that this consistency remains when including DES data. In the following most of our analyses are performed in the effective fluid description.

We can assess the goodness-of-fit of each model by comparing the values of χ^2 at the minimum. We find that the difference between Λ CDM and EDE scenarios is concentrated in the CMB part of the data vector: $\chi_{\text{CMB}}^2(\Lambda\text{CDM}) = 966.3$ and $\chi_{\text{CMB}}^2(\text{EDE}) = 957.0$, with difference $\Delta\chi_{\text{CMB}}^2 = \chi_{\text{CMB}}^2(\text{EDE}) - \chi_{\text{CMB}}^2(\Lambda\text{CDM}) = -9.3$. We remark that our CMB data vector consists of 911 components. Assuming $\Delta\chi^2$ is χ^2 -distributed with 3 degrees of freedom due to the extra EDE parameters, this difference corresponds to approximately a 2.2σ preference for EDE over Λ CDM, or a 97.5% significance.

The simplest way of quantifying tensions in the parameter constraints between two analyses is by the 1D standardized difference [195, 78]:

$$T = \frac{|\mu_1 - \mu_2|}{\sqrt{\sigma_1^2 + \sigma_2^2}}, \quad (6.17)$$

where μ_i is the marginalized mean value of the parameter posterior distribution for each analysis and σ_i is the marginalized 68% confidence limit. If the posteriors are skewed, we take the average of the upper and lower limits. We remark that this simple tension metric does not capture the multidimensional correlations between different parameters and it only reflects a statistical significance when the posteriors are approximately Gaussian, which is the case for H_0 and S_8 but not for f_{EDE} .

In Fig. 6.2 we show the tensions arising from our analysis compared with a recent H_0 constraint reported by SH0ES [21] and the DES-Y3 constraints for S_8 [127], using the simple 1D metric of Equation 6.17. As expected, the Hubble tension is decreased from roughly 4.5σ in Λ CDM to less than 1σ in EDE models

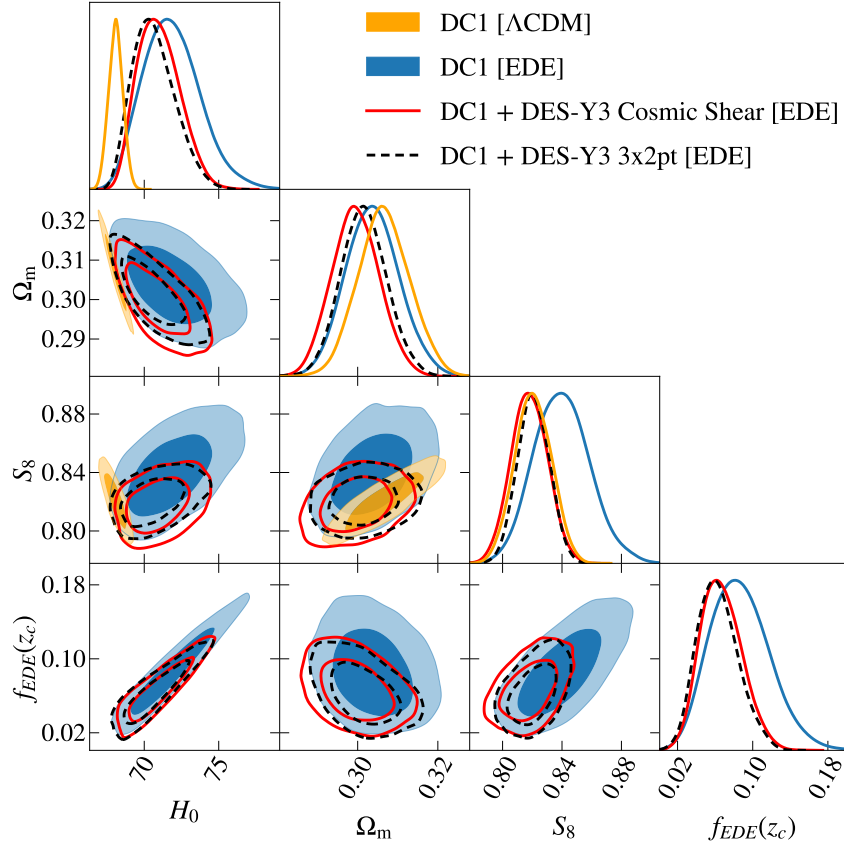


Figura 6.1: Constraints for the Λ CDM and effective fluid early dark energy models using the dataset combination DC1: ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum. We also include DES-Y3 3x2-point correlation function as well as cosmic shear alone.

and the different EDE models are in reasonable agreement. Regarding the S_8 parameter, one notices that the S_8 tension increases from roughly 2σ to $2.3 - 2.5\sigma$ when EDE is included. Thus, data from galaxy surveys should limit the amount of EDE in order to accommodate lower S_8 values. We find similar results for the other datasets that we show as robustness tests in appendix C.1.

We now turn our attention to the effects of including DES data on EDE constraints. Previous works such as [152] and [153] concluded that the evidence for EDE decreases when including galaxy clustering or cosmic shear data. Such works have used Planck 2018 CMB data for primary CMB and DES-Y1 or KiDS data for large-scale structure. We confirm their conclusions by reanalysing early dark energy models with recent data from DES-Y3. A word of caution is needed since, as mentioned earlier, there is an internal tension in DES-Y3 analysis using the REDMAGIC lens sample, which could introduce biases in the dark energy parameter constraints. For this reason in addition to the complete 3x2pt analysis we also present an analysis using cosmic shear data only, which is insensitive to this tension that appears only in the clustering amplitude.

Figure 6.1 shows confidence contours using the dataset DC1 combined with DES-Y3 data. More details are presented in Table 6.4, where we show the marginalized constraints on the parameters H_0 , S_8 and f_{EDE} for DC1 and DC2 comparing the effect of including DES-Y3 3x2pt and cosmic shear-only data. We observe no significant differences between 3x2pt and cosmic shear only constraints and thus conclude that the REDMAGIC internal tension does not significantly affect the EDE constraints. We plan a future in-depth analysis comparing EDE constraints from each of the galaxy lens samples and using a X_{lens} bias correction factor [127] in order to assess this robustness.

Due to the S_8 tension and its positive correlation with f_{EDE} , adding large-scale structure data decreases the EDE contribution and worsens the Hubble tension. For the combination DC1, we find:

$$\begin{aligned} f_{\text{EDE}} &= 0.087^{+0.028}_{-0.035} \text{ (DC1),} \\ f_{\text{EDE}} &= 0.067^{+0.019}_{-0.025} \text{ (DC1+DES-Y3 } \xi_{\pm}), \\ f_{\text{EDE}} &= 0.063^{+0.019}_{-0.024} \text{ (DC1+DES-Y3 3x2pt).} \end{aligned} \quad (6.18)$$

As expected, including DES-Y3 data results in a significant decrease on the estimated amount of EDE during recombination, disfavoring f_{EDE} values which solve the Hubble tension, i.e. around 10%.

We also compare our results of including either Y1 or Y3 data in our analyses below. For the combination DC1, the EDE constraints are

$$\begin{aligned} f_{\text{EDE}} &= 0.072^{+0.022}_{-0.029} \text{ (DC1+DES-Y1 } \xi_{\pm}), \\ f_{\text{EDE}} &= 0.057^{+0.018}_{-0.023} \text{ (DC1+DES-Y1 3x2pt).} \end{aligned} \quad (6.19)$$

In the Y1 analysis, we observe a small difference in the posterior means between 3x2pt and cosmic shear constraints, as the former imposes tighter constraints on f_{EDE} than the latter. This difference is smaller in the Y3 analysis. The same happens for the combination DC2, without CMB lensing:

$$\begin{aligned}
 f_{\text{EDE}} &= 0.081^{+0.022}_{-0.031} \text{ (DC2+DES-Y1 } \xi_{\pm}), \\
 f_{\text{EDE}} &= 0.064^{+0.017}_{-0.024} \text{ (DC2+DES-Y1 3x2pt),} \\
 f_{\text{EDE}} &= 0.075^{+0.019}_{-0.030} \text{ (DC2+DES-Y3 } \xi_{\pm}), \\
 f_{\text{EDE}} &= 0.068^{+0.020}_{-0.026} \text{ (DC2+DES-Y3 3x2pt).}
 \end{aligned} \tag{6.20}$$

The inclusion of DES-Y3 3x2pt correlation functions shifts H_0 by -0.6σ (increasing the tension with SH0ES data) and S_8 by -1.3σ (decreasing the tension with DES-Y3-only constraints on S_8). Figure 6.2 shows that the inclusion of DES-Y3 data worsens the H_0 tension solution, now above 1σ level. Figure 6.3 also shows that the inclusion of DES data slightly worsens the CMB fit. This effect is the main motivation to further extend the EDE scenario. In the following section, we explore whether substituting smooth dark energy for the cosmological constant can increase again the EDE contribution that results in a smaller H_0 tension.

6.4.2 Marginalization over Late-time Expansion

In this section we are interested in the study of models with modifications to the standard Λ CDM model that account simultaneously for both early dark energy and a generic late dark energy parametrization, the latter characterized by a piecewise constant equation of state in different redshift bins. This parametrization will be tested with the different datasets described in section 6.3.5.

Analysing the dark energy equation of state in detail during the so-called rise of dark energy age [196] is an ambitious task by itself. Since this study is not directly related to EDE, we describe it in appendix C.2, where we show an estimation of the reconstruction of the late dark energy equation of state and a principal component analysis on its components w_i .

Since we are interested in the possible impact of these models on the EDE parameter estimations together with the H_0 and S_8 tensions, we focus our attention on the results obtained from marginalizing over the late-time dark energy parameters. More specifically, we show results marginalized for 3, 5 and 10 redshift bins of constant $w(z)$, using the effective fluid EDE model with $n = 3$.

Our investigations are summarized in Fig. 6.4, which shows marginalized 1D constraints (mean and 68% limits) for the parameters H_0 , S_8 and f_{EDE} for the dataset combinations DC1 and DC2, without and with DES data and for three different number of bins for late dark energy. Results for DES-Y1 and DES-Y3 are shown in order to assess the impacts of the updated data set and analysis in our

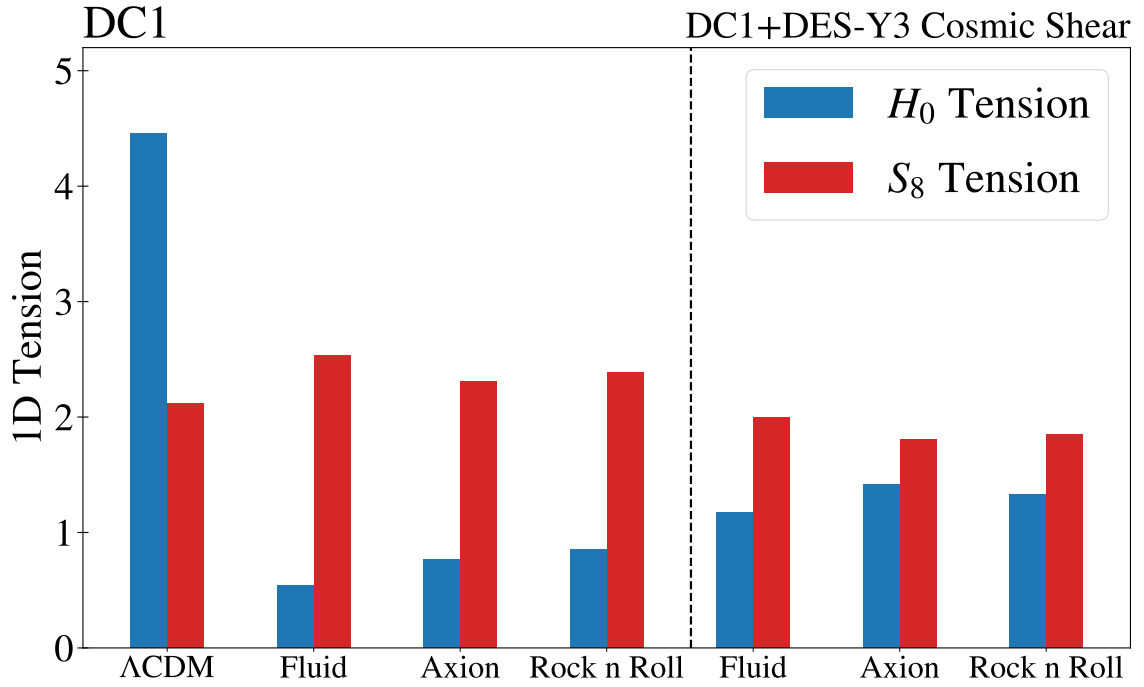


Figure 6.2: 1D tensions between our analysis and [21] (for the H_0 tension) or [127] (for the S_8 tension). To the left of the vertical dashed line, we are using the dataset combination DC1 ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum; to the right, we add DES-Y3 cosmic shear data. The horizontal axis represents different early dark energy model choices.

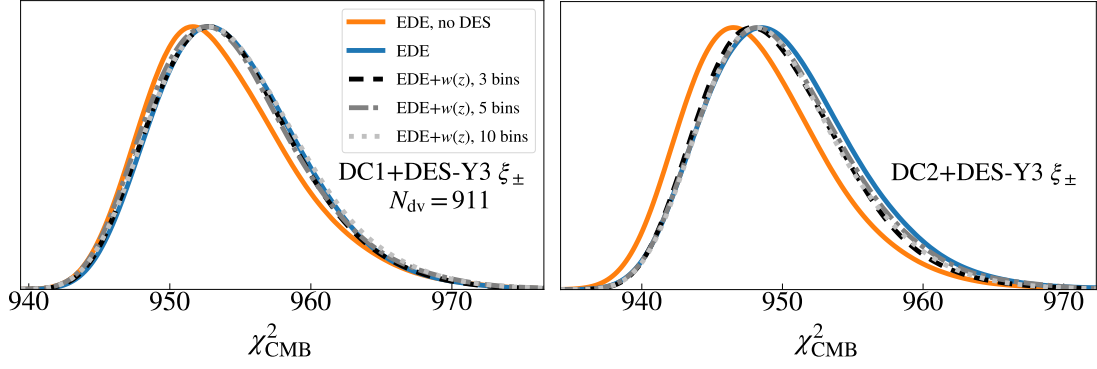


Figure 6.3: χ^2_{CMB} (911 points) distributions in the MCMCs using the dataset combinations DC1 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) and DC2 (same as DC1 without CMB Lensing), combined with DES-Y3 cosmic shear data, under the effective fluid EDE model and EDE + $w(z)$ with 3, 5 and 10 bins. We also include EDE results without DES data.

results. The values for the posterior means and 68% limits are shown in Table 6.4. Constraints for the datasets DC3, DC4 and DC5 are shown in appendix C.1 as robustness tests.

For DC1, DC3, DC4 and DC5 combined with DES data, we have found that adding the binned $w(z)$ model does not make a significant difference in f_{EDE} constraints, regardless of the number of redshift bins.

Interestingly, for the DC2 dataset (i.e. without CMB lensing) combined with DES data, the inclusion of a dynamical smooth dark energy fluid at late-times does slightly affect the S_8 and f_{EDE} constraints. The effect, although very small, can be seen in all DES analyses and redshift binning choices. As shown in Table 6.4, when including the binned $w(z)$ model, the f_{EDE} posterior mean is increased by 0.01. This corresponds to a 0.5σ shift, well within the error bars. The S_8 posterior mean also slightly decreases by approximately 0.4σ , which improves the fit to DES data. Figure 6.3 also shows that, for the combination of DC2 and DES-Y3 cosmic shear, the late-time modification can also slightly improve the CMB fit. However, this increase in f_{EDE} does not come with an increase in H_0 : we observe no significant shift in H_0 posterior. It seems the $w(z)$ models that are able to decrease S_8 also tend to decrease H_0 . As CMB lensing further constrains the dark energy equation of state in redshifts $z < 3$, no f_{EDE} shifts can be detected in the other dataset combinations.

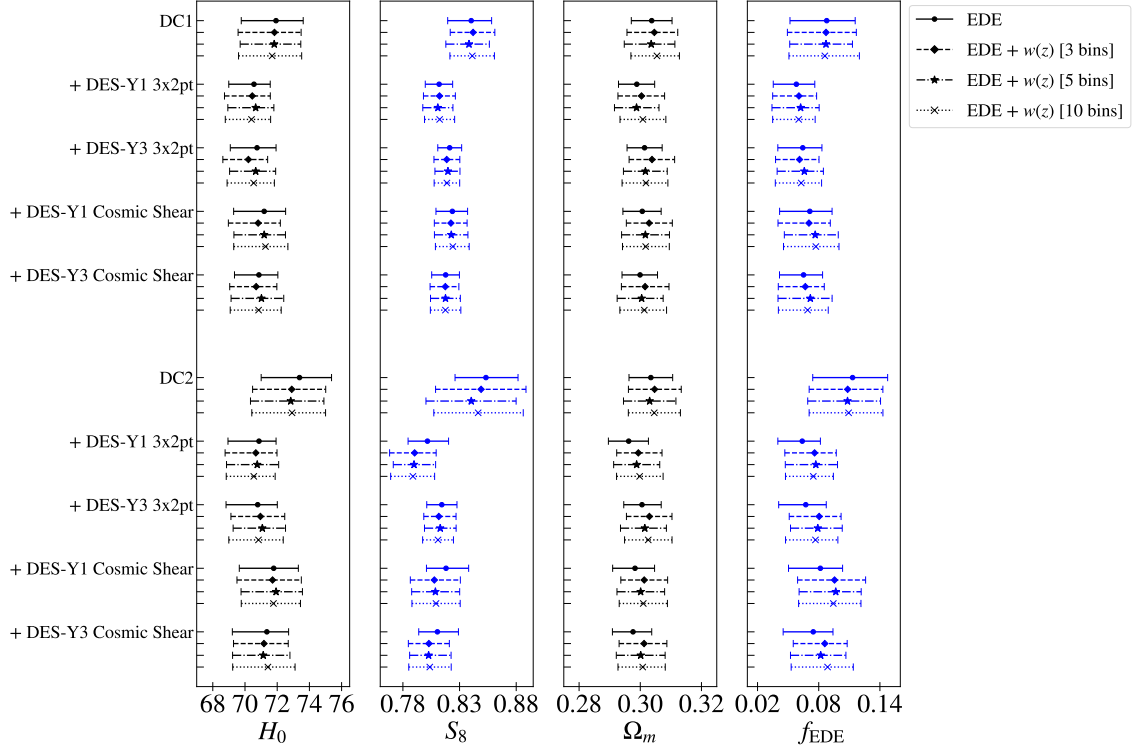


Figure 6.4: Marginalized constraints for H_0 (in $\text{km s}^{-1} \text{Mpc}^{-1}$), S_8 , Ω_m and f_{EDE} , using the dataset combinations DC1 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) and DC2 (same as DC1 without CMB Lensing). For each combination, we add DES 3x2-point correlation functions and cosmic shear-only data. DES-Y1 and DES-Y3 are shown in order to assess the impacts of the updated data set and analysis in our results. We use the effective fluid EDE model presented in section 6.2.1 combined with a late-time fluid with piecewise equation of state, described in section 6.2.2, using 3, 5 and 10 redshift bins. We observe no significant shifts in the parameter constraints due to the modification of smooth dark energy at late times, regardless of the number of redshift bins in our model.

Model/Dataset	H_0 (km s ⁻¹ Mpc ⁻¹)	$10 \times S_8$	$100 \times f_{\text{EDE}}$
DC1			
Λ CDM	$68.09^{+0.49}_{-0.49}$	8.21 ± 0.13	—
EDE	$71.9^{+1.6}_{-2.1}$	$8.40^{+0.18}_{-0.20}$	$8.7^{+2.8}_{-3.5}$
EDE + 3-bin $w(z)$	$71.8^{+1.7}_{-2.3}$	8.41 ± 0.19	$8.7^{+2.9}_{-3.8}$
EDE + 5-bin $w(z)$	$71.8^{+1.7}_{-2.1}$	8.38 ± 0.19	$8.7^{+2.8}_{-3.5}$
EDE + 10-bin $w(z)$	$71.6^{+1.8}_{-2.1}$	$8.41^{+0.18}_{-0.20}$	$8.4^{+3.2}_{-3.6}$
DC1+DES-Y3 $\xi_{\pm}$			
EDE	$71.0^{+1.2}_{-1.6}$	8.18 ± 0.12	$6.7^{+1.9}_{-2.5}$
EDE + 3-bin $w(z)$	$70.6^{+1.3}_{-1.7}$	8.17 ± 0.13	$6.7^{+1.9}_{-2.7}$
EDE + 5-bin $w(z)$	$71.0^{+1.3}_{-1.9}$	8.17 ± 0.13	$7.2^{+2.0}_{-3.1}$
EDE + 10-bin $w(z)$	$70.9^{+1.4}_{-1.8}$	8.18 ± 0.13	$7.0^{+2.1}_{-2.9}$
DC1+DES-Y3 3x2pt			
EDE	$70.7^{+1.1}_{-1.6}$	8.21 ± 0.10	$6.3^{+1.9}_{-2.4}$
EDE + 3-bin $w(z)$	$70.3^{+1.3}_{-1.6}$	8.19 ± 0.11	$6.3^{+1.9}_{-2.5}$
EDE + 5-bin $w(z)$	$70.7^{+1.2}_{-1.6}$	8.19 ± 0.11	$6.6^{+1.9}_{-2.4}$
EDE + 10-bin $w(z)$	$70.6^{+1.2}_{-1.6}$	8.19 ± 0.11	$6.4^{+2.0}_{-2.6}$
DC2			
Λ CDM	$68.06^{+0.56}_{-0.56}$	8.22 ± 0.17	—
EDE	$73.3^{+2.1}_{-2.5}$	$8.53^{+0.27}_{-0.31}$	$11.2^{+3.6}_{-4.3}$
EDE + 3-bin $w(z)$	$73.0^{+2.1}_{-2.6}$	8.49 ± 0.41	$11.0^{+3.3}_{-4.1}$
EDE + 5-bin $w(z)$	$72.8^{+2.0}_{-2.5}$	8.38 ± 0.39	$10.7^{+3.3}_{-3.9}$
EDE + 10-bin $w(z)$	$72.9^{+2.1}_{-2.5}$	8.46 ± 0.40	$10.9^{+3.4}_{-3.9}$
DC2+DES-Y3 $\xi_{\pm}$			
EDE	$71.4^{+1.3}_{-2.1}$	8.11 ± 0.17	$7.5^{+1.9}_{-3.0}$
EDE + 3-bin $w(z)$	$71.2^{+1.6}_{-2.0}$	$8.03^{+0.19}_{-0.17}$	$8.6^{+2.4}_{-3.2}$
EDE + 5-bin $w(z)$	$71.2^{+1.6}_{-1.9}$	$8.02^{+0.20}_{-0.17}$	$8.4^{+2.4}_{-3.2}$
EDE + 10-bin $w(z)$	$71.3^{+1.6}_{-2.2}$	8.03 ± 0.19	$8.7^{+2.5}_{-3.5}$
DC2+DES-Y3 3x2pt			
EDE	$70.9^{+1.3}_{-1.9}$	8.15 ± 0.13	$6.8^{+2.0}_{-2.6}$
EDE + 3-bin $w(z)$	$70.9^{+1.5}_{-1.8}$	$8.12^{+0.15}_{-0.13}$	$8.0^{+2.1}_{-2.9}$
EDE + 5-bin $w(z)$	$71.1^{+1.5}_{-1.8}$	8.13 ± 0.14	$7.9^{+2.6}_{-2.6}$
EDE + 10-bin $w(z)$	$71.0^{+1.5}_{-1.9}$	8.12 ± 0.14	$7.9^{+2.2}_{-2.9}$

Tabela 6.4: Marginalized constraints (mean and 68% limits) for the parameters H_0 , S_8 and f_{EDE} for the dataset combinations DC1 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) and DC2 (same as DC1 without CMB Lensing). We also combine both P1 and Base with DES-Y3 3x2-point correlations and cosmic shear.

6.5 Conclusions

Cosmological tensions in H_0 and, to a lesser extent, in S_8 , are challenging the standard Λ CDM model. If not explained by systematic effects, they may point to new physics. The presence of a non-negligible amount of dark energy around the recombination era, postulated in early dark energy models, has become a candidate solution for the Hubble tension, especially in light of new CMB data from ACT and SPT-3G. Cosmic shear and galaxy clustering data, however, disfavor the presence of EDE, since they aggravate the S_8 tension with CMB. This has been observed in previous analysis using Planck 2018, DES-Y1, KiDS and HSC data [152, 153]. Our work extends previous ones in several directions: incorporating the recent DES-Y3 data, analysing different combination of datasets and modifying the late dark energy model by allowing a smooth (unperturbed) dark energy completely characterized by its equation of state.

We also find that including recent large-scale structure data from DES-Y3 decreases the contribution for EDE and that this is robust for different combinations of datasets. For the combination DC1 we find $f_{\text{EDE}} = 0.087^{+0.028}_{-0.035}$, compared to $f_{\text{EDE}} = 0.067^{+0.019}_{-0.025}$ when DES-Y3 cosmic shear data is included, and $f_{\text{EDE}} = 0.063^{+0.019}_{-0.023}$ using DES-Y3 3x2pt data. This effect makes EDE more unlikely as a Hubble tension solution. Our main conclusion is that smooth, late-time dark energy modifications cannot restore the EDE contribution to its significance without large-scale structure data. Using the DC1 combination and DES-Y3 cosmic shear data, we find $f_{\text{EDE}} = 0.067^{+0.019}_{-0.027}$ for 3 redshift bins, $f_{\text{EDE}} = 0.072^{+0.020}_{-0.031}$ for 5 bins and $f_{\text{EDE}} = 0.070^{+0.021}_{-0.029}$ for 10 bins. Varying the number of redshift bins does not add information to early-time dark energy constraints.

If we are to consider EDE as a solution to the Hubble tension, we must address the S_8 tension with either systematic effects or theoretical models beyond the smooth dark energy paradigm, for instance changing the mechanisms for clustering of matter, as done in [165, 197, 198]. In future works, we will analyse the combination between EDE and more general dark energy paradigms such as including anisotropic stress, modifying the sound speed, adding interactions between dark energy and CDM, among others. Our results drives future research to other mechanisms affecting S_8 beyond the smooth dark energy paradigm combined with early dark energy models.

Chapter 7

Late-time Dark Energy Dynamics and Massive Neutrinos In Light of DESI Y1 BAO

This chapter discusses the recent DESI Y1 BAO results which indicate a strong preference for dynamical dark energy [50], which could represent the first hint for dynamical dark energy. This chapter also presents the article "Investigating Late-time Dark Energy and Massive Neutrinos in Light of DESI Y1 BAO" [24], which is reproduced below with permission from the Journal of Cosmology and Astroparticle Physics.

7.1 Introduction

The nature of dark energy persists as one of the greatest mysteries in current physics. Ever since the discovery of accelerated expansion in 1998 [199, 200], the cosmological constant Λ has become the accepted model of dark energy, due to its simplicity and ability to fit various independent observables: Type Ia supernovae luminosity distances [201, 202, 181, 36, 37, 39, 40], distance measurements from Baryonic Acoustic Oscillations (BAOs) [9, 66, 203, 60, 204, 205, 67, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 50, 217], Cosmic Microwave Background (CMB) temperature and polarization anisotropies [10, 43, 11, 218, 44, 5, 45, 48], two-point correlation functions of galaxy shapes and positions [219, 80, 58, 54, 53, 8], among other probes. The success of the Λ CDM model, which assumes a cosmological constant as dark energy, has ushered in an era of precision cosmology, in which increasingly ambitious surveys can track the expansion of the Universe and the growth of large-scale structure with great precision. However, the Λ CDM model faces several challenges. From a theoretical standpoint, its connection with the Standard Model of Particle Physics (SM) is not well understood: the dark energy density is orders of magnitude lower than the vacuum energy density of the SM fields [220, 221]. Furthermore, in recent years, different datasets have disagreed in their measured values of the Λ CDM cosmological parameters. The most pressing tension is in the H_0 parameter, the current expansion rate of the universe, between

local distance measurements [41] and those inferred by CMB measurements (see [222] for a recent review). Less statistically significant tensions, such as the S_8 parameter tension between CMB and cosmic shear surveys [223, 54], aggravate the Λ CDM crisis. In this context, the last decade witnessed an explosion of alternative cosmological models trying to alleviate tensions and provide insights about the fundamental nature of dark energy [142, 224, 225, 226, 227, 228, 229, 230, 231, 99, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 122, 242].

A recent hint on deviations from the Λ CDM model arising from new type Ia supernovae analyses from both Dark Energy Survey 5-year dataset (DESY5) [40] and Union3 [38] became more prominent with the new BAO distance measurements from DESI [50]. The dataset combination of DESI BAO with Planck 2018 CMB anisotropies [5] and Type Ia supernovae distances from either Pantheon+ [36], Union3 [37], or DESY5 [39] significantly prefers a dynamical dark energy behavior, with confidence ranging from $2.5\sigma - 3.9\sigma$ depending on which supernovae catalog is being used. DESI analysis relied on the widely used w_0w_a parametrization of dark energy: a phenomenological model where the equation of state evolves linearly with scale factor as $w(a) = w_0 + w_a(1 - a)$. The preferred dark energy behavior in the DESI analysis has a phantom behavior ($w < -1$) [243] for redshifts $z > 0.5$ and a thawing behavior with $w > -1$ nowadays. The main driver of this evidence is still under debate [244, 245, 246]. While [50] points that the Luminous Red Galaxy samples between redshifts $0.6 < z < 0.8$ drive this preference [247], reference [248] has shown that under the Λ CDM model there is a mild tension in the Ω_m parameter between DESI BAO and the Pantheon+, Union3, and DESY5 supernovae catalogs, which is alleviated by thawing dynamical dark energy. Parameter constraints using the Pantheon supernovae catalog, which agrees with DESI on Ω_m , are consistent with Λ CDM. However, the Pantheon+ analysis improves over the original Pantheon on several aspects, such as an updated light curve model, which takes into account galactic dust and an improved model for intrinsic brightness evolution [249], among others. It has also been noted that the preference for an evolving dark energy equation of state depends on priors for w_0 and w_a [250, 251, 252].

These intriguing clues for dynamical dark energy resulted in a flurry of studies considering more complex behaviors for the dark energy equation of state than the monotonic w_0w_a parametrization. Some examples are scalar field quintessence models [248, 253, 254, 255, 256], higher order terms in the Taylor expansion of the equation of state of dark energy around the present epoch [257], different 2-parameter descriptions of the equation of state [258] and other generalizations [259], modified gravity [260, 261], Gaussian Processes [262, 263, 264], interacting dark energy models [265], non-minimally coupled gravity [266], emergent dark energy model [267] and a modified recombination history [268], sterile neutrinos and modified gravity [269], a negative cosmological constant [270], early dark energy [271], among others [272].

A preference for dynamical dark energy over a cosmological constant also

has implications for other model components. Cosmological probes have been putting increasingly stringent constraints on the neutrino mass sum [273, 274, 275, 276, 277, 278, 279, 280, 281, 282], culminating with the recent constraints from the dataset combination of Planck 2018 CMB data and DESI BAO, assuming Λ CDM: $\sum m_\nu \leq 0.072$ eV at 95% confidence level (CL) [50]. These results are close to the lower bounds inferred from neutrino oscillation experiments, either for the normal-ordered hierarchy ($\sum m_\nu \geq 0.057$ eV) or for an inverted-ordered hierarchy ($\sum m_\nu \geq 0.10$ eV) [283, 284, 285]. One could argue that the inverted hierarchy has been ruled out in the context of the Λ CDM model. In addition, as large-scale structure surveys obtain more precise measurements, a tension between cosmological and laboratory neutrino mass constraints could arise [286, 287, 288, 289, 290, 291, 292, 293, 294]. Therefore, studying the bounds on the sum of neutrino masses in other cosmological models and datasets and their robustness under model assumptions and analysis choices is essential [295, 296]. Previous studies have pointed to a preference for negative cosmological neutrino masses, which tighten the neutrino mass constraints and could be a hint for new physics [290, 291, 297]. Several works on neutrino masses, taking into account the DESI data, appeared recently. For example, [289] and [290] study the robustness of the DESI results concerning neutrino masses; neutrino mass constraints under Λ CDM, w CDM and w_0w_a CDM and with a non-phantom w_0w_a CDM with the different hierarchy choices have been addressed in [286] and [287], and modifications due to new interactions between neutrinos and dark matter were considered in [288].

This work investigates general dark energy models using DESI BAO data alongside Type Ia supernovae distance catalogs and CMB anisotropy and lensing data. We test three models: a phenomenological model with a transition of $w(z)$ between two values, a model-agnostic parametrization in which $w(z)$ is a piecewise-constant function over given redshift bins, and a scalar field model. Quintessence models, where dark energy is related to a scalar field minimally coupled to gravity with a canonical kinetic term, are restricted to have an equation of state $w \geq -1$. To reproduce a phantom behavior, we focus on the monodromic k-essence (MKE) model introduced in [298], in which the dark energy equation of state can be oscillatory. After assessing the model parameter constraints and the $w(z)$ dynamical behavior preferred by different combinations of datasets, we compare the dark energy models by how they can improve the goodness-of-fit to each dataset, penalizing models with an increased number of parameters. Furthermore, we reassess the constraints on the neutrino mass sum considering the model-agnostic parametrization of dark energy as compared to the usual w_0w_a CDM model, obtaining constraints for $\sum m_\nu$ that are marginalized over the dark energy equation of state at late times.

7.2 Dark Energy Models

To perform tests of dynamical dark energy, we consider models that allow a phantom crossing of $w(z)$. The transition parametrization in Section 7.2.1 captures the transition between two values of $w(z)$; the binned $w(z)$ parametrization in Section 7.2.2 is a more general model that is agnostic to the redshift evolution of dark energy. Alongside these phenomenological choices, in Section 7.2.3, we also analyze the monodromic k-essence model: a scalar field with non-canonical lagrangian.

7.2.1 Transition model

This model represents an equation of state that smoothly transitions between two values: w_1 at early times and w_0 at late times. The dark energy equation of state is parametrized as

$$w(z) = w_0 + \left(\frac{w_1 - w_0}{2} \right) \left(1 + \tanh \left(\frac{z - z_c}{\sigma} \right) \right). \quad (7.1)$$

For high redshifts, $z - z_c \gg \sigma$, $w(z) \approx w_1$; conversely, for $z < z_c$ and $|z - z_c| \gg \sigma$, $w(z) \approx w_0$. The parameter z_c is the redshift in which the transition is at its midpoint: $w(z_c) = (w_0 + w_1)/2$. σ is a parameter that controls the redshift width of the transition: smaller values of σ represent faster transitions, while larger values of σ represent slower transitions. The energy density of this model is obtained via the integral

$$\rho_{\text{DE}} = \Omega_{\text{DE}} \rho_{\text{cr}} \exp \left(3 \int_0^z \frac{1 + w(z')}{1 + z'} dz' \right), \quad (7.2)$$

where $\rho_{\text{cr}} = 3H_0^2/(8\pi G)$, $\Omega_{\text{DE}} = 1 - \Omega_m - \Omega_r$ and the integral is calculated numerically. This model has four parameters: w_0 , w_1 , z_c and σ . We choose to fix $\sigma = 0.05$ throughout our analysis: this value is sufficiently small to guarantee a fast transition within a redshift window of $\Delta z < 0.1$. For completeness, in Appendix D.3 we present results for varying σ .

This model crosses the phantom barrier at $w = -1$ if w_0 and w_1 are chosen such that $(1 + w_0)(1 + w_1) < 0$. To avoid instabilities, we use the Parametrized Post-Friedmann (PPF) approach to calculate the dark energy perturbations [299, 94, 300].

7.2.2 Binned $w(z)$

In this model, the dark energy equation of state is given by constant values inside several redshift bins with limits $\{0, z_1, z_2, \dots, z_N\}$. The equation of state can be written as

$$w(z) = \begin{cases} w_0, & \text{if } z < z_1; \\ w_1, & \text{if } z_1 \leq z < z_2; \\ w_2, & \text{if } z_2 \leq z < z_3; \\ \dots & \\ w_{N-1}, & \text{if } z_{N-1} \leq z < z_N; \\ -1, & \text{if } z > z_N. \end{cases} \quad (7.3)$$

At redshifts larger than the last bin, we set $w = -1$. This model can approximate any smooth dark energy model that varies slowly inside each redshift bin. Increasing the number of redshift bins improves the generality of this parametrization by making the bins narrower. However, adding many extra parameters to the model makes the analysis more computationally expensive. We focus on the dark energy behavior at very low redshifts $z < 1$, when dark energy becomes dominant in the background energy density and many supernovae are detected.

Thus, we choose two strategies of redshift binning, with 5 and 10 bins, respectively, with constant redshift intervals:

- $z_i = 0.3 \times i, i = 1, \dots, 5;$
- $z_i = 0.1 \times i, i = 1, \dots, 10.$

Even though there are SN and BAO distance measurements at higher redshifts, we restrained ourselves to the low redshift windows of $z < 1$ and $z < 1.5$. For $z > 2$, dark energy comprises less than 10% of the Universe's energy density, having a reduced impact on the expansion history. Furthermore, there are fewer supernovae measurements for redshifts $z > 1$ and no DESY5 supernovae for $z > 1.13$, degrading the dark energy constraints above those redshifts. In addition, it is claimed by [50] that the DESI measurements that cause the preference for dynamical dark energy are those inferred from the Luminous Red Galaxy samples at redshifts $0.6 < z < 0.8$. As previous analyses from literature (e.g., [301]) suggest a phantom crossing at redshifts $z \approx 0.5$, we focus on the dynamics close to this redshift.

By imposing the continuity of the dark energy density in the edge of two consecutive redshift bins, we obtain the following expression for the evolution of the energy density

$$\rho_{\text{DE}}(z_i < z < z_{i+1}) = \Omega_{\text{DE}} \rho_{\text{cr}} \left(\prod_{j=1}^i (1 + z_j)^{3(w_{j-1} - w_j)} \right) (1 + z)^{3(1 + w_i)}. \quad (7.4)$$

As before, we use the PPF framework to compute the dark energy perturbations for this model. For robustness, we have implemented a continuous version of the discontinuous binned $w(z)$ given in Equation (7.3). In Appendix D.2, we compare results between the discontinuous and continuous versions of the model, assessing differences in parameter constraints and goodness-of-fit. We conclude that the discontinuity in $w(z)$ does not affect our analysis.

7.2.3 Monodromic k-essence

K-essence is a scalar field, minimally coupled to gravity, differing from quintessence by having a non-canonical lagrangian [86, 302, 88, 303, 304]. Assuming the flat Friedmann-Robertson-Walker metric with signature $(-, +, +, +)$, a general scalar field action can be written as

$$S = \int d^4x \sqrt{-g} P(X, \phi), \quad (7.5)$$

where X is the kinetic term of the scalar field given by

$$X = -\frac{1}{2} \nabla_\mu \phi \nabla^\mu \phi. \quad (7.6)$$

Non-canonical kinetically-driven fields [86], in which $P(X, \phi)$ is of the form

$$P(X, \phi) = V(\phi)(-X + X^2), \quad (7.7)$$

can exhibit tracking behavior and scaling solutions as in some quintessence models but are not restricted to an equation of state $w \geq -1$. We use the monodromic k-essence (MKE) model introduced in [298], where the function $V(\phi)$ is given by

$$V(\phi) = C \left(\frac{\phi}{\phi_0} \right)^{-\alpha} (1 - A \sin(\nu\phi)). \quad (7.8)$$

The energy density and equation of state of the field are given by

$$\rho_K = 2X \frac{\partial P}{\partial X} - P = V(\phi)X(-1 + 3X), \quad (7.9a)$$

$$w_K = \frac{P(X, \phi)}{\rho_K} = \frac{1 - X}{1 - 3X}. \quad (7.9b)$$

To find the field evolution in time, we must integrate a second-order differential equation for ϕ , a generalization of the Klein-Gordon equation for quintessence. Considering the specific form of the lagrangian $P(X, \phi)$ in Equation 7.7, the equa-

tion of motion is

$$\dot{X} = \frac{-V'(\phi)\sqrt{2X}(-X + 3X^2) - 6HV(\phi)X(-1 + 2X)}{V(\phi)(6X - 1)}, \quad (7.10)$$

where overdots indicate derivatives with respect to cosmic time t and H is the Hubble factor. Our implementation solves the equation above numerically for X , alongside the equation for the homogeneous background field ϕ

$$\dot{\phi} = \sqrt{2X}. \quad (7.11)$$

Like quintessence, this scalar field model exhibits tracking behavior: many initial conditions quickly converge to an attractor that determines the field evolution [305]. This makes today's dark energy behavior highly insensitive to the field's initial conditions. Thus, we choose initial conditions according to the tracking solution [298]. We adjust the parameter C to ensure the closure relation today, $\sum_{\text{all species}} \rho_i / \rho_{\text{cr}} = 1$, using the secant method. The remaining model parameters are α , A , and ν , as ϕ_0 is fixed to $1 M_{\text{pl}}$ without loss of generality. The MKE equation of state w_K is approximately constant at high redshifts; when dark energy starts dominating the background density, w_K begins oscillating. Figure 7.1 shows evolutions of w_K varying each parameter α , A and ν individually. The parameter α controls the mean value of w_K , denoted by $\bar{w}_K$, which is approximated by

$$\bar{w}_K = -1 + \frac{\alpha}{2}. \quad (7.12)$$

While the original reference [298] restricted its description for $\alpha > 0$, we also consider the cases where $\alpha < 0$, in which the function $V(\phi)$ has a positive power law. This makes the equation of state w_K oscillate around $\bar{w}_K < -1$, which is relevant in light of the DESI results. The parameter A controls the amplitude of the oscillations, and ν controls the frequency of the oscillations. Frequency values $\nu \lesssim 1 M_{\text{pl}}^{-1}$ are too small such that $w_K(z)$ does not perform a complete oscillation, providing a monotonic behavior as shown in the bottom panel of Figure 7.1.

The perturbations of the k-essence field $\delta\phi$ in the synchronous gauge are governed by the equation [87]

$$A\delta\phi'' + B\delta\phi' + C\delta\phi + D = 0, \quad (7.13)$$

where the primes $'$ denote derivatives with respect to conformal time $d\tau = dt/a$,

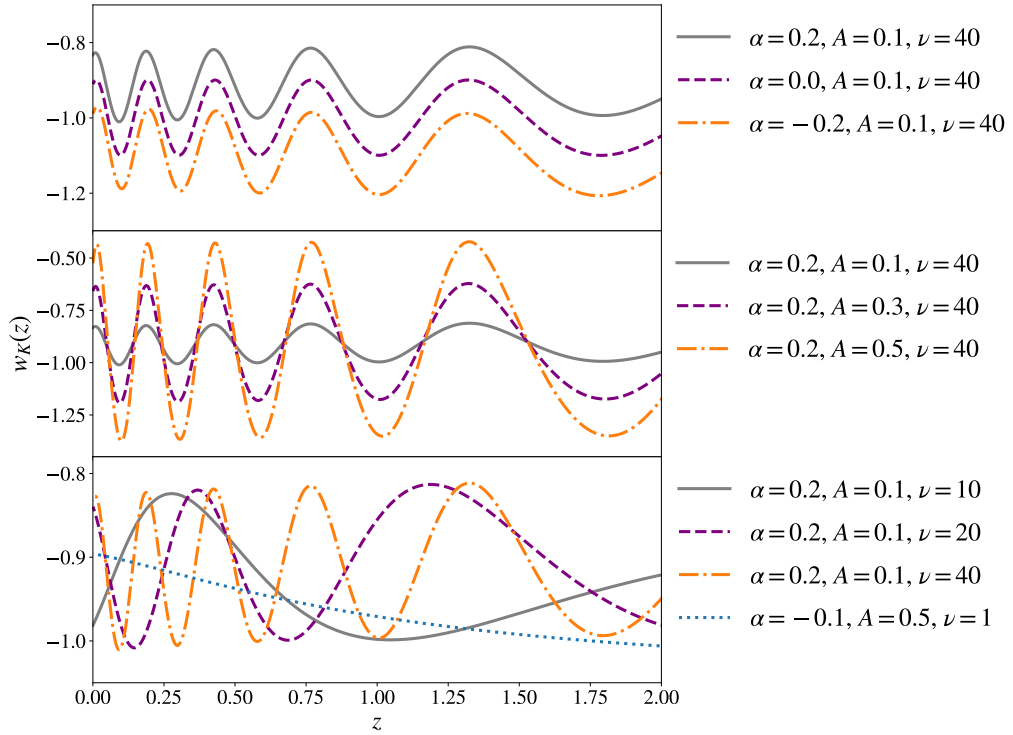


Figure 7.1: Evolution of the monodromic k-essence equation of state w_K for selected potential parameter values. The top row shows variations of the α parameter, the middle row shows variations of A and the bottom row shows variations of ν (in units of M_{pl}^{-1}).

and the coefficients are

$$A = P_{,XX} \frac{\phi'^2}{a^2} + P_{,X}, \quad (7.14a)$$

$$B = 2\mathcal{H}P_{,X} + P_{,XXX} \frac{X'\phi'^2}{2} + P_{,XX\phi} \frac{\phi'^3}{a^2} + P_{,XX} \left(3 \frac{\phi'\phi''}{a^2} - \frac{\mathcal{H}\phi'^2}{a^2} \right) + P_{,X\phi}\phi', \quad (7.14b)$$

$$C = -a^2 P_{,\phi\phi} + k^2 P_{,X} + P_{,XX\phi} X'\phi' + P_{,X\phi}\phi'' + P_{,X\phi\phi}\phi'^2 + 2\mathcal{H}P_{,X\phi}\phi', \quad (7.14c)$$

$$D = 3P_{,X}h\phi', \quad (7.14d)$$

where the commas represent partial derivatives (i.e. $P_{,X} = \partial P / \partial X$), $\mathcal{H} = a' / a$ is the conformal Hubble factor and h is the synchronous gauge curvature perturbation. The perturbed energy-momentum tensor components in synchronous gauge can be written as

$$\delta\rho_K = P_{,X}\delta X - P_{,\phi}\delta\phi + 2XP_{,XX}\delta X + 2XP_{,X\phi}\delta\phi, \quad (7.15a)$$

$$\delta P_K = P_{,X}\delta X - P_{,\phi}\delta\phi, \quad (7.15b)$$

$$(\rho_K + P_K)v_K = P_{,X}k\phi'\delta\phi/a^2, \quad (7.15c)$$

where $\delta X = \phi'\delta\phi'/a^2$. While we are interested in its background properties, this model is also interesting for having a sound speed $c_s^2 \approx 0$, which can induce dark energy perturbations and impact structure formation significantly. We include the k-essence perturbations in our numerical implementation of the model. While a phantom crossing for a general scalar field lagrangian would evoke instabilities in its perturbations [96, 97], these instabilities are avoided by the fact that the effective sound speed c_s^2 vanishes at the phantom crossing [306].

7.3 Datasets and Analysis Methodology

7.3.1 DESI 2024 BAO

The Dark Energy Spectroscopic Instrument has measured the baryonic acoustic oscillation signal from galaxy clustering correlations using three different tracers of matter: galaxies, quasars [64] and the Lyman- α forest [307]. The tracers are spread over a redshift range $0.1 < z < 4.2$, divided into seven bins. Measuring the 2-point correlation function of tracer positions, one can identify the sound horizon at the baryon drag epoch, z_d , defined as

$$r_d = \int_{z_d}^{\infty} \frac{c_s(z)}{H(z)} dz, \quad (7.16)$$

where $c_s(z)$ is the baryon-photon fluid sound speed. This physical scale can be used as a ruler to measure the transverse comoving distance to the tracers at each redshift bin, which, in a flat Universe, is given by

$$D_M(z) = c \int_0^z \frac{dz'}{H(z')}, \quad (7.17)$$

and the Hubble factor at the tracer redshift, which can be mapped to a distance measurement via

$$D_H(z) = \frac{c}{H(z)}. \quad (7.18)$$

The BAO measurements constrain the quantities $D_M(z)/r_d$ and $D_H(z)/r_d$. Throughout the rest of this work, we refer to this dataset simply as DESI.

7.3.2 Type Ia Supernovae Catalogs

Type Ia supernovae catalogs provide luminosity distance measurements, given by

$$D_L(z) = c(1+z) \int_0^z \frac{dz'}{H(z')}. \quad (7.19)$$

In this work, we use four different catalogs. The Pantheon light-curve sample is a collection of 1048 Type Ia supernovae, covering the redshift range $0.01 < z < 2.3$ [308]. The Pantheon+ catalog comprises 1701 light curves measured from 1550 Type Ia supernovae over the redshift range $0.001 < z < 2.26$. The Union3 catalog consists of 2087 Type Ia supernovae over the redshift range $0.01 < z < 2.26$, and the public data consists of binned distance measurements [38]. The Dark Energy Survey Year 5 (DESY5) catalog consists of 1635 Type Ia supernovae over the redshift range $0.1 < z < 1.13$ [40]. We will refer to these supernovae catalogs for conciseness as Pan, Pan+, Uni3, and DESY5, respectively.

7.3.3 Planck 2018 CMB

We use the Planck 2018 CMB temperature and polarization angular power spectra, including the `plik` likelihood for the TT, TE and EE spectra at multipoles $30 \leq \ell \leq 2508$, and the low multipole likelihoods `Commander` and `Small` for TT and EE spectra at multipoles $\ell < 30$ [309]. For conciseness, we will refer to this dataset as P18.

7.3.4 ACT DR4 CMB Temperature and Polarization Anisotropies

We use the ACT TT, TE, and EE power spectra from their Data Release 4, up to multipoles $\ell = 4000$. Due to the lack of large-scale polarization measurements,

ACT CMB data alone cannot constrain the reionization optical depth τ . Following [47], we supplement ACT data with Planck 2018 power spectra up to multipole $\ell = 650$. We will refer to this combination of ACT and Planck CMB data as ACT+P650.

7.3.5 ACT DR6 CMB Lensing Power Spectrum

The CMB lensing power spectrum, $\hat{C}_\ell^{\phi\phi}$, with multipoles range of $40 < \ell < 763$ in 10 bandpowers, are reported by the Atacama Cosmology Telescope (ACT) Data Release 6 (DR6) [310, 311]. ACT is a ground-based CMB survey that minimizes foreground and noise using a new pipeline, and from a lensing mass map covering 9400 deg^2 of the sky, they report measurements of the CMB lensing amplitude with a precision of 2.3%.

The theoretical prediction for the CMB lensing power spectrum, $C_\ell^{\phi\phi}$, is given by the line-of-sight integral projected onto the non-linear power spectrum P_{NL} [311]

$$C_\ell^{\phi\phi} = \int dz \frac{H}{c\chi(z)^2} [W^\kappa(z)]^2 P_{\text{NL}}(\ell/\chi(z), z) \quad (7.20)$$

where $W^\kappa(z)$ is the lensing kernel

$$W^\kappa(z) = \frac{3}{2} \Omega_m H_0^2 \frac{1+z}{H(z)} \frac{\chi(z)}{c} \left[\frac{\chi(z_\star) - \chi(z)}{\chi(z_\star)} \right]. \quad (7.21)$$

Since massive neutrinos suppress the matter power spectrum on scales smaller than the free-streaming, and dark energy also impacts the structure formation, CMB lensing is a good source of information for these components. We will refer to the ACT DR6 lensing dataset as ACTL.

7.3.6 Dataset Combinations

Among the individual datasets, several combinations can be analyzed. BAO measurements alone have a degeneracy between H_0 and r_d , which can be broken by the inclusion of CMB data. Supernovae distance measurements add extra geometric information, constraining the dark energy behavior at low redshifts. Thus, we consider combinations of CMB, BAO, and SN datasets. To assess the differences in parameter constraints among the multiple supernovae datasets, we combine each SN catalog with Planck 2018 CMB data and DESI BAO data, forming four different dataset combinations:

- Planck 2018 (P18) + DESI-Y1 BAO (DESI) + Pantheon (Pan);
- Planck 2018 (P18) + DESI-Y1 BAO (DESI) + Pantheon + (Pan+);

- Planck 2018 (P18) + DESI-Y1 BAO (DESI) + Union-3 (Uni3);
- Planck 2018 (P18) + DESI-Y1 BAO (DESI) + DES-Y5 (DESY5).

We also assess neutrino mass constraints changing the CMB dataset from Planck 2018 to ACT+P650, as described in Section 7.3.4:

- ACT DR4 (ACT) + Planck 2018 $\ell < 650$ (P650) + DESI + Pan;
- ACT DR4 (ACT) + Planck 2018 $\ell < 650$ (P650) + DESI + Pan+;
- ACT DR4 (ACT) + Planck 2018 $\ell < 650$ (P650) + DESI + Uni3;
- ACT DR4 (ACT) + Planck 2018 $\ell < 650$ (P650) + DESI + DESY5.

As a probe of large-scale structure, CMB lensing provides tight constraints on the neutrino mass sum. We also include ACT DR6 CMB Lensing (ACTL) data with the ACT+P650 anisotropy data:

- ACT + P650 + ACT DR6 Lensing (ACTL) + DESI + Pan;
- ACT + P650 + ACT DR6 Lensing (ACTL) + DESI + Pan+;
- ACT + P650 + ACT DR6 Lensing (ACTL) + DESI + Uni3;
- ACT + P650 + ACT DR6 Lensing (ACTL) + DESI + DESY5.

We neglect correlations between datasets; thus, the total likelihood is simply the product of each likelihood. The different supernovae catalogs cannot be trivially combined since they significantly overlap in supernovae.

7.3.7 Analysis Methodology

The three dark energy models discussed in Section 7.2 were implemented in a modified version of CAMB¹ [118] and are publicly available. The phenomenological models (transition and binned $w(z)$ models) are in the same code², while the scalar field monodromic k-essence model is implemented in a different one³.

For every dataset combination and each dark energy model, we sample over the parameter posterior distribution with Markov Chain Monte Carlo (MCMC) methods, specifically using the Metropolis-Hastings algorithm implemented in the Cobaya⁴ code [312, 313, 113]. We use CoCoA⁵, the Cobaya-Cosmolike Joint Architecture [120] framework, to run our two modified CAMBs with Cobaya. We make use of GetDist⁶ [110] to perform statistical analysis of the MCMC samples and produce the figures shown in this work.

¹<https://github.com/cmbant/CAMB>

²<https://github.com/SBU-COSMOLIKE/CAMBLateDE>

³<https://github.com/SBU-COSMOLIKE/CAMB-Monodromic>

⁴<https://github.com/CobayaSampler/cobaya>

⁵<https://github.com/CosmoLike/cocoa>

⁶<https://github.com/cmbant/getdist>

Model	Parameters	Priors
Λ CDM	$\Omega_c h^2$	$\mathcal{U}[0.001, 0.99]$
	$\Omega_b h^2$	$\mathcal{U}[0.005, 0.1]$
	$\ln(10^{10} A_s)$	$\mathcal{U}[1.61, 3.91]$
	n_s	$\mathcal{U}[0.8, 1.2]$
	τ	$\mathcal{U}[0.01, 0.8]$
	$100 \times \theta_*$	$\mathcal{U}[0.5, 10]$
	Σm_ν (eV)	$\mathcal{F}[0.06]$ or $\mathcal{U}[0.01, 0.6]$
$w_0 w_a$	w_0	$\mathcal{U}[-3, -0.01]$
	w_a	$\mathcal{U}[-3, 1]$
Transition	w_0	$\mathcal{U}[-3, -0.01]$
	w_1	$\mathcal{U}[-3, 1]$
	z_c	$\mathcal{U}[0.2, 1.0]$
	σ	$\mathcal{F}[0.05]$
Binned $w(z)$	w_0	$\mathcal{U}[-3, -0.01]$
	$w_{i>0}$	$\mathcal{U}[-3, 1]$
k-essence	α	$\mathcal{U}[0.01, 3]$
	A	$\mathcal{U}[0.01, 0.9]$
	ν (M_{pl}^{-1})	$\mathcal{U}[\nu_i - 2, \nu_i + 2], i = 1, 2, 3, 4$ ^a

^a See Section 7.4.1 for the values for ν_1, ν_2, ν_3 and ν_4 .

Tabela 7.1: Priors for Λ CDM and dark energy parameters. $\mathcal{U}[a, b]$ represents an uniform distribution from a to b , whereas $\mathcal{F}[x]$ represents a fixed value.

The MCMCs are performed in two scenarios: fixing $\sum m_\nu = 0.06$ eV or varying $\sum m_\nu$. We use a single massive neutrino and two massless neutrinos in the former case. In the latter, we adopt three degenerate massive neutrinos to avoid the choice of a given mass hierarchy [314, 315]. We explore the dark energy parameter posteriors, as well as the six cosmological parameters $\{\theta_*, \Omega_c h^2, \Omega_b h^2, A_s, n_s, \tau\}$ with/without varying $\sum m_\nu$ according to priors shown in Table 7.1. We choose to sample over θ_* , the angular scale of the sound horizon at recombination, instead of H_0 . Since CMB data puts very stringent constraints on θ_* , this choice optimizes the number of accepted points during the MCMC. We also run MCMCs considering the cosmological constant and $w_0 w_a$ parametrization models for dark energy. We use the Casarini prescription [316, 317] for including nonlinear effects in the matter power spectrum. We use the Gelman-Rubin criterion to assess whether the chains converged, stopping when $|R - 1| < 0.01$. For datasets with ACT DR4 or CMB lensing from ACT DR6, we use increased CAMB accuracy settings: `lmax = 7000`, `lens_potential_accuracy = 4`, `lens_margin = 1250`, `lSampleBoost = 1`, and `lAccuracyBoost = 1` as recommended by [310].

To compare how well each dark energy model fits the datasets, we maximize the likelihood and find the minimum value of χ^2 starting from the maximum a posteriori sample obtained in the MCMCs. Recent works [112, 318, 319] have shown that classical minimizers, such as `Py-BOBYQA`, fail to reach the global minimum of χ^2 , getting stuck in local minima. Simulated annealing, a stochastic minimization heuristic, has been proposed as a means to reach global minima of cosmological likelihood functions, outperforming deterministic minimizers. We have implemented a simple simulated annealing optimizer in `Cobaya` and we use it to find the minimum values of χ^2 and assess the goodness-of-fit of each model.

During our initial MCMC runs, we observed that the ν parameter, representing the oscillatory frequency in the MKE model, has a multimodal posterior distribution. The Metropolis-Hastings algorithm cannot explore the ν modes efficiently. To avoid this issue, one can employ a nested sample algorithm such as `PolyChord` [320, 321] or perform a minimization procedure; we opted for the latter. We minimize the total χ^2 with fixed values of $\nu \in [0.1, 1, 2, \dots, 50]$, finding the four frequency values with lowest χ^2_{tot} . Then, we run MCMCs varying ν by $\pm 2M_{\text{pl}}^{-1}$ around each of those values. We validate our pipeline by reproducing the DESI results for the $w_0 w_a$ parametrization.

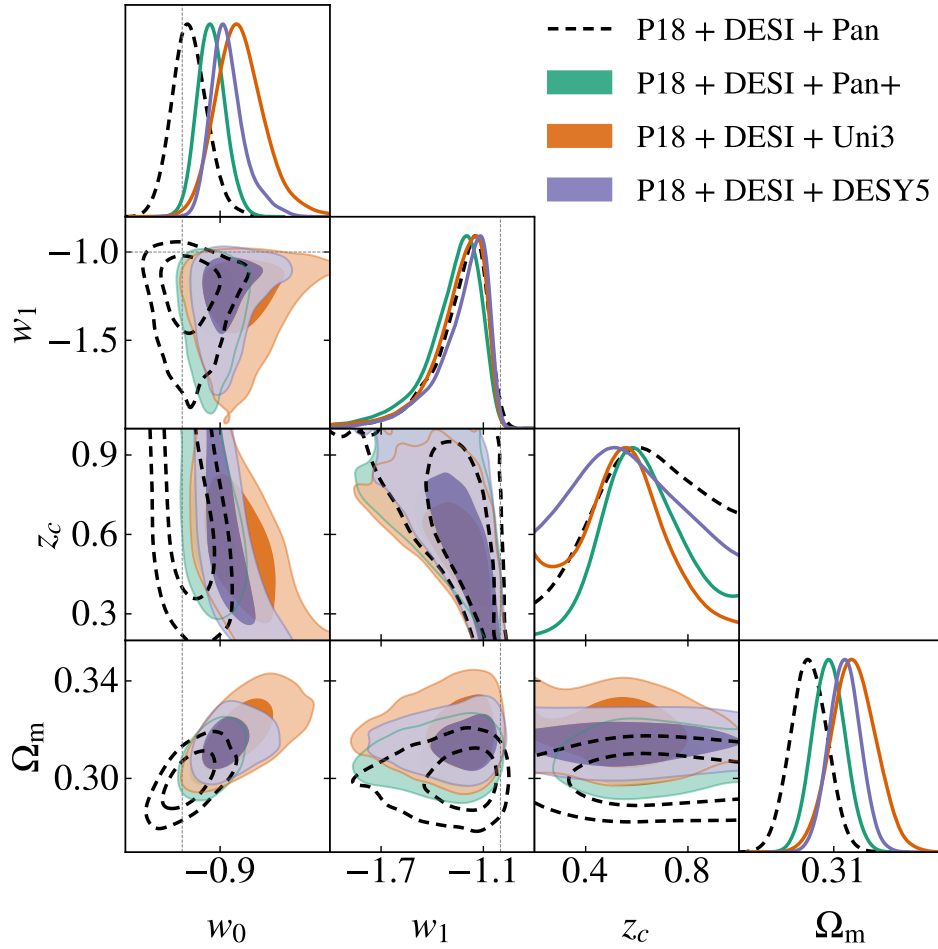


Figura 7.2: 2D confidence contours (68% and 95%) of dark energy parameters w_0 , w_1 and z_c from the transition parametrization in Equation 7.1, as well as Ω_m .

7.4 Results

7.4.1 Model Parameter Constraints

Transition model

Figure 7.2 shows confidence contours for the transition model described in Section 7.2.1. For Pantheon+, Union3, and DESY5, the 95% confidence region is contained in the quadrant of the $w_0 - w_1$ plane where $w_0 > -1$ and $w_1 < -1$, suggesting a transition between a phantom regime to a non-phantom behavior. Recent works [322] show that quintessence models that satisfy $w \geq -1$ can mimic the phantom crossing $w_0 w_a$ models preferred by DESI BAO. Our result corroborates the mild preference for phantom crossing using an alternative parametrization that directly probes the equation of state via w_0 and w_1 . Results considering Pantheon

SN are compatible with $w_0 = -1$ but also show a mild preference for $w_1 < -1$. The difference in w_0 constraints between the different SN datasets are caused by the correlation between w_0 and Ω_m observed in the lower left panel of Figure 7.2. As with the $w_0 w_a$ parametrization, SN datasets that prefer higher Ω_m values will also prefer higher w_0 values. The transition redshift z_c is weakly constrained at around $z_c \approx 0.6$. The 1D marginalized constraints (68% limits) for the dark energy parameters are:

- P18 + DESI + Pan: $w_0 = -0.982 \pm 0.044$, $w_1 = -1.24^{+0.18}_{-0.08}$, $z_c = 0.65^{+0.25}_{-0.18}$;
- P18 + DESI + Pan+: $w_0 = -0.924^{+0.034}_{-0.038}$, $w_1 = -1.30^{+0.20}_{-0.09}$, $z_c = 0.63^{+0.15}_{-0.18}$;
- P18 + DESI + Uni3: $w_0 = -0.848^{+0.053}_{-0.068}$, $w_1 = -1.28^{+0.21}_{-0.07}$, $z_c = 0.56 \pm 0.17$;
- P18 + DESI + DESY5: $w_0 = -0.878^{+0.033}_{-0.047}$, $w_1 = -1.24^{+0.19}_{-0.06}$, $z_c = 0.57^{+0.18}_{-0.27}$.

Figure 7.3 shows the constraints in the equation of state as a function of redshift, $w(z)$, and the dark energy density $\rho_{DE}(z)$. Compared with Λ CDM, the phantom crossing behavior implies increased dark energy at redshifts $z < 0.5$ and a smaller density at higher redshifts. These results agree with previous literature analyses using the $w_0 w_a$ parametrization and other reconstruction methods such as [301].

We have also assessed constraints with varying values of σ with a prior $\mathcal{U}[0.01, 0.5]$, and the results are qualitatively equivalent, with wider posteriors for all parameters. The results are shown in Appendix D.3.

We have verified by running the corresponding chains changing Planck 2018 CMB data by ACT data, as well as the inclusion of ACT CMB lensing, have no significant effect on the dark energy parameter constraints.

Binned $w(z)$

Due to the large number of dark energy parameters and the complex correlations among them in the binned $w(z)$ model, it is difficult to visualize and interpret the constraints on the individual w_i 's for each redshift bin i . For this purpose, we perform a principal component analysis (PCA) [323, 324, 325, 326, 327] of the w_i samples obtained in the MCMCs. This process consists of extracting the sample covariance matrix of the w_i parameters from the MCMC. Since this matrix is real and symmetric, it can be diagonalized. The eigenvectors of the sample covariance are the principal components e_i , $i = 1, \dots, N_{\text{bins}}$. Any given sample of parameters $\{w_0, \dots, w_{N_{\text{bins}}-1}\}$ represents a $w(z)$ evolution given by Equation 7.3 which can be rewritten in terms of the principal components as

$$w(z) = -1 + \sum_{i=1}^{N_{\text{bins}}} \alpha_i e_i(z), \quad (7.22)$$

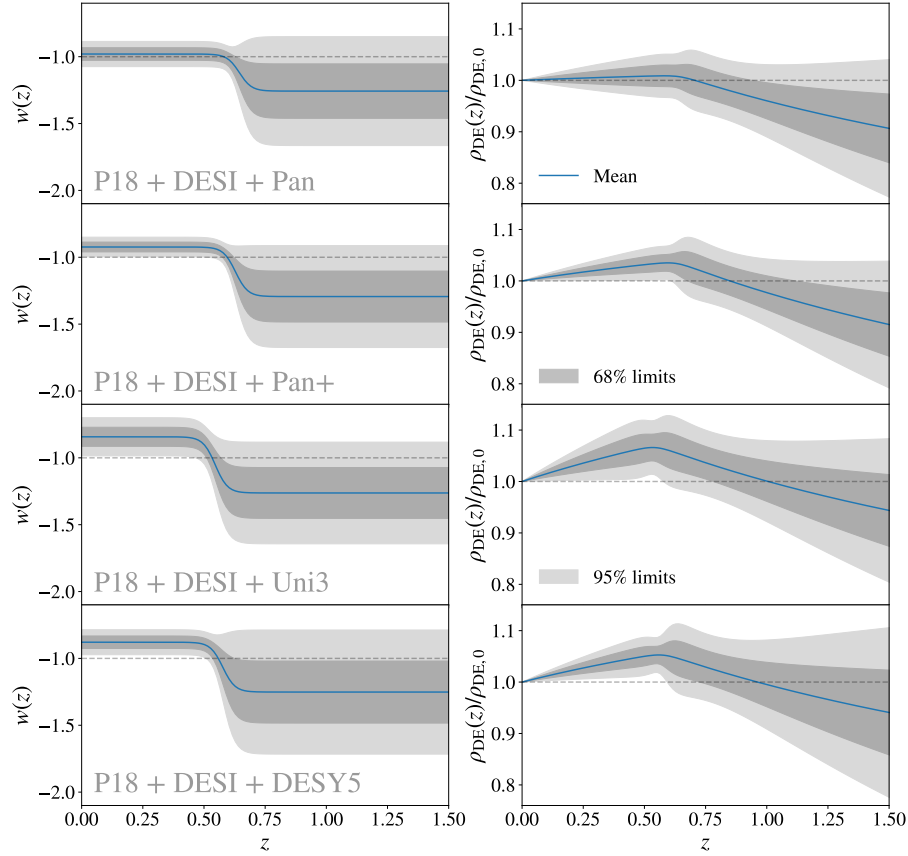


Figure 7.3: Reconstruction of the dark energy equation of state and density considering the transition dark energy parametrization, Equation 7.1. The blue line represents the mean model, and the darker and lighter gray bands represent the 68% and 95% confidence regions, respectively. The dashed black line indicates the corresponding Λ CDM values. Each row indicates a different dataset combination, all containing DESI BAO and Planck 2018 CMB data but using a different SN dataset.

where we choose $\alpha = (0, \dots, 0)$ to be equivalent to $w(z) = -1$ ⁷. Figure 7.4 shows the principal components $e_i(z)$. We order the principal components by increasing variance. We remark that, for both $N_{\text{bins}} = 5$ and $N_{\text{bins}} = 10$, the first principal component e_1 represents a thawing behavior, progressively deviating the dark energy equation of state from -1 in the lowest redshift bins.

Figure 7.5 shows the 1D marginalized distributions for the α_i components for both binning choices, $N_{\text{bins}} = 5$ and $N_{\text{bins}} = 10$. We observe that Pantheon+, Union3, and DESY5 show a mild preference for the thawing principal component, $\alpha_1 > 0$, which is not observed in the Pantheon analysis. This is connected to previous analyses from the literature using the $w_0 w_a$ parametrization [50, 37, 40]

⁷In implementations of PCA, the null vector in the principal component space maps to the mean value of the parameters in the feature space. This translation of the α_i parameters does not affect the eigenvectors e_i since the covariance matrix is invariant by translations.

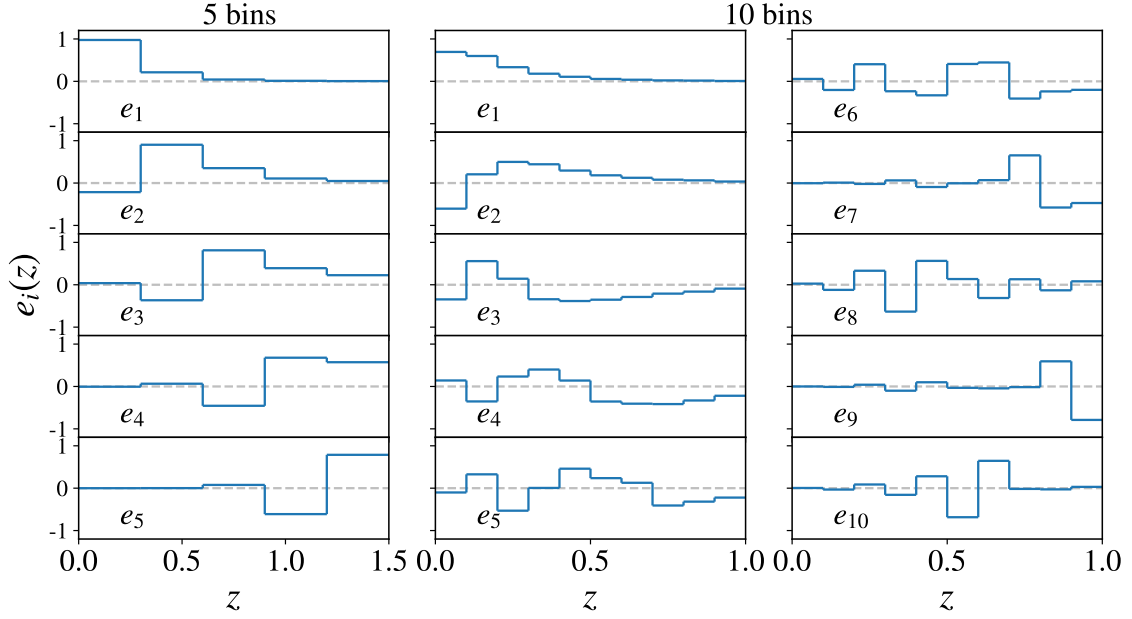


Figure 7.4: Principal Components $e_i(z)$ of the binned $w(z)$ model, defined in Equation 7.3, obtained from the samples using the P18 + DESI + Pan+ dataset. The left panel shows the PCs for the case with 5 bins, while the middle and right panels show the PCs for the 10 bins case.

and the results from the transition model, in which all supernovae except for Pantheon show a preference for $w_0 > -1$. Reference [248], which uses thawing quintessence models, argues that this signal is caused by a mild discrepancy in the Ω_m parameter between P18+DESI and the newer SN datasets: Pantheon SN, which prefers a value of Ω_m compatible with BAO and CMB, does not prefer thawing behavior.

For $N_{\text{bins}} = 5$, we also observe a preference for a negative amplitude of the e_3 principal component, $\alpha_3 < 0$, and other components are compatible with zero amplitude. The 1D marginalized constraints (68% limits) on α_3 are:

- P18 + DESI + Pan: $\alpha_3 = -0.94 \pm 0.35$;
- P18 + DESI + Pan+: $\alpha_3 = -1.17 \pm 0.31$;
- P18 + DESI + Uni3: $\alpha_3 = -0.86 \pm 0.33$;
- P18 + DESI + DESY5: $\alpha_3 = -0.47^{+0.31}_{-0.28}$.

With negative amplitude, the behavior of e_3 , depicted in Figure 7.4, increases the equation of state in the bin $0.3 < z < 0.6$ and decreases the equation of state in the subsequent bins, slowly converging to $w = -1$ at the last bins. This behavior is non-monotonic and cannot be described by a monotonic model such as the $w_0 w_a$ parametrization. To visualize this non-standard $w(z)$ behavior being picked up by

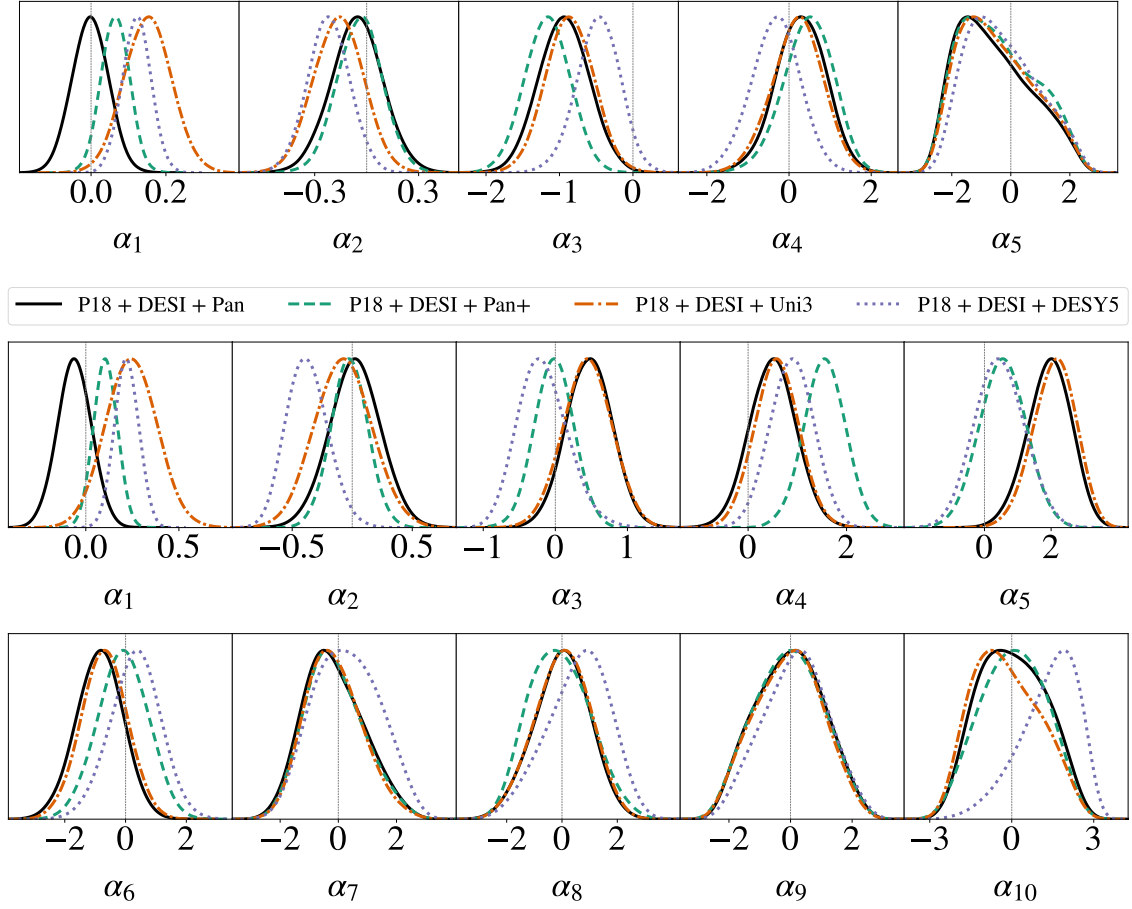


Figure 7.5: 1D marginalized constraints on the Principal Component amplitudes α_i . The top row shows constraints for $N_{\text{bins}} = 5$, while the middle and bottom rows show constraints for $N_{\text{bins}} = 10$. Each panel shows the constraints for a single PC amplitude α_i , and each line type corresponds to a different dataset combination. At each panel, a vertical line indicates $\alpha_i = 0$.

data, we present in the left panels of Figure 7.6 the filtered constraints on the dark energy equation of state, where the mean and error bars are inferred solely from α_1 and α_3 , i.e., setting the other amplitudes to zero. We emphasize that the error bars shown in Figure 7.6 correspond to the uncertainties of physically motivated models only if they have vanishing projections on the noisier principal components. In Appendix D.1, we show the full reconstruction of $w(z)$, with the full error bars on w_i . Although Figure 7.6 shows noticeable differences on the filtered $w(z)$ constraints across the datasets, the full error bars indicate that there is no tension between the predicted evolution of $w(z)$ from different datasets. For Pantheon, Pantheon+, and Union3, we notice an increase of $w(z)$ in the second redshift bin $0.3 < z < 0.6$, followed by a decrease in the third bin $0.6 < z < 0.9$. Interestingly, assuming the binned $w(z)$ model, the dark energy equation of state today is consistently lower than that of the best-fit $w_0 w_a$ model, with $w(z)$ peaking at the

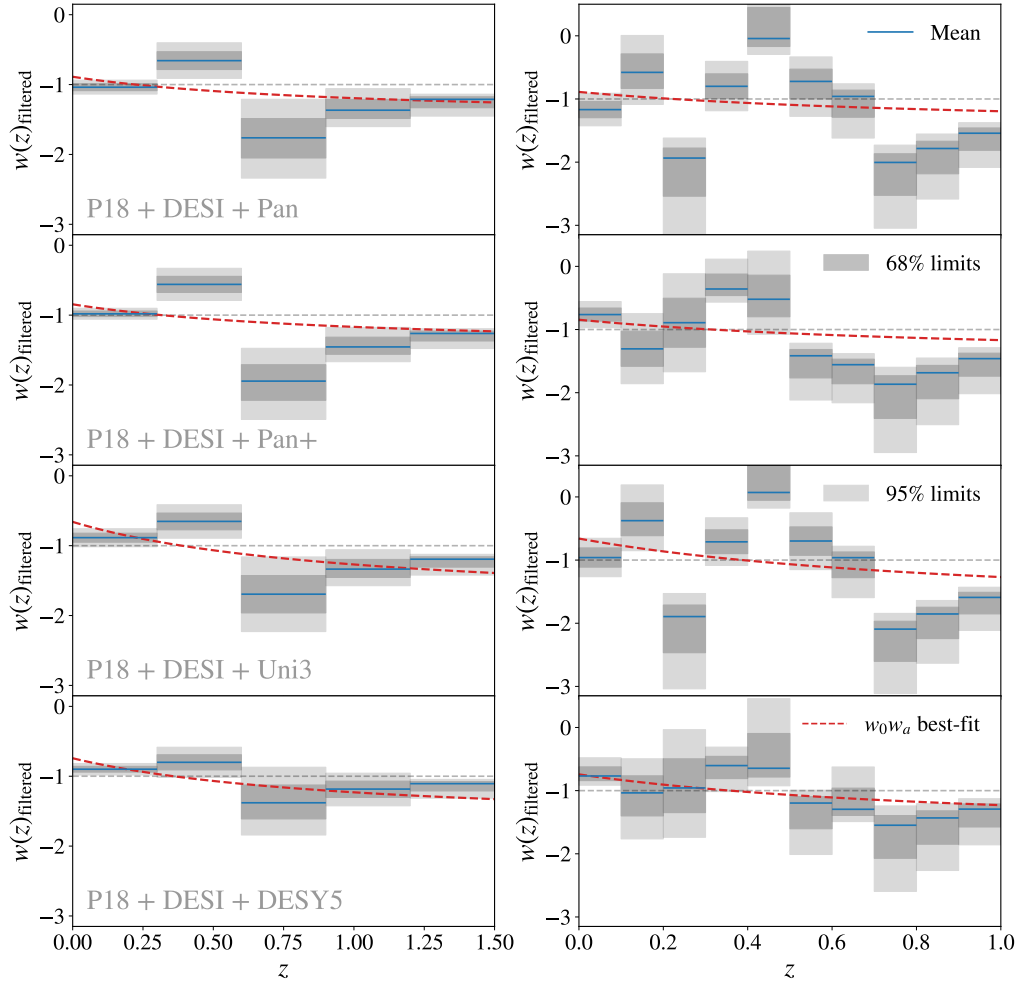


Figure 7.6: Filtered constraints of the dark energy equation of state using the binned $w(z)$, Equation 7.3, for the different SN datasets. Here, we only show the effect of the principal components whose amplitude constraints deviate from zero: for the 5 bins, we only show the effect of e_1 and e_3 , while for 10 bins we show the effect of e_1 , e_4 and e_5 . The mean and confidence intervals are inferred from the corresponding PC amplitudes α_i . The blue line indicates the mean value, and the darker and lighter gray bands indicate 68% and 95% limits. We also include the best-fit $w_0 w_a$ model as a red dashed line for comparison purposes. The left panels show the filtered constraints for $N_{\text{bins}} = 5$, while the right panels show the filtered constraints for $N_{\text{bins}} = 10$. Each row corresponds to a different dataset combination. We emphasize that, since we are discarding principal components amounting to noise, the error bars shown in this Figure are smaller than the actual constraints obtained from the MCMCs, and therefore there isn't necessarily a tension between the reconstructed $w(z)$ across different datasets. See Appendix D.1 for the full reconstruction of $w(z)$.

second bin. Looking forward at the 10 bins result, in the right panels of Figure 7.6,

we can further localize bins with increased $w(z)$ at redshifts $0.3 < z < 0.5$. The DESY5 case shows the least preference for the e_3 principal component and is consistent with a monotonic behavior.

For $N_{\text{bins}} = 10$, apart from the thawing principal component e_1 , we observe a mild preference for the two additional principal components: Pantheon+ and DESY5 show evidence for $\alpha_4 > 0$, whereas Pantheon and Union3 show evidence for $\alpha_5 > 0$. Finally, DESY5 also slightly prefers $\alpha_2 < 0$. The 1D marginalized constraints (68% limits) are:

- P18 + DESI + Pan: $\alpha_4 = 0.50 \pm 0.48, \alpha_5 = 1.94^{+0.71}_{-0.61}$,
- P18 + DESI + Pan+: $\alpha_4 = 1.55 \pm 0.42, \alpha_5 = 0.55 \pm 0.70$;
- P18 + DESI + Uni3: $\alpha_4 = 0.58 \pm 0.45, \alpha_5 = 2.09^{+0.69}_{-0.60}$,
- P18 + DESI + DESY5: $\alpha_4 = 0.89 \pm 0.44, \alpha_5 = 0.45 \pm 0.75, \alpha_2 = -0.38^{+0.16}_{-0.19}$.

The two principal components e_4 and e_5 represent oscillatory behavior with multiple phantom crossings. In the right panels of Figure 7.6 we show the filtered constraints on $w(z)$ inferred from α_1, α_4 and α_5 . We remark that we choose the same filtered principal components for all datasets. As in the case of $N_{\text{bins}} = 5$, we also observe an increase of $w(z)$ in the redshift window $0.3 < z < 0.5$. Once again, DESY5 is the SN dataset that shows the least preference for an oscillatory behavior, consistent with the $w_0 w_a$ behavior. The full constraints on w_i are shown in Appendix D.1.

In Figure 7.7, we show the 2-dimensional marginalized distributions of χ^2_{BAO} versus the amplitudes of the principal components listed above. For the 5 bins case, we observe a clear trend that χ^2_{BAO} is minimized at around $\alpha_3 \approx -1$. For the 10 bins case, considering Pantheon+ or DESY5, χ^2_{BAO} is minimized for $\alpha_4 \approx 1.5$, whereas for Pantheon and Union3, the minimum occurs for $\alpha_5 \approx 2$. In all cases, DESI BAO is decisive to push the amplitude constraints away from zero.

One may be concerned that the discontinuities in $w(z)$ plague the analysis. In Appendix D.2, we present a continuous version of the binned $w(z)$ model and we show that the impact of the discontinuities in χ^2 does not lead to significant differences.

Monodromic k-essence

Due to the multimodal posterior distribution of the parameter ν , we minimize the total χ^2 over all other cosmological parameters with fixed values of the frequency $\nu \in [0.1, 1, 2, 3, \dots, 50]$, finding the values preferred by data. The results of this minimization process are shown in Figure 7.8, showing $\chi^2_{\text{SN}}, \chi^2_{\text{BAO}}, \chi^2_{\text{CMB}}$ and χ^2_{tot} for each value of ν for all datasets. Out of the tested frequency values, those that minimize χ^2_{tot} are, in M_{pl}^{-1} :

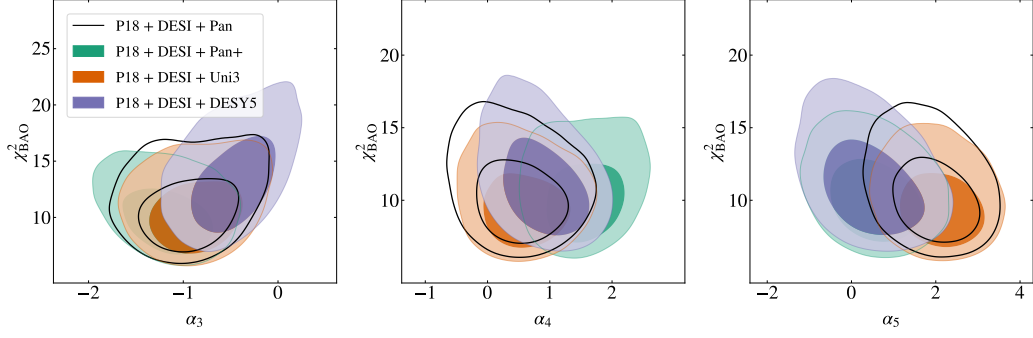


Figure 7.7: 2-dimensional marginalized distributions of χ^2_{BAO} and the principal component amplitudes whose mean deviates from zero. In the left panel, we show α_3 for the 5 bins case, in the middle panel we show α_4 for the 10 bins case and in the right panel we show α_5 , also for the 10 bins case.

- P18 + DESI + Pan: $\nu \in [1, \nu_1 = 10, \nu_2 = 24, \nu_3 = 30, \nu_4 = 38]$;
- P18 + DESI + Pan+: $\nu \in [1, \nu_1 = 10, \nu_2 = 22, \nu_3 = 29, \nu_4 = 36]$;
- P18 + DESI + Uni3: $\nu \in [1, \nu_1 = 9, \nu_2 = 24, \nu_3 = 30, \nu_4 = 37]$;
- P18 + DESI + DESY5: $\nu \in [1, \nu_1 = 9, \nu_2 = 23, \nu_3 = 30, \nu_4 = 36]$.

As shown in Figure 7.1, with a frequency $\nu = 1M_{\text{pl}}^{-1}$, $w(z)$ doesn't complete a full oscillation during the cosmological history, thawing at low redshifts, a behavior similar to w_0w_a . We remark that, for DESY5, $\nu = 1M_{\text{pl}}^{-1}$ is the frequency value that overall minimizes χ^2 . However, higher frequency values can yield lower χ^2 values for other supernovae, improving the overall fit. To explore the low-frequency region of the parameter space, we run MCMCs varying the frequency with a prior of $\nu \in [0, 3]$ in M_{pl}^{-1} .

It is interesting to notice that, for the different datasets, the preferred frequencies are similar, differing by at most $2M_{\text{pl}}^{-1}$. However, since the minima of χ^2 are very narrow, this difference can be enough to make one frequency value not be preferred by another dataset: for instance, $\nu = 24M_{\text{pl}}^{-1}$, which minimizes χ^2 under Pantheon, is not preferred by Pantheon+. We run MCMCs varying the ν parameter by $\pm 2M_{\text{pl}}^{-1}$ around the four preferred values of each dataset with $\nu > 3$. We label the central values them in ascending order as ν_1, ν_2, ν_3 , and ν_4 .

Figure 7.9 show a triangle plot with k-essence parameter constraints for the low frequency prior. All of the frequency posteriors peak at $\nu \approx 1$. Interestingly, the α posterior is shifted towards negative values, indicating oscillations around $w < -1$. Finally, the posterior peaks towards high values of A . Except for the results using Pantheon, a zero amplitude value is excluded at above 2σ confidence level. These parameter combinations suggest a behavior similar to the preferred w_0w_a behavior from the DESI results, in which the equation of state is below -1

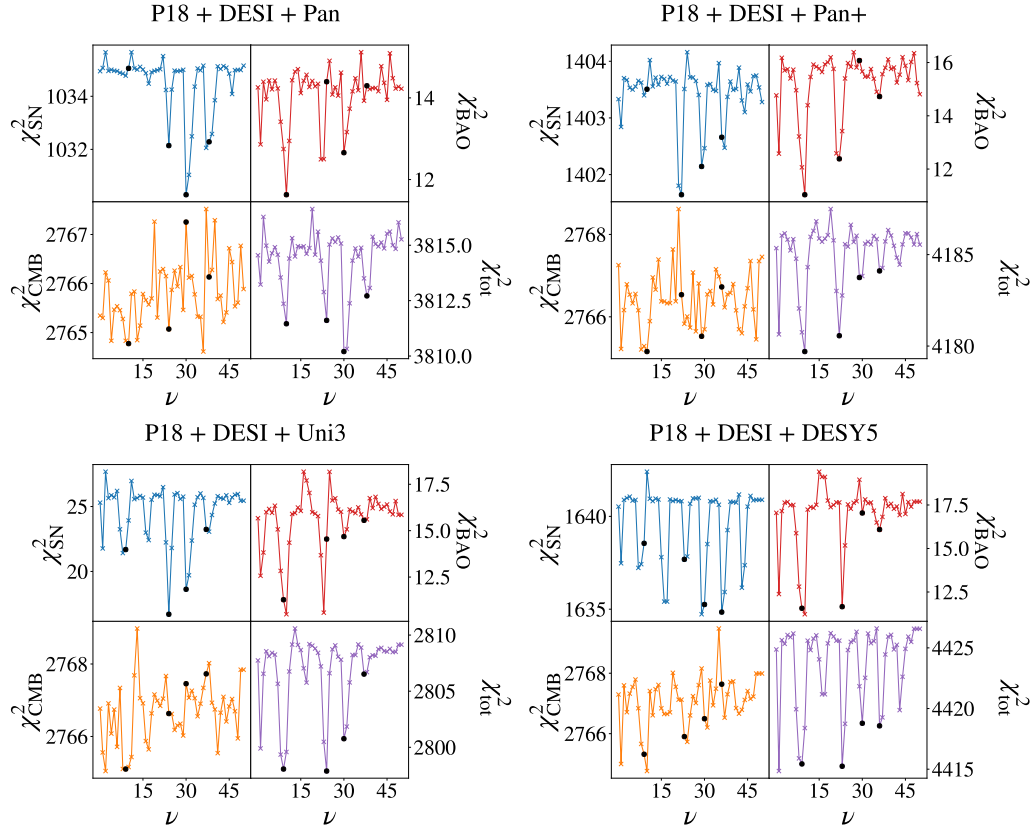


Figura 7.8: Minimum χ^2 values for different fixed frequencies ν . The black circles indicate the four frequency values that minimize χ^2_{tot} and were chosen to run the MCMCs.

in the past and starts oscillating slowly in the present, reaching values above -1 . The constraints at 68% confidence level are:

- P18 + DESI + Pan: $A > 0.405, \alpha = -0.37^{+0.32}_{-0.15}, \nu = 1.13 \pm 0.62;$
- P18 + DESI + Pan+: $A > 0.596, \alpha = -0.40^{+0.34}_{-0.23}, \nu = 1.11^{+0.52}_{-0.42};$
- P18 + DESI + Uni3: $A > 0.754, \alpha = -0.59^{+0.26}_{-0.36}, \nu = 1.28^{+0.41}_{-0.24};$
- P18 + DESI + DESY5: $A > 0.753, \alpha = -0.56^{+0.26}_{-0.36}, \nu = 1.23^{+0.36}_{-0.25}.$

Figure 7.10 shows 2D confidence contours for the MKE parameters α and A . For ν varying around ν_1 , all datasets present a mild preference for oscillations, $A > 0$, with constraints (68% limits):

- P18 + DESI + Pan: $A = 0.146^{+0.060}_{-0.10};$
- P18 + DESI + Pan+: $A = 0.169^{+0.066}_{-0.088};$
- P18 + DESI + Uni3: $A = 0.266^{+0.081}_{-0.098};$

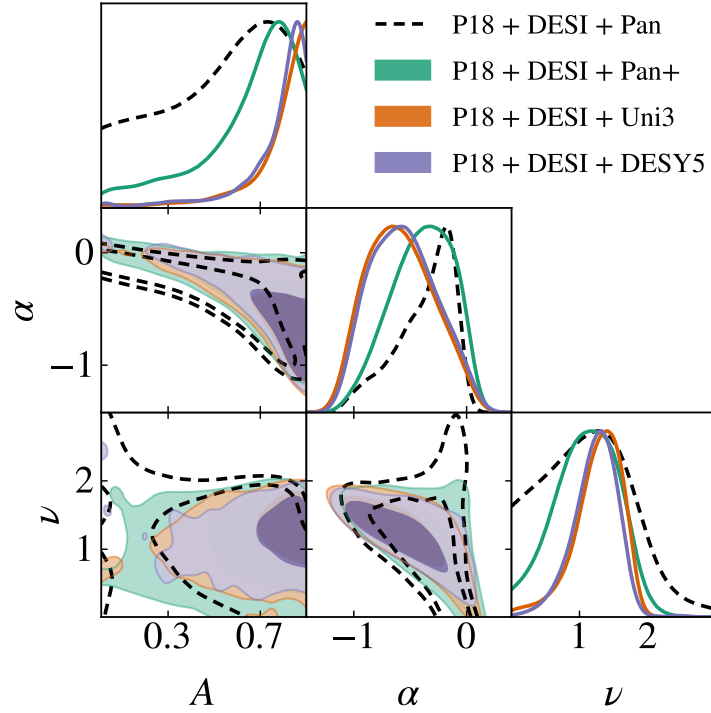


Figure 7.9: 2D confidence contours (68% and 95%) of monodromic k-essence parameters α , A and ν . Here, we impose a prior on the frequency ν of $\mathcal{U}[0, 3]$.

- P18 + DESI + DESY5: $A = 0.226^{+0.068}_{-0.084}$.

For ν varying around the next frequency ν_2 , the posteriors are shifted towards higher values of the amplitude A . Except for Pantheon, all dataset combinations exclude $A = 0$ with over 95% confidence, with a strong preference for $A > 0$ when either Union3 or DESY5 SN are considered. The 1D marginalized constraints on A are:

- P18 + DESI + Pan: $A = 0.29^{+0.14}_{-0.20}$,
- P18 + DESI + Pan+: $A = 0.36^{+0.16}_{-0.19}$,
- P18 + DESI + Uni3: $A = 0.58^{+0.20}_{-0.14}$,
- P18 + DESI + DESY5: $A = 0.50^{+0.16}_{-0.15}$.

No significant preference for $A > 0$ is observed for the other frequency values, although the posterior distribution is compatible with high amplitude values. Since the energy density is an integral of $w(z)$, and the luminosity distance is an integral containing the energy density, high-frequency oscillations are averaged and A has limited impact on the distance calculations. As for the α parameter, all datasets are consistent with $\alpha = 0$, suggesting oscillations around $w = -1$, see Eq. (7.12).

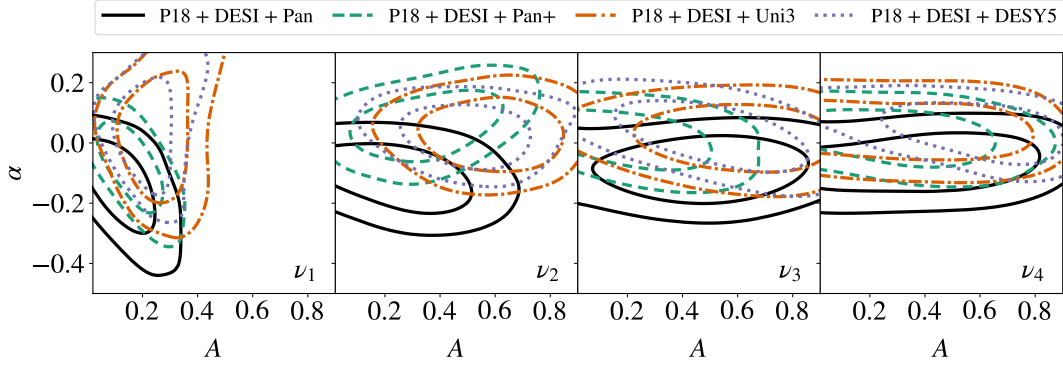


Figure 7.10: 2D confidence contours (68% and 95%) of monodromic k-essence parameters α and A . Each panel represents a different ν prior (see Figure 7.8) while each line type corresponds to a different dataset combination.

To visualize the $w(z)$ behavior being preferred by the data, in Figure 7.11 we show $w(z)$ for different parameter samples in the MCMCs⁸, color-coded by their $\chi^2_{\text{BAO+SN}}$. The oscillation feature of $w(z)$ in this model is noticeable, and are more pronounced for the ν values that yield a lower χ^2 according to Figure 7.8.

7.4.2 Goodness-of-Fit

Using the MCMC samples, we can use a simulated annealing algorithm as described in e.g. [112], finding the global minimum of χ^2 and the difference with the minimum χ^2 obtained assuming ΛCDM . To assess which specific dataset drives the results, we report the χ^2 value divided into three components: $(\chi^2_{\text{BAO}}, \chi^2_{\text{SN}}, \chi^2_{\text{CMB}})$. For each dark energy model, we assess $\Delta\chi^2 = \chi^2_{\text{model}} - \chi^2_{\Lambda\text{CDM}}$, as a measure of the performance of the model to fit the data when compared to ΛCDM ; the $\Delta\chi^2$ is divided into three components similarly. Table 7.2 shows the minimization results for each dark energy model and each dataset. For MKE, we perform minimizations starting at the minima for each MCMC with different ν prior and select the one that yields the minimum χ^2 .

Despite having one additional parameter, the transition parametrization fits the BAO and SN datasets similarly to the w_0w_a parametrization. For the analyses using Pantheon, Pantheon+ and Union3, the transition parametrization can fit DESI BAO slightly better than w_0w_a . We observe that the binned $w(z)$ parametrization can fit DESI BAO data considerably better than w_0w_a : using 5 bins, the binned $w(z)$ model can reduce χ^2_{BAO} by -5.4 , -5.3 and -4.2 when compared to w_0w_a in the Pantheon, Pantheon+ and Union3 analyses, respectively. However, except for Pantheon+, the binned $w(z)$ with 5 bins cannot improve the fit to the SN datasets. For this reason, we conclude that the non-monotonic features observed in Figure 7.6 are driven by DESI BAO data rather than the SN datasets. Due to the increased generality,

⁸We burn-in and thin the MCMC samples to ensure uncorrelated samples.

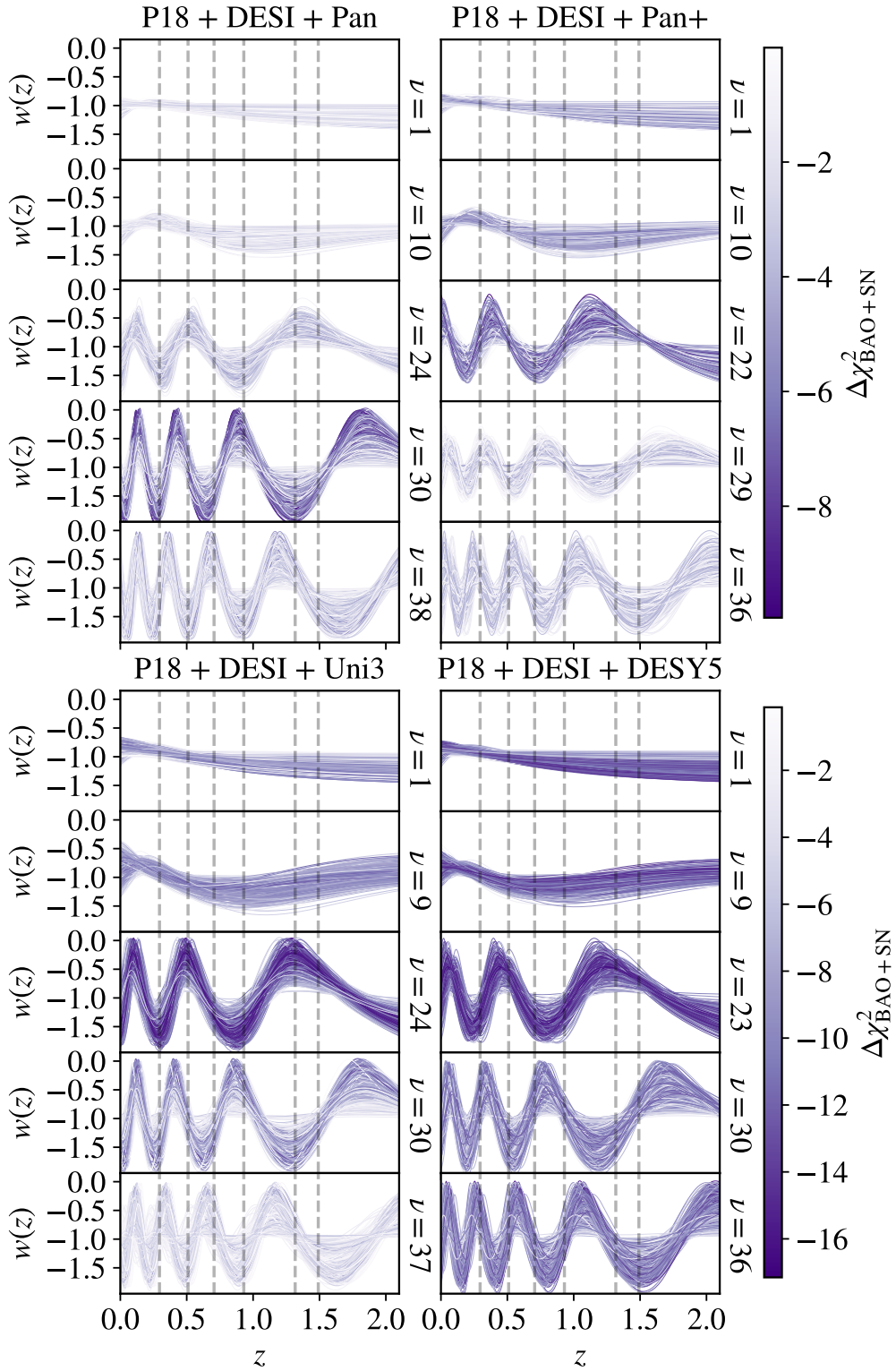


Figure 7.11: K-essence equation of state evolution for various MCMC samples of the model parameters A and α . Each panel corresponds to a different dataset combination and is divided into five subpanels, one for each frequency prior: $\nu \approx 1$ indicates $\nu \in [0, 3]$ and the other values indicate $\nu \in [\nu_i - 2, \nu_i + 2]$. Each $w(z)$ curve is color-coded by $\Delta\chi^2_{\text{BAO+SN}} = \chi^2_{\text{BAO+SN}}(\alpha, A, \nu) - \min_{\Lambda\text{CDM}} \chi^2_{\text{BAO+SN}}$, with darker shades indicating lower values of $\Delta\chi^2_{\text{BAO+SN}}$. The vertical dashed lines represent the BAO effective redshifts.

	P18 + DESI + Pan	P18 + DESI + Pan+
$\Delta\chi^2_{w_0w_a}$	-2.5 (-0.7, 0.2, -2.0)	-7.0 (-2.1, -2.6, -2.2)
$\Delta\chi^2_{\text{trans}}$	-3.7 (-1.5, 0.3, -2.5)	-8.6 (-2.9, -3.3, -2.4)
$\Delta\chi^2_{5\text{-bin } w(z)}$	-6.7 (-6.1, 1.0, -1.6)	-14.9 (-7.4, -5.8, -1.7)
$\Delta\chi^2_{10\text{-bin } w(z)}$	-15.6 (-9.3, -5.2, -1.1)	-20.0 (-8.9, -9.7, -1.5)
$\Delta\chi^2_{\text{MKE}}$	-6.8 (-3.0, -4.4 +0.5) ($\nu \approx \nu_2$)	-7.2 (-2.6, -4.9, +0.4) ($\nu \approx \nu_2$)
	P18 + DESI + Uni3	P18 + DESI + DESY5
$\Delta\chi^2_{w_0w_a}$	-11.9 (-3.0, -6.7, -2.2)	-15.4 (-4.0, -10.3, -1.0)
$\Delta\chi^2_{\text{trans}}$	-11.1 (-3.5, -6.2, -1.4)	-15.0 (-3.3, -11.3, -0.5)
$\Delta\chi^2_{5\text{-bin } w(z)}$	-13.7 (-7.2, -5.2, -1.3)	-15.0 (-5.3, -8.6, -1.2)
$\Delta\chi^2_{10\text{-bin } w(z)}$	-26.7 (-10.7, -14.3, -1.7)	-25.2 (-5.8, -20.3, +0.8)
$\Delta\chi^2_{\text{MKE}}$	-10.3 (-2.9, -6.7, -0.7) ($\nu \in [0, 3]$)	-13.8 (-4.1, -10.4, -0.7) ($\nu \in [0, 3]$)

Tabela 7.2: $\Delta\chi^2 = \chi^2_{\text{model}} - \chi^2_{\Lambda\text{CDM}}$ of the dark energy models, compared to the best-fit ΛCDM model. The value is broken down into $(\Delta\chi^2_{\text{BAO}}, \Delta\chi^2_{\text{SN}}, \Delta\chi^2_{\text{CMB}})$. The reference $\chi^2_{\Lambda\text{CDM}}$ for each dataset combination is the format P18+DESI+“SNIa” where “SNIa” refers to one of the Supernovae datasets from Pantheon: $\chi^2 = 3804.6$ ($\chi^2_{\text{BAO}} = 13.6, \chi^2_{\text{SN}} = 1034.7, \chi^2_{\text{CMB}} = 2756.3$); Pantheon+: $\chi^2 = 4176.0$ ($\chi^2_{\text{BAO}} = 14.4, \chi^2_{\text{SN}} = 1405.5, \chi^2_{\text{CMB}} = 2756.1$); Union3: $\chi^2 = 2798.7$ ($\chi^2_{\text{BAO}} = 14.5, \chi^2_{\text{SN}} = 28.1, \chi^2_{\text{CMB}} = 2756.1$); and DESY5: $\chi^2 = 4418.7$ ($\chi^2_{\text{BAO}} = 15.9, \chi^2_{\text{SN}} = 1647.8, \chi^2_{\text{CMB}} = 2755.0$).

10 redshift bins can fit both BAO and SN datasets better than all other models. Even in the P18 + DESI + DESY5 dataset, in which no other dark energy model could improve on the w_0w_a fit, the 10-bins model showed an improvement of $\Delta\chi^2 = -9.8$ over w_0w_a . Finally, the MKE model performs similarly or better than w_0w_a with respect to the SN fit: comparing χ^2_{SN} between both models, MKE reduces χ^2_{SN} by -4.6 considering Pantheon and -2.3 considering Pantheon+, with no significant difference in χ^2_{SN} for the other SN datasets. However, the MKE model has a considerably worse fit to CMB than the other dynamical dark energy models: while most dynamical DE models present a $\Delta\chi^2_{\text{CMB}}$ with respect to ΛCDM ranging from -1 to -2.5 , MKE has a $\Delta\chi^2_{\text{CMB}}$ ranging from -0.7 to $+0.5$.

To penalize models with an increased number of parameters, we transform the $\Delta\chi^2_{\text{model}}$ value into a z-score, the same measure used by DESI to quote the w_0w_a significance levels over ΛCDM [50]. Under the assumption that the likelihood is Gaussian, the quantity χ^2 is a random variable following a χ^2 distribution with $N_{\text{dv}} - N_{\text{params}}$ degrees of freedom, where N_{dv} is the number of elements in the data vector and N_{params} is the number of model parameters. Due to the additivity property of the of the χ^2 distribution, the random variable $X = \chi^2_{\Lambda\text{CDM}} - \chi^2_{\text{model}}$ is also χ^2 -distributed with ΔN_{params} degrees of freedom, where ΔN_{params} is the

difference in number of parameters between the dark energy model and Λ CDM. We have $\Delta N_{\text{params}}^{w_0 w_a} = 2$, $\Delta N_{\text{params}}^{\text{trans}} = 3$, $\Delta N_{\text{params}}^{\text{binw}} = 5$ or 10, and $\Delta N_{\text{params}}^{\text{MKE}} = 3$. We then calculate p , the probability of $X > |\Delta\chi^2_{\text{model}}|$. Defining Z as another random variable following a standard normal distribution, the z-score is the value z such that $P(-z < Z < z) = p$. We refrain, however, from interpreting the z-score as a statistical significance, only using this technique to quantitatively compare dark energy models while penalizing extra parameters.

The z-score of each dark energy model is shown in Figure 7.12. We recover similar z-score for $w_0 w_a$ reported by the DESI collaboration [50]. For Union3 and DESY5, $w_0 w_a$ is the model with the highest z-score. Even though the binned $w(z)$ model improves the fit significantly, the increased amount of parameters overall amounts to a lower z-score. However, one could conceive a dark energy model that reproduces the filtered $w(z)$ behavior shown in Figure 7.6: this model would have a similar $\Delta\chi^2$ to the binned $w(z)$ model but with less parameters, and therefore would be less penalized by statistical model comparison techniques. We also remark that the z-score of all models is below 2 when Pantheon is considered, pointing to the fact that the discrepancy in Ω_m between DESI BAO and the newer SN datasets is a decisive factor for the observed dynamical dark energy preference [248].

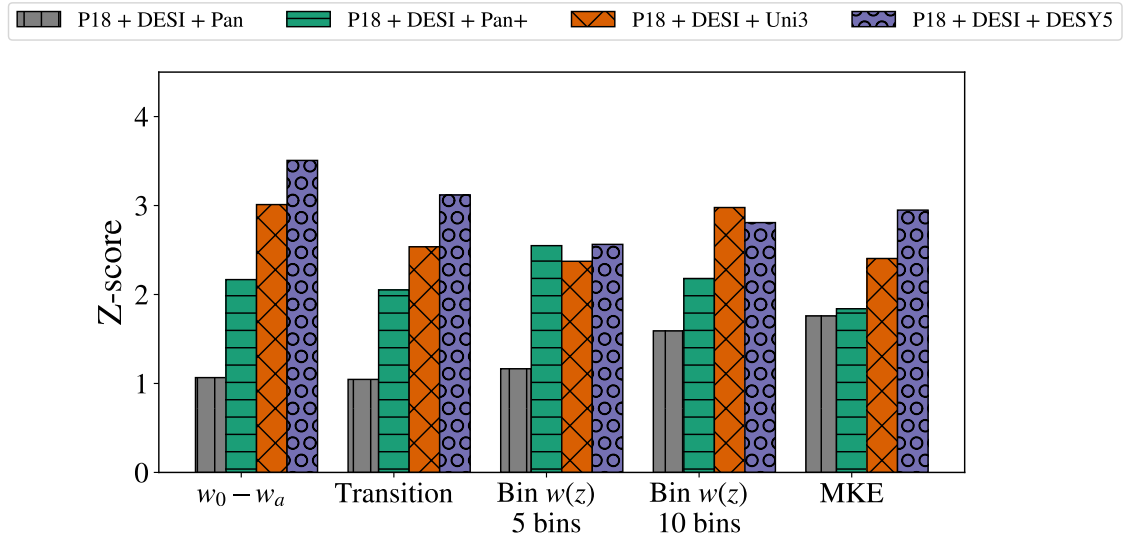


Figure 7.12: Z-score for each dark energy model and each dataset combination.

Another way to penalize extra parameters is to use the Akaike Information Criterion, $AIC = 2N_{\text{params}} + \chi^2$. The preferred models are those with the minimum value of AIC, representing a better fit with few parameters. For this purpose, we calculate $\Delta AIC_{\text{model}} = AIC_{\text{model}} - AIC_{\Lambda\text{CDM}}$ for each dataset and model, and the results are shown in Table 7.3. For Union3 and DESY5, $w_0 w_a$ is the model with the least AIC, with $\Delta AIC = -7.9$ and -11.4 , respectively. For Pantheon+

the binned $w(z)$ with $N_{\text{bins}} = 5$ has a lower AIC, with $\Delta\text{AIC} = -4.9$ compared to $\Delta\text{AIC} = -3.0$ for w_0w_a . These results are consistent with those shown in Figure 7.12, indicating that w_0w_a is still the most cost-effective model in terms of goodness-of-fit.

	P18 + DESI + Pan	P18 + DESI + Pan+
$\Delta\text{AIC}_{w_0w_a}$	+1.5	-3.0
$\Delta\text{AIC}_{\text{trans}}$	+2.3	-2.6
$\Delta\text{AIC}_{5\text{-bin } w(z)}$	+3.3	-4.9
$\Delta\text{AIC}_{10\text{-bin } w(z)}$	+4.4	0.0
$\Delta\text{AIC}_{\text{MKE}}$	-0.8 ($\nu \approx \nu_2$)	-1.2 ($\nu \approx \nu_2$)
	P18 + DESI + Uni3	P18 + DESI + DESY5
$\Delta\text{AIC}_{w_0w_a}$	-7.9	-11.4
$\Delta\text{AIC}_{\text{trans}}$	-5.1	-9.0
$\Delta\text{AIC}_{5\text{-bin } w(z)}$	-3.7	-5.0
$\Delta\text{AIC}_{10\text{-bin } w(z)}$	-6.7	-5.2
$\Delta\text{AIC}_{\text{MKE}}$	-4.3 ($\nu \in [0, 3]$)	-7.8 ($\nu \in [0, 3]$)

Tabela 7.3: $\Delta\text{AIC} = \Delta\chi^2_{\text{model}} + 2\Delta N_{\text{params}}$ of the dark energy models, compared to the best-fit ΛCDM model.

7.4.3 Constraints on $\sum m_\nu$

Hitherto, our analysis has assumed two massless neutrinos and one massive neutrino with $\sum m_\nu = 0.06$ eV, i.e. the minimal value for the sum mass in the normal hierarchy scenario. This assumption is recurrent in the literature [5, 310, 50] when $\sum m_\nu$ is kept fixed. In this Section, we consider the neutrino mass sum $\sum m_\nu$ as a free parameter, assuming three massive neutrinos and a degenerate hierarchy with priors shown in Table 7.1. For these constraints, it is interesting to assess the difference among the CMB datasets and the effect of including CMB lensing data. The constraints on $\sum m_\nu$ are assessed for different dark energy equations of state models of $w = -1$, w_0w_a , and binned $w(z)$ models.

The results are illustrated in Figure 7.13, which shows the marginalized constraints on the neutrino mass sum assuming different dark energy models; Table 7.4 shows the 95% upper limit. Previous works have shown that constraints on $\sum m_\nu$ under the ΛCDM model prefer negative neutrino masses [290]. This effect is aggravated by the “lensing anomaly” present on the Planck 2018 temperature and polarization power spectra in the `Planck` likelihood⁹: the lensing of the spectra

⁹The Planck collaboration has released two likelihoods in which the lensing anomaly is diminished: `CamSpec` and `HiLLiPop`. Analyses using the new likelihoods show relaxed constraints

Upper limit (95% C. L.) on $\sum m_\nu$ (eV)				
P18 + DESI +	Pan	Pan+	Uni3	DESY5
Λ CDM	0.10	0.11	0.11	0.12
w_0w_a	0.18	0.17	0.21	0.19
5 – bin $w(z)$	0.19	0.19	0.19	0.18
10 – bin $w(z)$	0.16	0.16	0.16	0.15
ACT+P650 + DESI +	Pan	Pan+	Uni3	DESY5
Λ CDM	0.16	0.18	0.18	0.20
w_0w_a	0.31	0.28	0.34	0.32
5 – bin $w(z)$	0.32	0.33	0.32	0.31
10 – bin $w(z)$	0.26	0.26	0.26	0.24
ACT+P650 + ACTL + DESI +	Pan	Pan+	Uni3	DESY5
Λ CDM	0.10	0.11	0.11	0.12
w_0w_a	0.22	0.21	0.24	0.23
5 – bin $w(z)$	0.23	0.23	0.23	0.22
10 – bin $w(z)$	0.17	0.18	0.17	0.17

Tabela 7.4: Upper limit on the sum of the neutrino mass at 2σ for different dataset combinations and dark energy models.

exceeds the theoretical Λ CDM lensing effect [5]. Extra lensing would be caused by an increased formation of structure. Therefore, the anomaly makes Planck 2018 data disfavor mechanisms that suppress the growth of structure; in particular, this anomaly causes a preference for even more negative neutrino masses, and the Bayesian posterior upper limit, assuming $\sum m_\nu > 0$, gets lower. ACT CMB data does not present a lensing anomaly [45], and we observe an increase in the upper bound on $\sum m_\nu$ compared to Planck 2018 [292]. The constraints obtained with the ACT+P650 dataset are wider by a factor of 1.5 – 1.9 compared to P18. However, including ACT DR6 lensing data puts the constraints on the same level as P18.

Assuming the w_0w_a parametrization, the $\sum m_\nu$ constraints are relaxed by a factor of 1.8-2.2 compared to Λ CDM, depending on the dataset considered. The binned $w(z)$ with 5 redshift bins shows similar constraints to w_0w_a ; however, although having an increased number of parameters, the case with 10 redshift bins has slightly tighter constraints on $\sum m_\nu$ than w_0w_a by 75% – 90%. One might expect that a more general model with many more parameters would yield relaxed parameter constraints; however, if the binned $w(z)$ model makes the preferred value of $\sum m_\nu$ become more negative than that of w_0w_a , the Bayesian posterior gets tighter as a consequence, since the physical prior excludes negative neutrino

on $\sum m_\nu$ when compared to the original `plik` likelihood [292, 289], but the preference for negative neutrino masses persist.

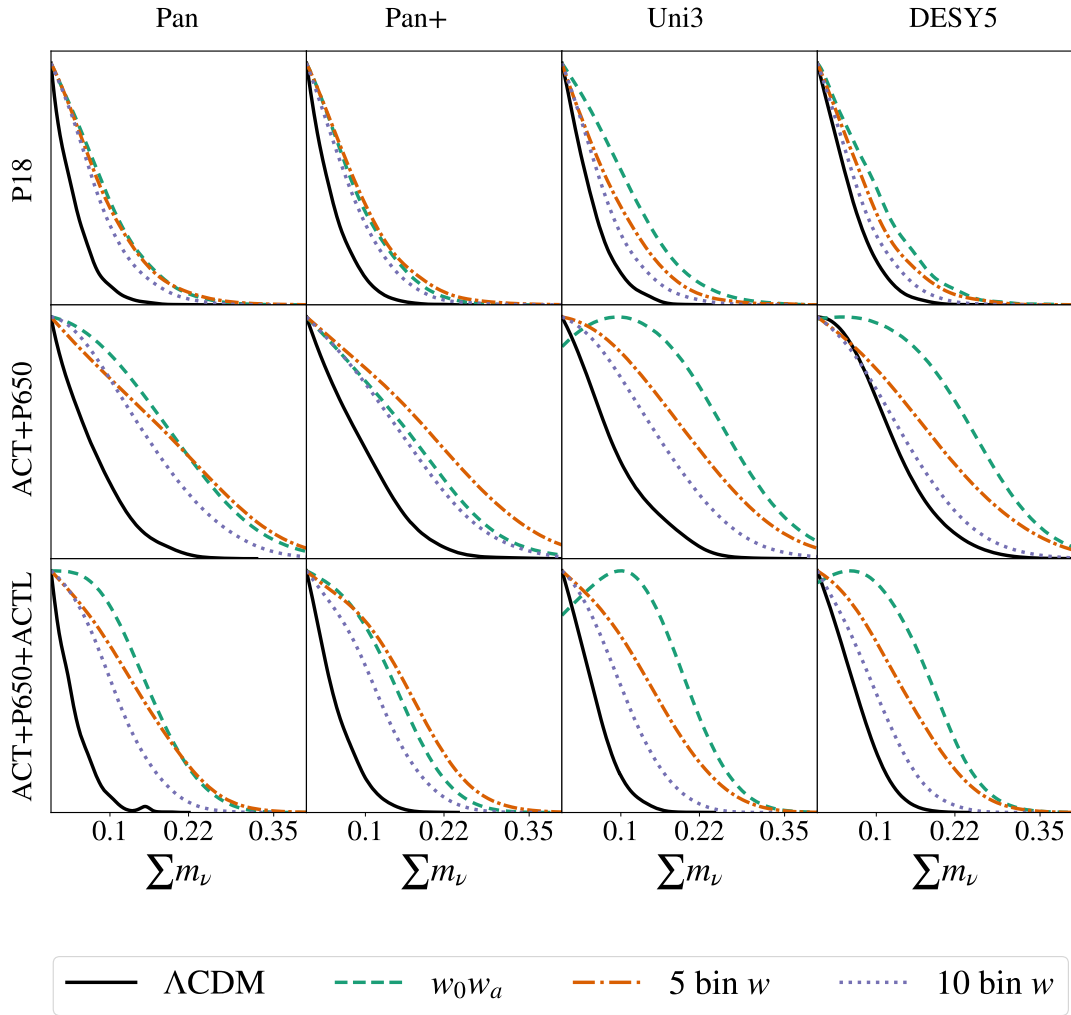


Figure 7.13: 1D marginalized posteriors for the neutrino mass sum Σm_ν for datasets and models presented in Table 7.4. Each panel represents a different dataset combination with BAO from DESI. The top row represents constraints with Planck 2018, the middle row shows constraints using ACT DR4 + Planck 2018 TT TE EE ($\ell < 650$), and the bottom row is the same as the middle row with the addition of CMB lensing from ACT DR6. Each column has a different supernovae catalog: Pantheon, Pantheon+, Union3, and DESY5.

masses¹⁰. Our current results cannot confirm such hypothesis, and we leave this for future investigations. A similar effect has been noted in [328], where the w_0w_a dark energy parametrization with priors such that $w_0 > -1$ and $w_0 + w_a > -1$ has tighter constraints on $\sum m_\nu$ than Λ CDM.

7.5 Conclusion

DESI 2024 BAO data, combined with recent supernovae data from Pantheon+, Union3, and DESY5 catalogs, has shown an intriguing hint in favor of a dynamical dark energy equation of state. Analysis of the w_0w_a parametrization, where $w(z)$ is a linear function of the scale factor, favors a transition from phantom dark energy at redshifts $z > 0.5$ to a quintessence behavior with $w > -1$ for $z < 0.5$. This exciting result, if confirmed, puts even more pressure on the Λ CDM model, and several studies have investigated this result using more general models that go beyond the simple w_0w_a parametrization. Another surprising result from DESI data is the constraints on the neutrino mass sum, whose upper limit in the Λ CDM model is not far from the minimum possible value allowed by neutrino oscillation experiments, $\sum m_\nu > 0.06$ eV. If the trend persists, the next generation of large-scale structure probes, such as Euclid and LSST, could put Λ CDM in tension with laboratory experiments. As cosmological data analyses show correlations between the inferred dark energy equation of state and neutrino mass sum, those constraints should be reassessed considering more general dark energy models.

To investigate the dynamical dark energy behavior preferred by DESI data, we have analyzed three general dark energy models: a transition parametrization, a model-agnostic parametrization with a binned $w(z)$, and an oscillating k-essence model. We investigate the dark energy parameter constraints from each dataset, assessing the preferred forms of $w(z)$ and pointing out differences and similarities among each supernovae catalog, especially between Pantheon and the other catalogs. We found that, for the transition parametrization, the transition redshift z_c is weakly constrained, and the overall $w(z)$ behavior is compatible with those obtained from a w_0w_a analysis. For the binned $w(z)$, we tested two choices of redshift binning, one with 5 bins and the other with 10 bins, and we performed a principal component analysis of the obtained MCMC samples. While the error bars on the equation of state $w(z_i)$ are large due to the increased number of parameters, we found a preference for non-monotonic principal components in both choices of redshift bins, driven by DESI data. To assess the non-trivial behavior preferred by data, we have filtered the principal components with nonzero amplitude means, finding an interesting non-monotonic signal. Furthermore, the thawing behavior discussed in reference [248] is parametrized by a single principal component, and all SN datasets prefer it except for Pantheon. For the monodromic k-essence model,

¹⁰We thank Daniel Green for this remark.

we have minimized χ^2 for fixed values of frequency ν , finding the values that yield a better fit to the data. Among the different SN datasets, the preferred frequency values are very similar, all showing evidence for a nonzero amplitude.

To assess the goodness-of-fit of each model, we have minimized the χ^2 for each dark energy model analyzed in the MCMC explorations, using the simulated annealing technique. Overall, the transition parametrization fits all datasets we investigated as well as w_0w_a , despite having one extra parameter. The binned $w(z)$ parametrization can improve the fit to DESI BAO significantly. The monodromic k-essence model, while having competitive goodness-of-fit to BAO and SN datasets, cannot improve the fit to CMB data. We penalize the increased parameters by translating the $\Delta\chi^2$ into a z-score and calculating the Akaike Information Criterion. Among all dark energy models, w_0w_a is the most cost-effective model, significantly improving the fit of all datasets with only two additional parameters compared to Λ CDM. However, a theoretical dark energy model that reproduces the dynamics shown in Figure 7.6 with fewer parameters than the binned $w(z)$ would be less penalized by model comparison techniques.

Furthermore, we have investigated the constraints on the neutrino mass sum $\sum m_\nu$ considering four different dark energy models: the cosmological constant Λ , w_0w_a , and the model-agnostic binned $w(z)$ with 5 and 10 redshift bins. The tight constraints on $\sum m_\nu$ under the Λ CDM model are greatly relaxed when w_0w_a or the binned $w(z)$ with 5 bins are assumed, while the two latter models show similar constraints. For the case with 10 bins, we observe an overall tightening of the constraints by 70% – 90% depending on the dataset combination.

Future DESI releases [64]¹¹, as well as BAO distance measurements from Euclid [62, 330], galaxy clustering, weak lensing and cross-correlation, as forecasted by Euclid [331, 332], in combination with future supernovae observations, such as from the Roman Space Telescope [333, 334] and the Vera C. Rubin Observatory [61] will be able to pinpoint the expansion history and the behavior of dark energy at low redshifts with increased precision. Determining the low redshift dark energy dynamics with general parametrizations is extremely important in the current era of precision cosmology: it can shed light on the standing cosmological tensions and point towards fundamental dark energy models that can reproduce the observed features.

¹¹During the review of this article, DESI has released its cosmological constraints from the full-shape power spectrum [329], which agrees with the BAO-only analysis.

Chapter 8

Conclusions

The field of cosmology has seen remarkable progress over the last few decades. Theoretically, cosmological perturbation theory has provided a robust framework to describe inhomogeneities and anisotropies in the matter distribution, enabling predictions of observable effects such as cosmic microwave background (CMB) anisotropies and cosmic shear. Observationally, ambitious surveys have measured cosmological probes with unprecedented precision, yielding vast amounts of data. Statistically, we have developed techniques to control systematic errors in observations and optimize the extraction of cosmological information. Computationally, advanced software has been created to produce fast and accurate theoretical predictions, facilitating efficient data analysis.

As is often the case in physics, progress has brought new questions and challenges. The standard cosmological model, Λ CDM, relies on the existence of dark matter and dark energy, whose fundamental nature remains unknown. Furthermore, tensions between different cosmological analyses, such as the Hubble and S_8 tensions, suggest potential shortcomings in the Λ CDM paradigm. These unresolved issues have motivated an extensive body of research, including the work presented in this thesis.

During my PhD at IFT-UNESP, I conducted an extensive study on the cosmological background and linear perturbation theories, detailed in Chapter 2. This theoretical foundation underpins our understanding of cosmological observables, discussed in Chapter 3, as well as extensions to the standard cosmological model, presented in Chapter 4. These extended models were analyzed using advanced statistical techniques and computational algorithms, as described in Chapter 5. This background enabled the original research I conducted in collaboration with researchers from Stony Brook University, Centro Brasileiro de Pesquisas Físicas, University of Arizona, University of Portsmouth, and University of Oslo.

In Chapter 6, our group explored whether the Hubble and S_8 tensions could be addressed simultaneously by employing Early Dark Energy to adjust the sound horizon at recombination and late-time dynamical dark energy to modify the growth of matter perturbations. We found that late-time smooth dark energy cannot simultaneously accommodate the high values of H_0 measured by the local cosmic distance ladder and the low values of S_8 inferred from galaxy surveys. Chapter 7 examines recent indications of dynamical dark energy reported by the DESI collaboration and multiple supernova datasets, including Pantheon+,

Union3, and DESY5. We analyzed complex dark energy models to identify the dynamics preferred by the data and reassessed neutrino mass constraints under these extended parametrizations. Our findings suggest a non-monotonic dark energy equation of state and relaxed neutrino mass constraints compared to Λ CDM.

In addition to the work presented in this thesis, I contributed to other projects during my PhD. In collaboration with Stony Brook University and CBPF, we developed an emulator for the nonlinear matter power spectrum using the Comoving Lagrangian Acceleration (COLA) algorithm, an approximation for N-body simulations. This work culminated in the article "Modelling Nonlinear Scales with COLA: Preparing for LSST-Y1" [25]. Additionally, I am analyzing interacting dark energy models as part of the Dark Energy Survey collaboration, using the complete dataset from six years of observations. I am also a member of the LSST DESC collaboration, where I am leading a project aiming to forecast constraints on the dark energy equation of state using LSST 3x2pt data.

In the coming years, Stage-IV cosmological surveys, such as those conducted by the Rubin Observatory's LSST, the Euclid mission, and the Roman Space Telescope, will provide an unprecedented volume of data about the Universe. These surveys will illuminate current challenges and likely reveal new ones. As precision increases, inconsistencies in the Λ CDM model may become more apparent, necessitating careful data analysis to isolate cosmological signals and the development of sophisticated methods to manage the growing data volume. Exploring extended cosmological models has never been more critical, as the potential falsification of Λ CDM could usher in new physics, shedding light on the fundamental nature of matter and gravity. I hope to contribute to these efforts by advancing theoretical models and analysis techniques to address the pressing challenges of modern cosmology.

Appendix A

Derivations

In this Appendix, I make specific derivations that were left from the main text for clarity and conciseness.

A.1 The Homogeneous and Isotropic Spatial Metric

The 3-space with zero curvature is the well-known Euclidean space, whose metric in cartesian coordinates is

$$ds_{(3)}^2 = dx^2 + dy^2 + dz^2. \quad (\text{A.1})$$

The positively curved 3-space can be thought as a sphere embedded in a 4-dimensional flat space. Let's add an auxiliary coordinate w and the embedding 4-dimensional flat space with metric

$$ds_{(4)}^2 = dw^2 + dx^2 + dy^2 + dz^2. \quad (\text{A.2})$$

Imposing the sphere equation $w^2 + x^2 + y^2 + z^2 = R^2$, we can write the auxiliary coordinate w in terms of the 3-space coordinates

$$w^2 = R^2 - x^2 - y^2 - z^2. \quad (\text{A.3})$$

We can also use the sphere equation to find the induced metric on the sphere. The sphere obeys the following equation

$$wdw + xdx + ydy + zdz = 0. \quad (\text{A.4})$$

Therefore, the induced metric becomes

$$ds_{(3)}^2 = \frac{(xdx + ydy + zdz)^2}{w^2} + dx^2 + dy^2 + dz^2. \quad (\text{A.5})$$

$$ds_{(3)}^2 = \frac{(\mathbf{r} \cdot d\mathbf{r})^2}{R^2 - x^2 - y^2 - z^2} + dx^2 + dy^2 + dz^2, \quad (\text{A.6})$$

where $\mathbf{r} = (x, y, z)$, $d\mathbf{r} = (dx, dy, dz)$ and $\cdot$ is a standard element-wise dot product. Introducing spherical coordinates, we can rewrite some terms as

$$dx^2 + dy^2 + dz^2 = dr^2 + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (\text{A.7a})$$

$$\mathbf{r} \cdot d\mathbf{r} = r dr, \quad (\text{A.7b})$$

and the metric becomes

$$ds_{(3)}^2 = \frac{r^2 dr^2}{R^2 - r^2} + dr^2 + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (\text{A.8a})$$

$$ds_{(3)}^2 = \frac{R^2 dr^2}{R^2 - r^2} + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (\text{A.8b})$$

$$ds_{(3)}^2 = \frac{dr^2}{1 - kr^2} + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (\text{A.8c})$$

where we introduce $k = 1/R^2$.

The negative curved space can be thought as a hyperbola in a flat Riemannian space. Let's again introduce an auxiliary dimension w and an embedding flat space with metric

$$ds_{(4)}^2 = -dw^2 + dx^2 + dy^2 + dz^2. \quad (\text{A.9})$$

The hyperbola in question is the hypersurface defined by

$$-w^2 + x^2 + y^2 + z^2 = -R^2. \quad (\text{A.10})$$

We take analogous steps as in the spherical case. The induced metric on the hyperbola is

$$-w dw + x dx + y dy + z dz = 0 \quad (\text{A.11a})$$

$$ds_{(3)}^2 = \frac{(x dx + y dy + z dz)^2}{R^2 + x^2 + y^2 + z^2} + dx^2 + dy^2 + dz^2 \quad (\text{A.11b})$$

$$ds_{(3)}^2 = \frac{(r dr)^2}{R^2 + r^2} + dx^2 + dy^2 + dz^2 \quad (\text{A.11c})$$

$$ds_{(3)}^2 = \frac{dr^2}{1 + kr^2} + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \quad (\text{A.11d})$$

where once again we have used $k = 1/R^2$. This metric only differs from the positively curved metric in the sign of k . Finally, notice that, for $k = 0$, the metric reduces to the usual euclidean space metric in spherical coordinates. Therefore,

we can describe all three cases with a single expression

$$ds_{(3)}^2 = \frac{dr^2}{1 - kr^2} + r^2(d\theta^2 + \sin^2 \theta d\phi^2), \text{ where } \begin{cases} k > 0 \rightarrow \text{positive curvature,} \\ k = 0 \rightarrow \text{no curvature,} \\ k < 0 \rightarrow \text{negative curvature.} \end{cases} \quad (\text{A.12})$$

A.2 Christoffel Symbols, Ricci and Einstein Tensors for FLRW Metric

For simplicity, I describe the FLRW metric as

$$ds^2 = -dt^2 + a^2 \gamma_{ij} dx^i dx^j. \quad (\text{A.13})$$

The Christoffel symbols are given by

$$\Gamma_{\alpha\beta}^{\mu} = \frac{1}{2} g^{\mu\nu} (\partial_{\alpha} g_{\nu\beta} + \partial_{\beta} g_{\nu\alpha} - \partial_{\nu} g_{\alpha\beta}). \quad (\text{A.14})$$

Two important remarks that simplify the calculations are:

- The metric components do not depend on spatial coordinates: $\partial_i g_{\mu\nu} = 0$, $i = 1, 2, 3$.
- The metric is diagonal: if $\mu \neq \nu$, then $g_{\mu\nu} = 0$.

We can then compute

$$\Gamma_{00}^0 = 0; \quad (\text{A.15a})$$

$$\Gamma_{0i}^0 = 0; \quad (\text{A.15b})$$

$$\Gamma_{00}^i = 0; \quad (\text{A.15c})$$

$$\Gamma_{0j}^i = \frac{1}{2} g^{ik} \partial_0 g_{jk} = \frac{1}{2} \frac{1}{a^2} \gamma^{ik} (2a\dot{a}) \gamma_{jk} = H \delta_j^i; \quad (\text{A.15d})$$

$$\Gamma_{ij}^0 = -\frac{1}{2} g^{00} \partial_0 g_{ij} = -\frac{1}{2} (-1) (2a\dot{a}) \gamma_{ij} = a\dot{a} \gamma_{ij}; \quad (\text{A.15e})$$

$$\Gamma_{jk}^i = \frac{1}{2} \gamma^{il} (\partial_j \gamma_{lk} + \partial_k \gamma_{lj} - \partial_l \gamma_{jk}). \quad (\text{A.15f})$$

The Ricci tensor is given by

$$R_{\mu\nu} = \partial_{\alpha} \Gamma_{\mu\nu}^{\alpha} - \partial_{\nu} \Gamma_{\alpha\mu}^{\alpha} + \Gamma_{\alpha\beta}^{\alpha} \Gamma_{\mu\nu}^{\beta} - \Gamma_{\beta\mu}^{\alpha} \Gamma_{\alpha\nu}^{\beta}. \quad (\text{A.16})$$

Fortunately, assuming isotropy, the components R_{i0} vanish. We then proceed to calculate the components

$$R_{00} = \partial_\alpha \Gamma_{00}^\alpha - \partial_0 \Gamma_{\alpha 0}^\alpha + \Gamma_{\alpha\beta}^\alpha \Gamma_{00}^\beta - \Gamma_{\beta 0}^\alpha \Gamma_{\alpha 0}^\beta \quad (\text{A.17})$$

$$R_{00} = -\partial_0 \Gamma_{i0}^i + \Gamma_{ji}^j \Gamma_{00}^i - \Gamma_{j0}^i \Gamma_{i0}^j \quad (\text{A.18})$$

$$R_{00} = -3\dot{H} - 3H^2 = -3\frac{\ddot{a}}{a}. \quad (\text{A.19})$$

There is a trick to simplify the calculation of R_{ij} . The Ricci tensor is a combination of first and second derivatives of the metric components. We can calculate the Ricci tensor at the origin, $R_{ij}(t, \mathbf{r} = 0)$ in terms of the metric $g_{ij}(t, \mathbf{r} = 0)$, and then use the fact that the origin is an arbitrary point to imply that our final result holds everywhere. Since we are only interested in first and second derivatives of the metric at $x_i = 0$, we may expand the metric components in second order in the spatial components x^i ,

$$\gamma_{ij} = \delta_{ij} + \frac{kx_i x_j}{1 - kx_k x^k} = \delta_{ij} + kx_i x_j + \mathcal{O}(x^4). \quad (\text{A.20})$$

Thus, its derivative is

$$\partial_k \gamma_{ij} = k(\delta_{ki} x_j + \delta_{kj} x_i), \quad (\text{A.21})$$

and the spatial Christoffel symbols are

$$\Gamma_{jk}^i = \frac{k}{2} \gamma^{il} (\delta_{jl} x_k + \delta_{jk} x_l + \delta_{kl} x_j + \delta_{kj} x_l - \delta_{lj} x_k - \delta_{lk} x_j); \quad (\text{A.22})$$

$$\Gamma_{jk}^i = \frac{k}{2} \delta^{il} (\delta_{jl} x_k + \delta_{jk} x_l + \delta_{kl} x_j + \delta_{kj} x_l - \delta_{lj} x_k - \delta_{lk} x_j); \quad (\text{A.23})$$

$$\Gamma_{jk}^i = \frac{k}{2} (\delta_{ji} x_k + \delta_{jk} x_i + \delta_{ki} x_j + \delta_{kj} x_i - \delta_{ij} x_k - \delta_{ik} x_j); \quad (\text{A.24})$$

$$\Gamma_{jk}^i = \frac{k}{2} (2\delta_{jk} x_i); \quad (\text{A.25})$$

$$\Gamma_{jk}^i = k\delta_{jk} x^i. \quad (\text{A.26})$$

$$(\text{A.27})$$

The spatial Christoffel symbols vanish at the origin $x^i = 0$, but their derivatives are

$$\partial_l \Gamma_{jk}^i = k\delta_l^i \delta_{jk}. \quad (\text{A.28})$$

We may now evaluate the spatial components R_{ij} at the origin,

$$R_{ij} = \partial_\alpha \Gamma_{ij}^\alpha - \partial_j \Gamma_{\alpha i}^\alpha + \Gamma_{\alpha\beta}^\alpha \Gamma_{ij}^\beta - \Gamma_{\beta i}^\alpha \Gamma_{\alpha j}^\beta. \quad (\text{A.29})$$

The first two terms reduce to

$$\partial_\alpha \Gamma_{ij}^\alpha - \partial_j \Gamma_{\alpha i}^\alpha = \partial_0 \Gamma_{ij}^0 + \partial_k \Gamma_{ij}^k - \partial_j \Gamma_{ki}^k \quad (\text{A.30})$$

$$\partial_\alpha \Gamma_{ij}^\alpha - \partial_j \Gamma_{\alpha i}^\alpha = \partial_0(a\dot{a})\gamma_{ij} + k\delta_k^k\delta_{ij} - k\delta_j^k\delta_{ki} \quad (\text{A.31})$$

$$\partial_\alpha \Gamma_{ij}^\alpha - \partial_j \Gamma_{\alpha i}^\alpha = (\dot{a}^2 + a\ddot{a})\delta_{ij} + 3k\delta_{ij} - k\delta_{ij} \quad (\text{A.32})$$

$$\partial_\alpha \Gamma_{ij}^\alpha - \partial_j \Gamma_{\alpha i}^\alpha = (\dot{a}^2 + a\ddot{a} + 2k)\delta_{ij}, \quad (\text{A.33})$$

where, evaluating at the origin, $\gamma_{ij} = \delta_{ij}$. The other two terms in the Ricci tensor expression evaluate to

$$\Gamma_{\alpha\beta}^\alpha \Gamma_{ij}^\beta - \Gamma_{\beta i}^\alpha \Gamma_{\alpha j}^\beta = \Gamma_{k0}^k \Gamma_{ij}^0 - \Gamma_{0i}^k \Gamma_{kj}^0 - \Gamma_{ki}^0 \Gamma_{0j}^k \quad (\text{A.34})$$

$$\Gamma_{\alpha\beta}^\alpha \Gamma_{ij}^\beta - \Gamma_{\beta i}^\alpha \Gamma_{\alpha j}^\beta = 3Ha\dot{a}\delta_{ij} - Ha\dot{a}\delta_{ij} - a\dot{a}\delta_{ki}H\delta_j^k \quad (\text{A.35})$$

$$\Gamma_{\alpha\beta}^\alpha \Gamma_{ij}^\beta - \Gamma_{\beta i}^\alpha \Gamma_{\alpha j}^\beta = \dot{a}^2\delta_{ij}. \quad (\text{A.36})$$

where we already use the fact that the pure spatial Christoffel symbols are zero at the origin. Finally, we obtain

$$R_{ij}(t, x^i = 0) = (a\ddot{a} + 2\dot{a}^2 + 2k)\delta_{ij} = \left[\frac{\ddot{a}}{a} + 2H^2 + 2\frac{k}{a^2} \right] g_{ij}(t, x^i = 0). \quad (\text{A.37})$$

Finally, we use the fact that if a proportionality relation between two tensors holds at the origin, it must hold at all spatial points, as the origin is not a special point in the homogeneous space. An alternative argument is that our homogeneous and isotropic spacetime is a maximally symmetric space, and a property of those spaces is that the Ricci tensor is proportional to the metric. Thus, we only need to calculate the proportionality constant in any point of space. Therefore,

$$R_{ij} = \left[\frac{\ddot{a}}{a} + 2H^2 + 2\frac{k}{a^2} \right] g_{ij}. \quad (\text{A.38})$$

The Ricci scalar is

$$R = g^{\mu\nu} R_{\mu\nu} = g^{00} R_{00} + g^{ij} R_{ij} \quad (\text{A.39})$$

$$R = (-1) \left(-3 \frac{\ddot{a}}{a} \right) + g^{ij} R_{ij} \quad (\text{A.40})$$

$$R = 3 \frac{\ddot{a}}{a} + 3 \left[\frac{\ddot{a}}{a} + 2H^2 + 2 \frac{k}{a^2} \right] \quad (\text{A.41})$$

$$R = 6 \frac{\ddot{a}}{a} + 6H^2 + 6 \frac{k}{a^2}. \quad (\text{A.42})$$

Finally, the Einstein tensor has components

$$G_{00} = R_{00} - \frac{1}{2} R g_{00} = -3 \frac{\ddot{a}}{a} - 3 \left(\frac{\ddot{a}}{a} + H^2 + \frac{k}{a^2} \right) (-1) = 3H^2 + 3k/a^2; \quad (\text{A.43})$$

$$G_{ij} = R_{ij} - \frac{1}{2} R g_{ij} = \left[\frac{\ddot{a}}{a} + 2H^2 + 2 \frac{k}{a^2} - 3 \frac{\ddot{a}}{a} - 3H^2 - 3 \frac{k}{a^2} \right] a^2 \gamma_{ij}; \quad (\text{A.44})$$

$$G_{ij} = \left[-2 \frac{\ddot{a}}{a} - H^2 - \frac{k}{a^2} \right] a^2 \gamma_{ij}. \quad (\text{A.45})$$

A.3 Gauge Transformations

In this Appendix, I calculate the gauge transformation equations 2.102 explicitly. Let's assume that we change the coordinate system from x^μ to $\tilde{x}^\mu$ such that

$$\tilde{x}^\mu = x^\mu + \zeta^\mu, \quad (\text{A.46})$$

where ζ^μ is a position-dependent linear perturbation. We define $\zeta^0 = T$, $\zeta^i = \partial^i L + \hat{L}^i$, where $\partial_i \hat{L}^i = 0$. For the metric, we use the coordinate transformation equation

$$\tilde{g}_{\mu\nu}(\tilde{x}) = \frac{\partial x^\alpha}{\partial \tilde{x}^\mu} \frac{\partial x^\beta}{\partial \tilde{x}^\nu} g_{\alpha\beta}(x). \quad (\text{A.47})$$

Since $x^\alpha = \tilde{x}^\alpha - \zeta^\alpha$, the partial derivatives are

$$\frac{\partial x^\alpha}{\partial \tilde{x}^\mu} = \delta_\mu^\alpha - \partial_\mu \zeta^\alpha. \quad (\text{A.48})$$

Each transformation equation comes from a different set of combinations of μ and ν . Let's start with $\mu = \nu = 0$. We have defined $g_{00} = -a^2(\tau)(1 + 2A)$, and thus $\tilde{g}_{00}(\tilde{x}) = -a^2(\tilde{\tau})(1 + 2\tilde{A})$. We are interested only in the first order part of the equation, and thus we can neglect any term that is not linear in the perturbations. We need to be careful, because the tilde part of the equation is calculated on transformed coordinates, and thus $a(\tilde{\tau}) = a(\tau + T) \approx a(\tau) + a'(\tau)T$

and $a^2(\tilde{\tau}) \approx a^2(\tau) + 2a(\tau)a'(\tau)T = a^2(\tau)(1 + 2\mathcal{H}T)$. Inserting these expressions into the coordinate transformation, we get

$$\begin{aligned}
\tilde{g}_{00} &= (\delta_0^\alpha - \partial_0 \tilde{\zeta}^\alpha)(\delta_0^\beta - \partial_0 \tilde{\zeta}^\beta)g_{00} \\
\tilde{g}_{00} &= g_{00} - \partial_0 \tilde{\zeta}^\alpha g_{\alpha 0} - \partial_0 \tilde{\zeta}^\beta g_{\beta 0} \\
\tilde{g}_{00} &= g_{00} - 2\partial_0 \tilde{\zeta}^\alpha g_{\alpha 0} \\
-a^2(\tilde{\tau})(1 + 2\tilde{A}) &= -a^2(\tau)(1 + 2A) + 2a^2(\tau)T' \\
-a^2(\tau)(1 + 2\mathcal{H}T)(1 + 2\tilde{A}) &= -a^2(\tau)(1 + 2A) + 2a^2(\tau)T' \\
-(1 + 2\mathcal{H}T)(1 + 2\tilde{A}) &= -(1 + 2A) + 2T' \\
-(1 + 2\mathcal{H}T + 2\tilde{A}) &= -(1 + 2A) + 2T' \\
\mathcal{H}T + \tilde{A} &= A - T' \\
\tilde{A} &= A - T' - \mathcal{H}T.
\end{aligned}$$

Now, $\mu = 0$ and $\nu = i$

$$\begin{aligned}
\tilde{g}_{0i} &= (\delta_0^\alpha - \partial_0 \tilde{\zeta}^\alpha)(\delta_i^\beta - \partial_i \tilde{\zeta}^\beta)g_{\alpha\beta} \\
\tilde{g}_{0i} &= g_{0i} - \partial_0 \tilde{\zeta}^\alpha g_{\alpha i} - \partial_i \tilde{\zeta}^\beta g_{0\beta} \\
a^2(\tilde{\tau})\tilde{B}_i &= a^2(\tau)B_i - \partial_0 \tilde{\zeta}^j g_{ji} - \partial_i \tilde{\zeta}^0 g_{00} \\
a^2(\tau)(1 + 2\mathcal{H}T)\tilde{B}_i &= a^2(\tau)B_i - a^2(\tau)\partial_0 L_i + a^2(\tau)\partial_i T \\
\tilde{B}_i &= B_i - L'_i + \partial_i T.
\end{aligned}$$

We may perform the SVT decomposition, separating divergence and divergenceless terms

$$\begin{aligned}
\tilde{B}_i &= \partial_i \tilde{B} + \hat{\tilde{B}}_i, \\
L_i &= \partial_i L + \hat{L}_i,
\end{aligned}$$

and defining the Fourier modes $B(k) = \partial_i B/k$, $L(k) = \partial_i L/k$, we obtain

$$\begin{aligned}
\partial_i \tilde{B} + \hat{\tilde{B}}_i &= \partial_i B + \hat{B}_i - \partial_i L' - \hat{L}'_i + \partial_i T \\
\begin{cases} \tilde{B} &= B - L' + kT, \\ \hat{\tilde{B}}_i &= \hat{B}_i - \hat{L}'_i. \end{cases}
\end{aligned}$$

For the spatial part, $\mu = i, \nu = j$, we have

$$\begin{aligned}\tilde{g}_{ij} &= (\delta_i^\alpha - \partial_i \xi^\alpha)(\delta_j^\beta - \partial_j \xi^\beta) g_{\alpha\beta} \\ \tilde{g}_{ij} &= g_{ij} - \partial_i \xi^\alpha g_{\alpha j} - \partial_j \xi^\beta g_{i\beta} \\ a^2(\tilde{\tau})(\gamma_{ij} + \tilde{h}_{ij}) &= a^2(\tau)(\gamma_{ij} + h_{ij}) - a^2(\tau)\partial_i \xi^m \gamma_{mj} - a^2(\tau)\partial_j \xi^m \gamma_{im} \\ a^2(\tau)(1 + 2\mathcal{H}T)(\gamma_{ij} + \tilde{h}_{ij}) &= a^2(\tau)(\gamma_{ij} + h_{ij}) - a^2(\tau)\partial_i L_j - a^2(\tau)\partial_j L_i \\ (1 + 2\mathcal{H}T)(\gamma_{ij} + \tilde{h}_{ij}) &= \gamma_{ij} + h_{ij} - \partial_i L_j - \partial_j L_i \\ \tilde{h}_{ij} &= h_{ij} - 2\mathcal{H}T\gamma_{ij} - \partial_i L_j - \partial_j L_i.\end{aligned}$$

Performing the SVT decomposition on $L_i = \partial_i L + \hat{L}_i$ and h_{ij} according to Equation 2.67, we obtain

$$\begin{aligned}2\tilde{H}_L\gamma_{ij} + \partial_{ij}^{TT}\tilde{H}_T + (\partial_i\tilde{H}_{Tj} + \partial_j\tilde{H}_{Ti}) + \tilde{H}_{Tij} &= 2H_L\gamma_{ij} + \partial_{ij}^{TT}H_T + (\partial_i H_{Tj} + \partial_j H_{Ti}) \\ &\quad + H_{Tij} - 2\mathcal{H}T\gamma_{ij} - \partial_i \hat{L}_j - \partial_j \hat{L}_i - 2\partial_i \partial_j L.\end{aligned}$$

The term $\partial_i \hat{L}_j - \partial_j \hat{L}_i$ is traceless, since $\gamma^{ij}\partial_i \hat{L}_j = \partial^j \hat{L}_j = 0$. The trace of the term $\partial_i \partial_j L$ is

$$\gamma^{ij}\partial_i \partial_j L = \nabla^2 L. \quad (\text{A.49})$$

Thus, separating trace and traceless parts, we have $2\partial_i \partial_j L = 2\nabla^2 L \gamma_{ij}/3 + 2\partial_{ij}^{TT} L$. Taking the trace part, that proportional to γ_{ij} , we get

$$\begin{aligned}2\tilde{H}_L\gamma_{ij} &= 2H_L\gamma_{ij} - 2\mathcal{H}T\gamma_{ij} - \frac{2}{3}\nabla^2 L\gamma_{ij}, \\ \tilde{H}_L &= H_L - \mathcal{H}T - \frac{1}{3}\nabla^2 L.\end{aligned}$$

Taking the terms inside ∂_{ij}^{TT} , we get

$$\tilde{H}_T = H_T - L. \quad (\text{A.50})$$

Taking the vector part, we get

$$\tilde{H}_{Ti} = H_{Ti} - \hat{L}_i. \quad (\text{A.51})$$

Finally, the pure tensor part is unchanged,

$$\tilde{H}_{Tij} = H_{Tij}. \quad (\text{A.52})$$

Let's turn our attention to the matter perturbations. The energy-momentum

tensor perturbations are given in terms of Equation 2.94, and transform as

$$\tilde{T}_\nu^\mu(\tilde{x}) = \frac{\partial \tilde{x}^\mu}{\partial x^\alpha} \frac{\partial x^\beta}{\partial \tilde{x}^\nu} T_\beta^\alpha(x). \quad (\text{A.53})$$

Therefore, we can repeat the same steps to derive the transformation equations. Starting with $\mu = \nu = 0$, we have

$$\begin{aligned} \tilde{T}_0^0(\tilde{x}) &= (\delta_\alpha^0 + \partial_\alpha \tilde{\xi}^0)(\delta_0^\beta - \partial_0 \tilde{\xi}^\beta) T_\beta^\alpha(x) \\ &\quad - (\rho(\tilde{\tau}) + \delta\tilde{\rho}) = -(\rho + \delta\rho) \\ \rho(\tau) + \rho'T + \delta\tilde{\rho} &= \rho + \delta\rho \\ \delta\tilde{\rho} &= \delta\rho - \rho'T. \end{aligned}$$

For $\mu = i$ and $\nu = 0$, we obtain

$$\begin{aligned} \tilde{T}_0^i(\tilde{x}) &= (\delta_\alpha^i + \partial_\alpha \tilde{\xi}^i)(\delta_0^\beta - \partial_0 \tilde{\xi}^\beta) T_\beta^\alpha(x) \\ &\quad - (\rho(\tilde{\tau}) + P(\tilde{\tau}))\tilde{v}^i = -(\rho(\tau) + P(\tau))v^i + T_0^\alpha \partial_\alpha \tilde{\xi}^i - T_\beta^i \partial_0 \tilde{\xi}^\beta \\ -(\rho(\tau) + \rho'T + P(\tau) + P'T)\tilde{v}^i &= -(\rho(\tau) + P(\tau))v^i + T_0^0 \partial_0 L^i - T_j^i \partial_0 L^j \\ -(\rho(\tau) + \rho'T + P(\tau) + P'T)\tilde{v}^i &= -(\rho(\tau) + P(\tau))v^i - \rho L'^i - P L'^i \\ \tilde{v}^i &= v^i + L'^i. \end{aligned}$$

This equation automatically works for each component of the SVT decomposition.

Finally, for $\mu = i$ and $\nu = j$, we obtain

$$\begin{aligned} \tilde{T}_j^i(\tilde{x}) &= (\delta_\alpha^i + \partial_\alpha \tilde{\xi}^i)(\delta_j^\beta - \partial_j \tilde{\xi}^\beta) T_\beta^\alpha(x) \\ \tilde{T}_j^i(\tilde{x}) &= T_j^i(x) + T_j^\alpha \partial_\alpha \tilde{\xi}^i - T_\beta^i \partial_j \tilde{\xi}^\beta \\ \tilde{T}_j^i(\tilde{x}) &= T_j^i(x) + P \delta_j^m \partial_m \tilde{\xi}^i - P \delta_\beta^i \partial_j \tilde{\xi}^\beta \\ \tilde{T}_j^i(\tilde{x}) &= T_j^i(x) + P \partial_j L^i - P \partial_j L^i. \end{aligned}$$

Decomposing into the trace and traceless parts, we obtain

$$\begin{aligned} \delta_j^i(P(\tilde{\tau}) + \delta\tilde{P}) + P(\tilde{\tau})\tilde{\Pi}_j^i &= \delta_j^i(P(\tau) + \delta P) + P(\tau)\Pi_j^i, \\ \delta_j^i(P(\tau) + P'T + \delta\tilde{P}) + P(\tilde{\tau})\tilde{\Pi}_j^i &= \delta_j^i(P(\tau) + \delta P) + P(\tau)\Pi_j^i, \\ \delta\tilde{P} &= \delta P - P'T, \\ \tilde{\Pi}_j^i &= \Pi_j^i. \end{aligned}$$

A.4 Klein-Gordon Equation in FLRW

$$S_\phi = \int d^4x \sqrt{-g} \left(-\frac{1}{2} \partial_\mu \phi \partial^\mu \phi - V(\phi) \right). \quad (\text{A.54})$$

The term $X = -\partial_\mu \phi \partial^\mu \phi / 2$ is the kinetic energy of the field. Assuming homogeneity, the kinetic term evaluates to

$$X = -\frac{1}{2} \partial_0 \phi \partial^0 \phi = -\frac{1}{2} g^{00} \dot{\phi}^2 = \frac{\dot{\phi}^2}{2}. \quad (\text{A.55})$$

The field potential $V(\phi)$ determines the evolution of the scalar field. By using the Euler-Lagrange equations, we obtain the classical equation of motion for the field ϕ in the FLRW spacetime

$$\begin{aligned} \sqrt{-g} &= a^3; \\ \frac{\partial \mathcal{L}}{\partial \phi} &= a^3 \frac{dV}{d\phi}; \\ \frac{\partial \mathcal{L}}{\partial \dot{\phi}} &= a^3 \dot{\phi}; \\ \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} &= 3a^2 \dot{a} \dot{\phi} + a^3 \ddot{\phi}; \\ a^3 (\ddot{\phi} + 3H\dot{\phi} + V'(\phi)) &= 0 \\ \ddot{\phi} + 3H\dot{\phi} + V'(\phi) &= 0. \end{aligned}$$

Appendix B

Perturbed Cosmological Equations using xPand

In this Appendix, I describe the process of using xPand to obtain the cosmological perturbation equations described in Section 2.

Notation and Definitions

xPand's FRW metric perturbations $\delta g_{\mu\nu}$ are given by (ϵ is the perturbation parameter, h_{ij} is the spatial metric γ_{ij} and $\bar{D}$ is the spatial covariant derivative)

	n	h
n	$-a^2 - 2 \epsilon a^2 \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} A \right)$	$\epsilon \left(a^2 \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} B_\nu \right) + a^2 \left(\bar{D}_\nu \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} B \right) \right)$
h	$\epsilon \left(a^2 \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} B_\mu \right) + a^2 \left(\bar{D}_\mu \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} B \right) \right)$	$a^2 \bar{h}_{\mu\nu} + \epsilon \left(2 a^2 \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} H_{T\mu\nu} \right) - 2 a^2 \bar{h}_{\mu\nu} \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix} H_L \right) + a^2 \left(\bar{D}_\mu \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} H_{T\nu} \right) + a^2 \left(\bar{D}_\nu \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} H_{T\mu} \right) + 2 a^2 \left(\bar{D}_\nu \bar{D}_\mu \begin{smallmatrix} 1 \\ 1 \end{smallmatrix} H_T \right) \right)$

Figura B.1: Metric output from xPand.

This translates to

$$g_{00} = -a^2(1 + 2A) \quad (\text{B.1a})$$

$$g_{0i} = a^2 B_i \quad (\text{B.1b})$$

$$g_{ij} = a^2(\gamma_{ij} - 2H_L \gamma_{ij} + 2\partial_i \partial_j H_T) \quad (\text{B.1c})$$

Note that xPand already did SVT decomposition in my quantities. **The signs of B_i and H_L are changed.** A very important thing to notice: xPand defines the scalar mode of H_{Tij} as $H_{Tij}^{(0)} = \nabla_i \nabla_j H_T^{(0)}$ instead of $H_{Tij}^{(0)} = (\nabla_i \nabla_j - \frac{1}{3} \gamma_{ij} \nabla^2) H_T^{(0)}$. This redefinition is important to make $H_{Tij}^{(0)}$ trace-free. The only thing we have to do is to add and subtract this $\frac{1}{3} \gamma_{ij} \nabla^2 H_T^{(0)}$, subtracting it on H_T and adding it on H_L , and **hence $H_L \rightarrow H_L - \frac{1}{3} \nabla^2 H_T$ is necessary to make equations right.**

Now, for the energy-momentum tensor (quantities with a red "(1)" are linear perturbations)

	n	h
n	$-\rho - \epsilon \left(\begin{smallmatrix} 1 \\ \rho \end{smallmatrix} \right)$	$\epsilon \left(\left(\begin{smallmatrix} 1 \\ B_v \end{smallmatrix} \right) P + P \left(\begin{smallmatrix} 1 \\ V_v \end{smallmatrix} \right) + \left(\begin{smallmatrix} 1 \\ B_v \end{smallmatrix} \right) \rho + \left(\begin{smallmatrix} 1 \\ V_v \end{smallmatrix} \right) \rho + P \left(\begin{smallmatrix} 1 \\ \bar{D}_v \begin{smallmatrix} 1 \\ B \end{smallmatrix} \end{smallmatrix} \right) + \rho \left(\begin{smallmatrix} 1 \\ \bar{D}_v \begin{smallmatrix} 1 \\ B \end{smallmatrix} \end{smallmatrix} \right) + P \left(\begin{smallmatrix} 1 \\ \bar{D}_v \begin{smallmatrix} 1 \\ V \end{smallmatrix} \end{smallmatrix} \right) + \rho \left(\begin{smallmatrix} 1 \\ \bar{D}_v \begin{smallmatrix} 1 \\ V \end{smallmatrix} \end{smallmatrix} \right) \right)$
h	$\epsilon \left(-P \left(\begin{smallmatrix} 1 \\ V^\mu \end{smallmatrix} \right) - \left(\begin{smallmatrix} 1 \\ V^\mu \end{smallmatrix} \right) \rho - P \left(\begin{smallmatrix} 1 \\ \bar{D}^\mu \begin{smallmatrix} 1 \\ V \end{smallmatrix} \end{smallmatrix} \right) - \rho \left(\begin{smallmatrix} 1 \\ \bar{D}^\mu \begin{smallmatrix} 1 \\ V \end{smallmatrix} \end{smallmatrix} \right) \right)$	$\bar{h}^\mu_\nu P + \epsilon \bar{h}^\mu_\nu \left(\begin{smallmatrix} 1 \\ P \end{smallmatrix} \right)$

Figura B.2: Energy-momentum tensor output from xPand.

This translates to

$$\delta T_0^0 = -\delta \rho \quad (\text{B.2a})$$

$$\delta T_0^i = -(\bar{\rho} + \bar{P})v^i \quad (\text{B.2b})$$

$$\delta T_i^0 = (\bar{\rho} + \bar{P})(v^i + B^i) \quad (\text{B.2c})$$

$$\delta T_j^i = \delta P \delta_j^i \quad (\text{B.2d})$$

xPand does not include anisotropic stress $\bar{P}\Pi_{ij}$.

Figure B.3 shows the list of rules that are used to convert xPand definitions to the definitions and notations used in this thesis. After every calculation, these rules (and other rules that may help simplify the equations) can be applied to xPand's output.

```

PrintAs[phi] ^= "A"; (*
PrintAs[psi] ^= "H_L ";
PrintAs[Esh] ^= "H_T ";
PrintAs[Evh] ^= "H_T ";
PrintAs[Eth] ^= "H_T ";
PrintAs[Vvhu] ^= "V ";
PrintAs[Vshu] ^= "V ";
eq00 = ExtractComponents[ExtractOrder[einsteineqs, 1] * ah[]^2, h, {"Time", "Time"}];
% /. cd[-alpha]@cd[alpha][x_] -> -k^2 * x;
% /. {psi[LI[z1_], LI[z2_]] -> -psi[LI[z1], LI[z2]]};
% /. {psi[LI[z1_], LI[z2_]] -> (psi[LI[z1], LI[z2]] + k^2 * Esh[LI[z1], LI[z2]] / 3)};
% /. {Esh[LI[z1_], LI[z2_]] -> Esh[LI[z1], LI[z2]] / k^2};
% /. {Vshu[LI[z1_], LI[z2_]] -> -Vshu[LI[z1], LI[z2]] / k};
% /. {Bsh[LI[z1_], LI[z2_]] -> -Bsh[LI[z1], LI[z2]] / k};
% /. {Bsh[LI[z1_], LI[z2_]] -> -Bsh[LI[z1], LI[z2]]};

```

Figura B.3: Commands to adjust notation and definitions

From xPand output to Wayne's equations

Let's start from the perturbed continuity equation. The raw output from xPand before applying the rules is given in Figure B.4.

$$3 \mathcal{H} \left(\overset{(1)}{P} \right) + 3 \mathcal{H} \left(\overset{(1)}{\rho} \right) + \overset{(1)}{\rho} - 6 \mathcal{H} P \left(\overset{(1)}{\phi} \right) - 6 \mathcal{H} \rho \left(\overset{(1)}{\phi} \right) - 2 \dot{\rho} \left(\overset{(1)}{\phi} \right) - 3 P \left(\overset{(1)}{\psi} \right) - 3 \rho \left(\overset{(1)}{\psi} \right) + P \left(\bar{D}_\alpha \bar{D}^\alpha \overset{(1)}{E} \right) + \rho \left(\bar{D}_\alpha \bar{D}^\alpha \overset{(1)}{E} \right) + P \left(\bar{D}_\alpha \bar{D}^\alpha \overset{(1)}{V}_u \right) + \rho \left(\bar{D}_\alpha \bar{D}^\alpha \overset{(1)}{V}_u \right)$$

Figura B.4: xPand output for the perturbed conservation equation

$$\left(4 k \mathcal{H} P \left(\overset{(1)}{V}^\gamma \right) + k \dot{P} \left(\overset{(1)}{V}^\gamma \right) + k P \left(\overset{(1)}{V}^\gamma \right) + 4 k \mathcal{H} \left(\overset{(1)}{V}^\gamma \right) \rho + k \left(\overset{(1)}{V}^\gamma \right) \dot{\rho} + k \left(\overset{(1)}{V}^\gamma \right) (P + \rho) + k \left(\overset{(1)}{V}^\gamma \right) (\dot{P} + \mathcal{H} (P + \rho)) + k \left(\overset{(1)}{V}^\gamma \right) \dot{\rho} + \mathcal{H} P \left(\bar{D}^\gamma \overset{(1)}{B} \right) + \dot{P} \left(\bar{D}^\gamma \overset{(1)}{B} \right) + \mathcal{H} \rho \left(\bar{D}^\gamma \overset{(1)}{B} \right) + P \left(\bar{D}^\gamma \overset{(1)}{B} \right) + \rho \left(\bar{D}^\gamma \overset{(1)}{B} \right) + k \left(\bar{D}^\gamma \overset{(1)}{P} \right) - 4 \mathcal{H} P \left(\bar{D}^\gamma \overset{(1)}{V} \right) - \dot{P} \left(\bar{D}^\gamma \overset{(1)}{V} \right) - 4 \mathcal{H} \rho \left(\bar{D}^\gamma \overset{(1)}{V} \right) - \dot{\rho} \left(\bar{D}^\gamma \overset{(1)}{V} \right) - P \left(\bar{D}^\gamma \overset{(1)}{V} \right) - \rho \left(\bar{D}^\gamma \overset{(1)}{V} \right) + k (P + \rho) \left(\bar{D}^\gamma \overset{(1)}{A} \right) \right)$$

Figura B.5: xPand output for the vector part of the conservation equation.

The output can be translated as

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) - 2A(\bar{\rho}' + 3\mathcal{H}(\bar{\rho} + \bar{P})) - 3(\bar{\rho} + \bar{P})H_L' + (\bar{\rho} + \bar{P})\nabla^2 v + (\bar{\rho} + \bar{P})\nabla^2 H_T' = 0 \quad (\text{B.3})$$

The Φ term is just the continuity equation for the background, and therefore vanishes. The remaining terms are

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) - 3(\bar{\rho} + \bar{P})H_L' + (\bar{\rho} + \bar{P})\nabla^2 v + (\bar{\rho} + \bar{P})\nabla^2 H_T' = 0 \quad (\text{B.4})$$

Now, we have to make the substitution $H_L \rightarrow H_L - \frac{1}{3}\nabla^2 H_T$. This can be made using a simple rule in Mathematica. When we do this, the laplacian of H_T cancels, and we obtain

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) - 3(\bar{\rho} + \bar{P})H_L' + (\bar{\rho} + \bar{P})\nabla^2 v = 0 \quad (\text{B.5})$$

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = (\bar{\rho} + \bar{P})(3H_L' - \nabla^2 v) \quad (\text{B.6})$$

The only thing to do now is using the Fourier modes. Since the ± 1 modes are transverse, we get

$$\nabla^2 v^{(0)} = \nabla \cdot \mathbf{v} = v^{(0)} \nabla^i (Q_i^{(0)}) = -v^{(0)} \frac{1}{k} \nabla^i \nabla_i Q^{(0)} = kv^{(0)} \quad (\text{B.7})$$

and we get the continuity equation,

$$\delta\rho' + 3\mathcal{H}(\delta\rho + \delta P) = (\bar{\rho} + \bar{P})(-kv + 3H_L'). \quad (\text{B.8})$$

As noted before, the sign of H_L is changed, so this result agrees exactly with Wayne. I remark that, due to our conventions for the laplacian eigenfunctions, we always substitute $v \rightarrow -\frac{1}{k}v$ and all other scalar modes of vector quantities. In the same way, scalar modes of tensor quantities need to be substituted as $H_T \rightarrow \frac{1}{k^2}H_T$.

After applying the rules from Figure B.3, we obtain the following result for the vector part of the conservation perturbation

The first terms are vector terms, and the rest are gradients of scalar terms. Since the vector parts are transverse and the gradient parts are longitudinal, they

separate due to linear independence. Therefore, we can pick only the gradient part and equal it to zero. If the gradient of a function is zero everywhere, then it's a constant function. After discarding the gradients, we obtain

$$(\mathcal{H}(\bar{\rho} + \bar{p}) + \bar{p}')B + (\bar{\rho} + \bar{p})B' + k\delta P - (4\mathcal{H}(\bar{\rho} + \bar{p}) + \bar{p}' + \bar{\rho}')v - (\bar{\rho} + \bar{p})v' + (\bar{\rho} + \bar{p})kA = 0 \quad (\text{B.9})$$

Using the continuity background equation $3\mathcal{H}(\bar{\rho} + \bar{p}) + \bar{\rho}' = 0$, we see that the coefficients of B and v are equal

$$[4\mathcal{H}(\bar{\rho} + \bar{p}) + \bar{p}' + \bar{\rho}'](B - v) + -(\bar{\rho} + \bar{p})(B' - v') + k\delta P + (\bar{\rho} + \bar{p})kA = 0 \quad (\text{B.10})$$

The first terms look like a product rule for the time derivative of $(\bar{\rho} + \bar{p})(\nabla B + \nabla v)$. In fact,

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [(\bar{\rho} + \bar{p})(B - \nabla v)] = [4\mathcal{H}(\bar{\rho} + \bar{p}) + \bar{p}' + \bar{\rho}'](B - v) + (\bar{\rho} + \bar{p})(B' - v') \quad (\text{B.11})$$

So, we can rewrite the equation as

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [(\bar{\rho} + \bar{p})(\nabla B - \nabla v)] + k\delta P + k(\bar{\rho} + \bar{p})A = 0 \quad (\text{B.12})$$

Therefore, we obtain

$$\left(\frac{d}{d\tau} + 4\mathcal{H}\right) [(\bar{\rho} + \bar{p})\frac{(v - B)}{k}] = \delta P + (\bar{\rho} + \bar{p})A \quad (\text{B.13})$$

Let's proceed to the Einstein equations. Figure B.6 shows the xPand output for the space/time equation.

$$\frac{1}{12k^2} \left(3k^2 \left(\overset{(1)}{B}{}^\mu \right) \left(k^2 + 4\gamma\mathcal{H}^2 - 4\gamma'\mathcal{H} + 2k \right) - 3 \left(\overset{(1)}{H_T}{}^\mu \right) \left(k^4 - 2k^2k \right) + \right. \\ \left. 4 \left(3k\gamma\mathcal{H}^2 \left(\bar{D}^\mu \overset{(1)}{B} \right) - 3k\gamma'\mathcal{H} \left(\bar{D}^\mu \overset{(1)}{B} \right) - k^2 \left(\bar{D}^\mu \overset{(1)}{H_T} \right) + 3k \left(\bar{D}^\mu \overset{(1)}{H_T} \right) + 12Gk\pi a^2 (P + \rho) \left(k \left(\overset{(1)}{V}{}^\mu \right) - \bar{D}^\mu \overset{(1)}{V} \right) + 3k^2\gamma\mathcal{H} \left(\bar{D}^\mu \overset{(1)}{A} \right) - 3k^2 \left(\bar{D}^\mu \overset{(1)}{H_L} \right) \right) \right)$$

Figura B.6: xPand output for the Einstein equation 0i.

Only the last terms are from scalar modes, and they can be set independently to zero since Fourier modes are independent. Dividing by $3k^2$, we get:

$$\mathcal{H}A - H'_L - \frac{H'_T}{3} - \frac{1}{k}(\mathcal{H}' - \mathcal{H}^2)B + \frac{K}{k^2}H'_T = 4\pi Ga^2 \frac{v}{k} \quad (\text{B.14})$$

Using the Friedmann equations, we get $\mathcal{H}' - \mathcal{H}^2 = -4\pi Ga^2(\bar{\rho} + \bar{p}) + K$. There-

fore,

$$\mathcal{H}A - H'_L - \frac{H'_T}{3} - \frac{1}{k}(-4\pi Ga^2(\bar{\rho} + \bar{P}) + K)B + \frac{K}{k^2}H'_T = 4\pi Ga^2(\bar{\rho} + \bar{P})\frac{v}{k} \quad (\text{B.15})$$

$$\mathcal{H}A - H'_L - \frac{H'_T}{3} - \frac{K}{k^2}(kB - H'_T) = 4\pi Ga^2(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right). \quad (\text{B.16})$$

The xPand output for the 00 Einstein equation is given in Figure B.7.

Figura B.7: xPand output for the Einstein equation 0i.

In the last term, we are going to substitute $\mathcal{H}A - H'_L = \frac{H'_T}{3} + \frac{K}{k^2}(kB - H'_T) + 4\pi Ga^2(\bar{\rho} + \bar{P})(\frac{v-B}{k})$ from the previous result. We then get

$$4\pi Ga^2\delta\rho = (k^2 - 3K)(H_L + \frac{H_T}{3}) - \mathcal{H}[-kB + 3(\mathcal{H}A - H'_L)], \quad (\text{B.17})$$

$$4\pi Ga^2\delta\rho = (k^2 - 3K)(H_L + \frac{H_T}{3}) - \mathcal{H}[-kB + 3\left(\frac{H'_T}{3} + \frac{K}{k^2}(kB - H'_T) + 4\pi Ga^2(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right)\right)], \quad (\text{B.18})$$

$$4\pi Ga^2\left(\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right)\right) = (k^2 - 3K)(H_L + \frac{H_T}{3}) - \mathcal{H}[-kB + (H'_T + \frac{3K}{k^2}(kB - H'_T))], \quad (\text{B.19})$$

$$4\pi Ga^2\left(\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right)\right) = (k^2 - 3K)(H_L + \frac{H_T}{3}) + \mathcal{H}(1 - \frac{3K}{k^2})(kB - H'_T), \quad (\text{B.20})$$

$$4\pi Ga^2\left(\delta\rho + 3\mathcal{H}(\bar{\rho} + \bar{P})\left(\frac{v - B}{k}\right)\right) = (k^2 - 3K)\left(H_L + \frac{H_T}{3} + \frac{\mathcal{H}}{k^2}(kB - H'_T)\right). \quad (\text{B.21})$$

Finally, the xPand output for the spatial part ij of the Einstein equation is shown in Figure B.8

Which is a mess, but we can always take the trace to eliminate all the trace-free components. Before we do that, the tensor part has only a few terms and can be obtained easily:

$$\frac{d^2}{d\tau^2}H_T^{(\pm 2)} + 2\mathcal{H}\frac{d}{d\tau}H_T^{(\pm 2)} + (k^2 + 2K)H_T^{(\pm 2)} = 0 \quad (\text{B.22})$$

$$\begin{aligned}
& \left(\overset{(1)}{H}_T^{\mu\nu} \right)' + k \left(\overset{(1)}{B} \right)' \overset{(1)}{h}_{\mu\nu} + \left(\overset{(1)}{H}_T^{\mu\nu} \right) (k^2 + 2k) + \\
& \frac{1}{6} \left(12 \left(\overset{(1)}{H}_T^{\mu\nu} \right)' \mathcal{H} - 2 \left(\overset{(1)}{H}_T \right)' \overset{(1)}{h}_{\mu\nu} (k^2 - 2k) - 3 \left(\bar{\nabla}^\mu \overset{(1)}{B}_\nu \right)' + 3 \left(\bar{\nabla}^\mu \overset{(1)}{H}_T \right)' - 3 \left(\bar{\nabla}_\nu \overset{(1)}{B}^\mu \right)' + 3 \left(\bar{\nabla}_\nu \overset{(1)}{H}_T^\mu \right)' + \frac{1}{k^2} 2 \left(k \left(\overset{(1)}{H}_T \right)' \overset{(1)}{h}_{\mu\nu} + 6 k^2 \left(\overset{(1)}{B} \right)' \overset{(1)}{h}_{\mu\nu} \mathcal{H} + 2 k \left(\overset{(1)}{H}_T \right)' \overset{(1)}{h}_{\mu\nu} \mathcal{H} - \right. \\
& \quad \left. 3 k \left(8 G \pi a^2 \overset{(1)}{h}_{\mu\nu} \left(\overset{(1)}{P} \right) + \overset{(1)}{h}_{\mu\nu} \left((k^2 - 2 \mathcal{H}^2 - 4 \mathcal{H}') \left(\overset{(1)}{A} \right) + (k^2 - 2k) \left(\overset{(1)}{H}_L \right) - 2 \mathcal{H} \left(\overset{(1)}{A}' - 2 \left(\overset{(1)}{H}_L \right)' \right) + 2 \left(\overset{(1)}{H}_L \right)' \right) + \mathcal{H} \left(\bar{\nabla}^\mu \overset{(1)}{B}_\nu - \bar{\nabla}_\nu \overset{(1)}{H}_T^\mu + \bar{\nabla}_\nu \overset{(1)}{B}^\mu - \bar{\nabla}_\nu \overset{(1)}{H}_T^\mu \right) \right) + \\
& \quad \left. 6 \mathcal{H} \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{B} \right) + 3 \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{B} \right)' \right) + 6 \mathcal{H} \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{H}_T \right) + 3 \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{H}_T \right)' - 2 \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{H}_T + 3 \left(\bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{A} + \bar{\nabla}_\nu \bar{\nabla}^\mu \overset{(1)}{H}_L \right) \right) \Big)
\end{aligned}$$

Figure B.8: xPand output for the Einstein equation ij .

Which, considering $\mathcal{H}$ slow-varying, is the equation for a damped harmonic oscillator: the tensor modes generate gravitational waves! It's also important to notice that these modes are gauge-invariant. Also, it's easy to generalize this to include anisotropic stress, since the only tensor modes are $\bar{P}\Pi^{(\pm 2)}$, so just add $8\pi G a^2 \bar{P}\Pi^{(\pm 2)}$ to the RHS.

Now, taking the trace (in Mathematica, just contract with the converse metric), we obtain

$$\begin{aligned}
& \frac{1}{2} k \left(\overset{(1)}{B} \right)' - \frac{1}{6} k^2 \left(\overset{(1)}{H}_T \right)' + \frac{1}{6} \left(\overset{(1)}{H}_T \right)' + k \left(\overset{(1)}{B} \right)' \mathcal{H} + \frac{1}{3} \left(\overset{(1)}{H}_T \right)' \mathcal{H} - 4 G \pi a^2 \left(\overset{(1)}{P} \right)' + \frac{1}{3} \left(\overset{(1)}{H}_T \right)' k - \frac{1}{2} k^2 \left(\overset{(1)}{A} \right)' + \mathcal{H}^2 \left(\overset{(1)}{A} \right)' + 2 \mathcal{H}' \left(\overset{(1)}{A} \right)' + \mathcal{H} \left(\overset{(1)}{A} \right)' - \\
& \frac{1}{2} k^2 \left(\overset{(1)}{H}_L \right)' + k \left(\overset{(1)}{H}_L \right)' - 2 \mathcal{H} \left(\overset{(1)}{H}_L \right)' - \overset{(1)}{H}_L + \frac{\mathcal{H} \left(\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{B} \right)}{3k} + \frac{\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{B}}{6k} - \frac{1}{18} \left(\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{H}_T \right)' + \frac{\mathcal{H} \left(\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{H}_T \right)}{3k^2} + \frac{\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{H}_T}{6k^2} - \frac{1}{6} \left(\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{A} \right)' - \frac{1}{6} \left(\bar{\nabla}_\mu \bar{\nabla}^\mu \overset{(1)}{H}_L \right)'
\end{aligned}$$

Figure B.9: xPand output for the trace of the Einstein equation ij .

Notice that the laplacian terms didn't vanish, because, as noted before, xPand defines the scalar mode of tensors as being just the laplacian, not the trace-free definition. However, all of the other modes did vanish. This is actually useful, since the laplacian terms are the trace-free scalar modes and the other are the trace terms, so it's easy to recognize and separate them. The traceless part is

$$k^2 \left(A + H_L + \frac{H_T}{3} \right) + \left(\frac{d}{d\tau} - 2\mathcal{H} \right) (kB - H'_T) = 0 \quad (\text{B.23})$$

It's easy to generalize this to include anisotropic stress, since the scalar trace-free part of the energy-tensor is only $\bar{P}\Pi$. Therefore, one should simply add $8\pi G a^2 \bar{P}\Pi$ to the RHS.

Our last equation is the spatial trace part, which can be written as

$$\left(-\frac{k^2}{2} + \mathcal{H}^2 + \mathcal{H}' + \mathcal{H} \frac{d}{d\tau} \right) A + \left(-\frac{k^2}{2} + K \right) \left(H_L + \frac{H_T}{3} \right) + \left(\frac{1}{2} \frac{d}{d\tau} + \mathcal{H} \right) \left(-kB + \frac{H'_T}{3} - 2H'_L \right) = \quad (\text{B.24})$$

There is actually some work to do here, since I need to insert the 00 equation to get to Wayne's equation. Now, instead of doing everything by hand, I am going to do the whole process in Mathematica, shown in Figure B.10.

```

eq00 = k (1)B  $\mathcal{H}$  + (1)HT  $\left(-\frac{\kappa^-}{3} + k\right)$  + 4 G  $\pi$  a2 (1) $\rho$  - (k2 - 3 k) (1)HL + 3  $\mathcal{H}$   $\left(\mathcal{H} \left(\frac{(1)}{A}\right) - \frac{(1)'}{H_L}\right)$ ;

eqspacetrace = - $\frac{1}{2}$  k (1)B -  $\frac{1}{6}$  k2 (1)HT +  $\frac{1}{6}$  (1)HT'' - k (1)B  $\mathcal{H}$  +  $\frac{1}{3}$  (1)HT'  $\mathcal{H}$  - 4 G  $\pi$  a2 (1)P +  $\frac{1}{3}$  (1)HT k -  $\frac{1}{2}$  k2 (1)A +  $\mathcal{H}^2$  (1)A + 2  $\mathcal{H}$  (1)A +
 $\mathcal{H}$  (1)A' -  $\frac{1}{2}$  k2 (1)HL + k (1)HL - 2  $\mathcal{H}$  (1)HL' - (1)HL'';

eqspacetrace = eq00 / 3 // FullSimplify
[simplifica completamente]

Also, I need to remove the traceless equation:

eqtraceless = - $\frac{\mathcal{H} \left(\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)}{B}\right)}{3 k}$  -  $\frac{\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)'}{B}}{6 k}$  -  $\frac{1}{18} \left(\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)}{H_T}\right)$  +  $\frac{\mathcal{H} \left(\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)'}{H_T}\right)}{3 k^2}$  +  $\frac{\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)''}{H_T}}{6 k^2}$  -  $\frac{1}{6} \left(\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)}{A}\right)$  -  $\frac{1}{6} \left(\bar{\partial}_\mu \bar{\partial}^\mu \frac{(1)}{H_L}\right)$  /. cd[-μ]@cd[μ][[x_]] → x

- $\frac{\frac{(1)'}{B}}{6 k}$  -  $\frac{1}{18} \left(\frac{(1)}{H_T}\right)$  +  $\frac{\frac{(1)''}{H_T}}{6 k^2}$  -  $\frac{\left(\frac{(1)}{B}\right) \mathcal{H}}{3 k}$  +  $\frac{\left(\frac{(1)'}{H_T}\right) \mathcal{H}}{3 k^2}$  -  $\frac{1}{6} \left(\frac{(1)}{A}\right)$  -  $\frac{1}{6} \left(\frac{(1)}{H_L}\right)$ 

eqspacetrace = eq00 / 3 - eqtraceless * k^2 // FullSimplify
[simplifica completamente]

 $\frac{1}{3} \left(-k \left(\frac{(1)'}{B}\right) - 3 k \left(\frac{(1)}{B}\right) \mathcal{H} - 4 G \pi a^2 \left(3 \left(\frac{(1)}{P}\right) + \frac{(1)}{\rho}\right) - \left(k^2 - 6 \mathcal{H}'\right) \left(\frac{(1)}{A}\right) + 3 \mathcal{H} \left(\frac{(1)'}{A} - \frac{(1)'}{H_L}\right) - 3 \left(\frac{(1)''}{H_L}\right)\right)$ 

```

Figura B.10: Treating the xPand output with Mathematica rules.

Which translates to

$$\left(2\frac{a''}{a} - 2\left(\frac{a'}{a}\right)^2 + \frac{d}{d\tau} - \frac{k^2}{3}\right) A - \left(\frac{d}{d\tau} + \mathcal{H}\right) \left(\frac{kB}{3} + H'_L\right) = 4\pi G a^2 \left(\delta P + \frac{\delta\rho}{3}\right). \quad (\text{B.25})$$

We then have the fundamental equations for cosmological perturbations in Λ CDM. The full Mathematica code can be accessed in [this link](#).

Appendix C

Appendices to Chapter 6

C.1 Constraints for Dataset Combinations 3, 4 and 5

In this appendix, we show results for DC3, DC4 and DC5, which corroborate our conclusions from the main text. In all dataset combinations, adding DES data does limit the amount of EDE during recombination and worsens the CMB fit. Furthermore, including the late-time modification does not restore the EDE detection to the significance it had without DES data. Figure C.1 shows the 1D marginalized constraints for the parameters H_0 , Ω_m , S_8 and f_{EDE} , including DES data. Figure C.2 shows the χ^2_{CMB} distribution in the DC3, DC4 and DC5 chains, including DES-Y3 cosmic shear data, and using the EDE and EDE+ $w(z)$ models.

C.2 Principal Component Analysis of Late Dark Energy

As a byproduct of our analysis, we present in this appendix constraints on the smooth, late-time dark energy behavior using our baseline dataset DC1, including DES-Y3 cosmic shear data. Figure C.3 shows constraints for $w(z_i)$, the dark energy equation of state at each redshift bin $[z_i, z_{i+1}]$ for the 5 and 10-bin cases. As expected, above $z = 1$ our constraining power decreases to the point that our constraints have no statistical significance. All constraints are well in agreement with a cosmological constant at late-times.

Since the values of $w(z_i)$ are correlated, we perform a Principal Component Analysis to find uncorrelated parameters. The procedure is as follows: from the MCMC sample, we compute the sample covariance matrix for the equations of state in each bin, $w(z_i)$. This matrix is real and symmetric, and can therefore be diagonalized. The principal components are the eigenvectors e_j of the sample covariance matrix. In the principal component basis, the covariance matrix is diagonal and thus the components are uncorrelated with each other. Thus, the dark energy equation of state can be expanded in the Principal Component basis as:

$$w(z) = -1 + \sum_{i=1}^{N_{\text{bins}}} \alpha_i e_i(z), \quad (\text{C.1})$$

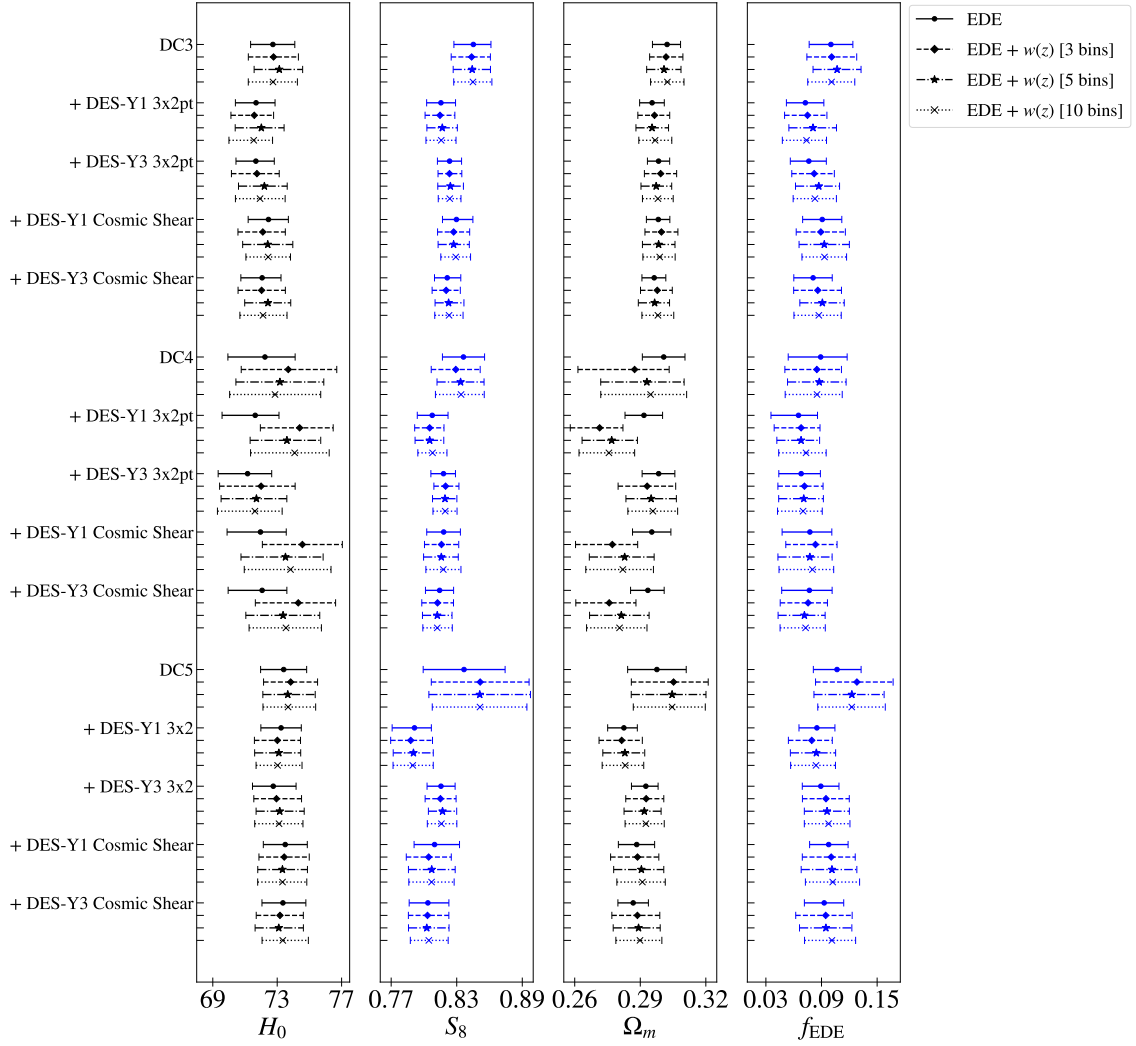


Figure C.1: Marginalized constraints for H_0 , S_8 , Ω_m and f_{EDE} , using the dataset combinations DC3 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae, Planck 2018 CMB Lensing spectrum and H0liCOW strong lensing time delays), DC4 (same as DC3 without BAO and strong lensing) and DC5 (same as DC3, without BAO and CMB Lensing). For each combination, we add DES 3x2-point correlation functions and cosmic shear-only data. DES-Y1 and DES-Y3 are shown in order to assess the impacts of the updated data set and analysis in our results. We use the effective fluid EDE model presented in section 6.2.1 combined with a late-time fluid with piecewise equation of state, described in section 6.2.2, using 3, 5 and 10 redshift bins. We observe no significant shifts in the f_{EDE} constraints due to the modification of smooth dark energy at late times, regardless of the number of redshift bins in our model.

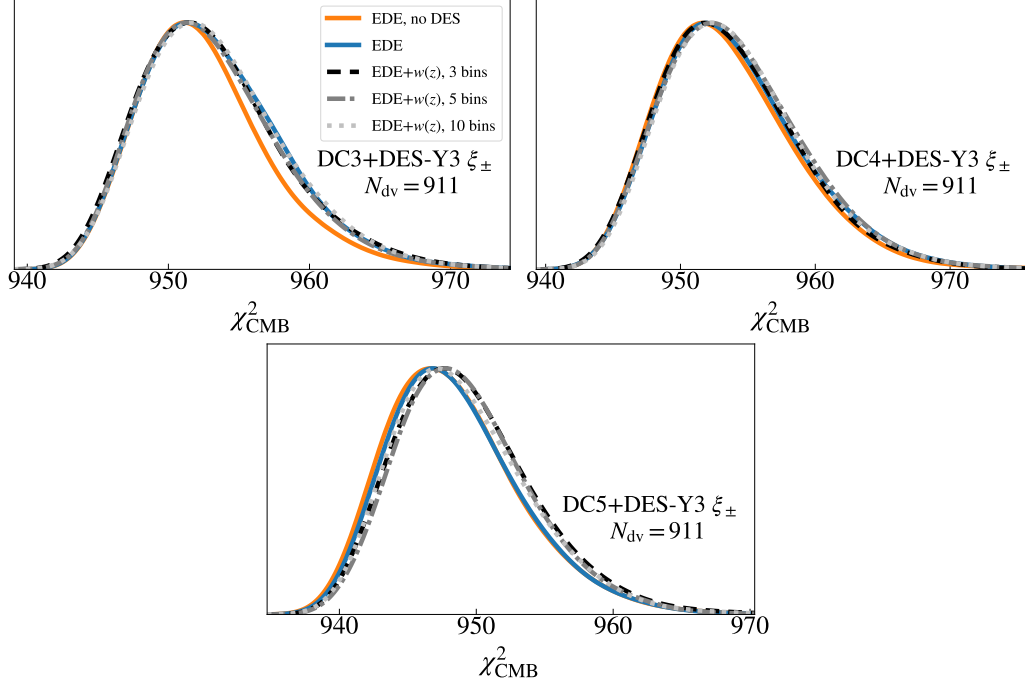


Figure C.2: χ^2_{CMB} (911 points) distributions in the MCMCs using the dataset combinations DC3 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae, Planck 2018 CMB Lensing spectrum and H0liCOW strong lensing time delays), DC4 (same as DC3 without BAO and strong lensing) and DC5 (same as DC3, without BAO and CMB Lensing), combined with DES-Y3 cosmic shear data, under the effective fluid EDE model and EDE + $w(z)$ with 3, 5 and 10 bins. We also include EDE results without DES data.

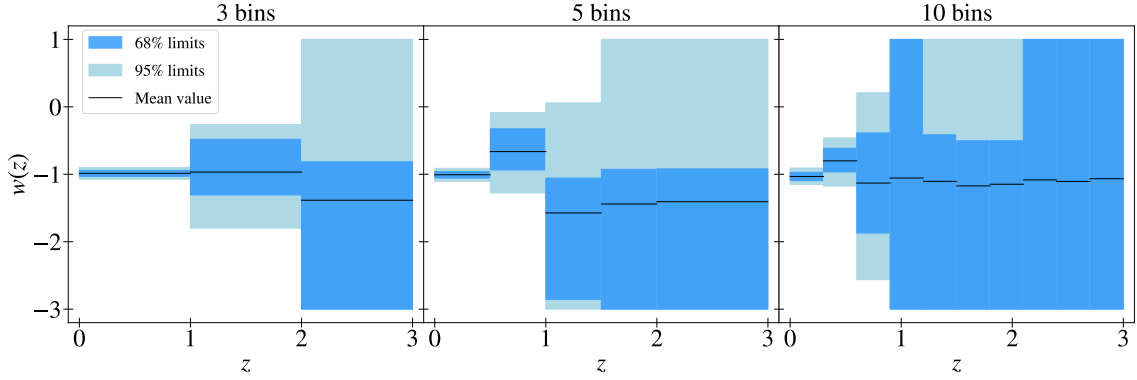


Figura C.3: Mean (black line), 68% and 95% limits (darker and lighter blue contours respectively) of the constraints for w_i , the dark energy equation of state within redshifts $z \in [z_i, z_{i+1}]$. Vertical widths represent the confidence limits and the horizontal widths represent the chosen redshift binning. The constraints are for the dataset combination DC1 (ACT TT, TE, EE spectra with $\ell_{\max} = 650$, Planck 2018 TT spectrum with $\ell_{\max} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) combined with DES-Y3 cosmic shear. We remind our MCMC priors $w_i \in [-3, 1]$ for $i > 0$. For redshifts $z > 1$, we have no constraining power. **Left panel:** constraints using the 3-bin model, with bin limits $z = [1, 2, 3]$. **Middle panel:** same constraints for the 5 bin analysis, where the bin limits are $[0.5, 1.0, 1.5, 2.0, 3.0]$. **Right panel:** same constraints for the binning $z_i = 0.3 \times i, i = 1, \dots, 10$.

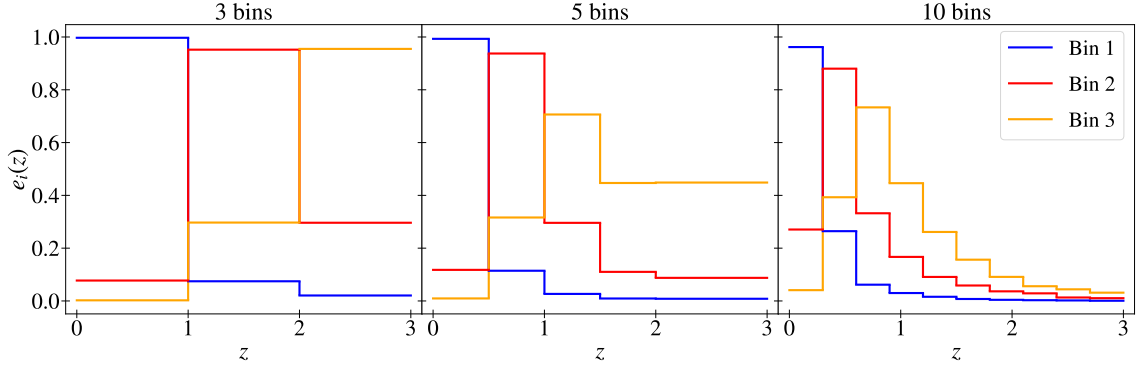


Figura C.4: First (ordered by least variance) three $w(z)$ principal components, $e_i(z)$, $i = 1, 2, 3$. The PCs are constructed using the MCMC sample from DC1 (ACT TT, TE, EE spectra with $\ell_{\max} = 650$, Planck 2018 TT spectrum with $\ell_{\max} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) combined with DES-Y3 cosmic shear. The components of each PC are focused on each redshift bin, which we use to label the PCs. **Left panel:** PCs for the 3 bin analysis, where the bin limits are $[1, 2, 3]$. **Middle panel:** First three PCs for the 5 bin analysis, where the bin limits are $[0.5, 1.0, 1.5, 2.0, 3.0]$. **Right panel:** First three PCs for the 10-bin analysis, where the bin limits are $z_i = 0.3 \times i, i = 1, \dots, 10$.

where N_{bins} is the number of redshift bins and α_i is the component of $w(z)$ in the Principal Component e_i direction. Figure C.4 shows the first three principal component basis functions. Each principal component is localized in a redshift bin but receive contributions from all other bins. The components α_i can then be interpreted as deviations from $w = -1$.

Figure C.5 shows marginalized constraints for the components α_i of the three first principal components. All constraints are compatible with the fiducial Λ CDM model.

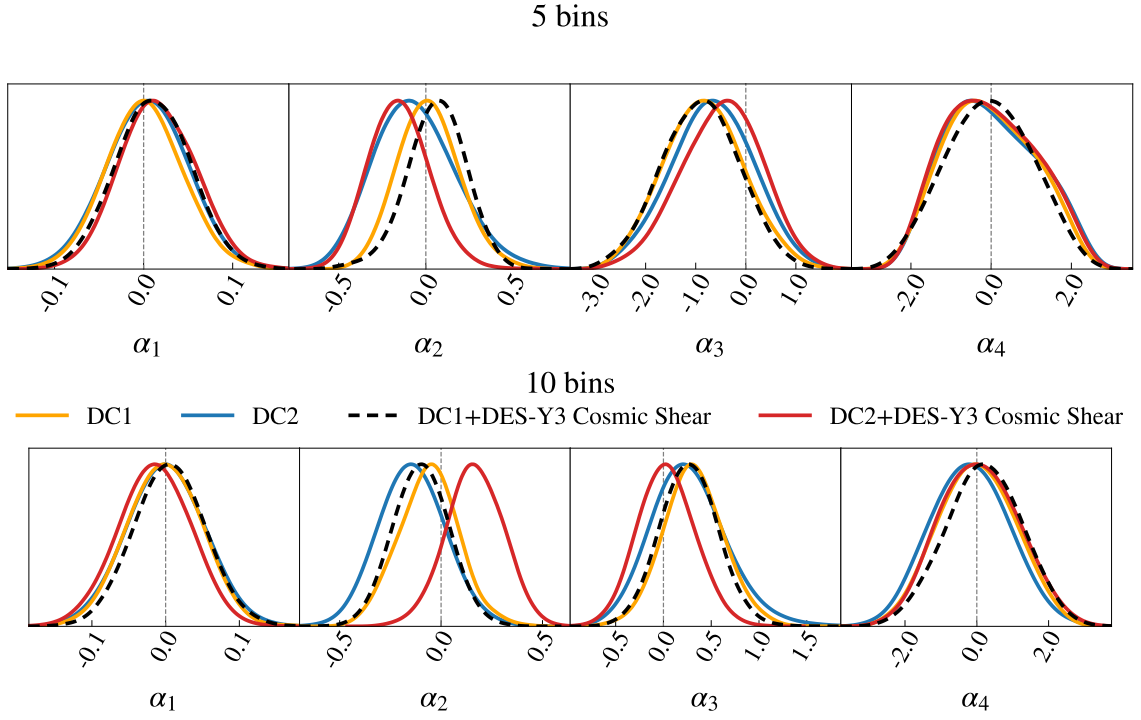


Figure C.5: Marginalized posterior distributions of the first four principal component weights, α_i , under the datasets DC1 (ACT TT, TE, EE spectra with $\ell_{\text{max}} = 650$, Planck 2018 TT spectrum with $\ell_{\text{max}} = 650$ + Planck 2018 low- ℓ EE spectrum, BAO from 6dFGS, SDSS DR7 main galaxy sample and SDSS BOSS DR12 consensus sample, Pantheon supernovae and Planck 2018 CMB Lensing spectrum) and DC2 (same as DC1, without CMB Lensing). We also show results including DES-Y3 cosmic shear data combined with DC1 and DC2. **Top Panel:** Constraints for the weights of the first four principal components for the 5 bin analysis. **Bottom Panel:** Same constraints as in top panel but for the 10 bin analysis.

Appendix D

Appendices to Chapter 7

D.1 Appendix: Full Reconstruction of the Equation of State

In Figure 7.6, we have presented the filtered constraints on w_i , the model-agnostic dark energy parameters in Equation 7.3. In this appendix, for completeness, we show the unfiltered reconstruction, i.e., the full reconstruction for $w(z)$ in both cases of 5 and 10 bins inferred directly from the w_i samples. The result is shown in Figure D.1.

We also classify the binned $w(z)$ MCMC samples into different categories according to the bins in which the first phantom crossing occurred and in Tables D.1 and D.2 we show the percentages of MCMC samples in each class.

	P18 + DESI +			
	Pan	Pan+	Uni3	DESY5
$1 \rightarrow 2$	70.1%	30.8%	17.0%	55.5%
$2 \rightarrow 3$	28.5%	69.1%	82.6%	41.9%
$3 \rightarrow 4$	0.82%	0.06%	0.5%	2.4%
$4 \rightarrow 5$	0.04%	0.03%	0.03%	0.2%
No crossing	0.02%	0	0	0

Tabela D.1: Percentages of 5-bin $w(z)$ MCMC samples that present the first phantom crossing between the bins. After burn-in, each MCMC contains around 300000 samples.

D.2 Appendix: Continuous Binned $w(z)$

The binned $w(z)$ model presented in Section 7.2.2 has discontinuities in the equation of state. To ensure that such discontinuities do not invalidate the model, we implement a continuous version, in which the equation of state is parametrized

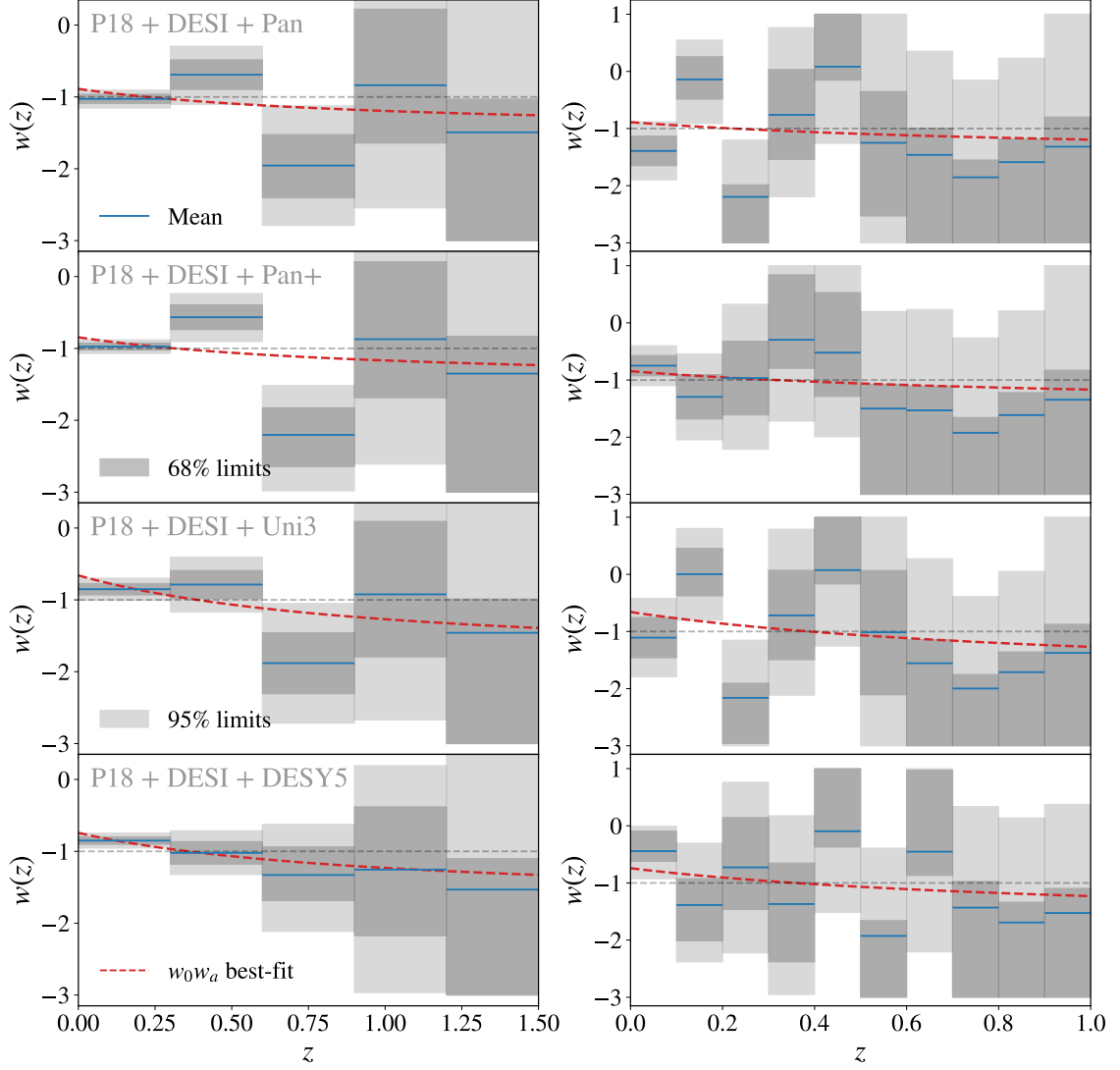


Figure D.1: Reconstruction of the dark energy equation of state using the binned $w(z)$, Equation 7.3, for the different SN datasets. The blue line indicates the mean value, and the darker and lighter gray bands indicate 68% and 95% limits. We also include the best-fit $w_0 w_a$ model as a red dashed line for comparison purposes. The left panels show the reconstruction for $N_{\text{bins}} = 5$, while the right panels show the filtered constraints for $N_{\text{bins}} = 10$. Each row corresponds to a dataset combination including a different SN catalog.

	P18 + DESI +			
	Pan	Pan+	Uni3	DESY5
$1 \rightarrow 2$	94.1%	83.4%	63.3%	79.5%
$2 \rightarrow 3$	5.7%	15.7%	35.1%	17.3%
$3 \rightarrow 4$	0.2%	0.6%	1.5%	3.0%
$4 \rightarrow 5$	0	0.2%	0.02%	0.1%
$5 \rightarrow 6$	0	0.1%	0.04%	0.1%
$6 \rightarrow 7$	0	0	0.02%	0
$7 \rightarrow 8$	0	0	0	0
$8 \rightarrow 9$	0	0	0	0
$9 \rightarrow 10$	0	0	0	0
No crossing	0	0	0	0

Tabela D.2: Percentages of 10-bin $w(z)$ MCMC samples that present the first phantom crossing between the bins. After burn-in, each MCMC contains around 500000 samples.

as

$$w(z) = \sum_{i=1}^N \left\{ w_{i-1} + \frac{w_i - w_{i-1}}{2} \left[1 + \tanh \left(\frac{z - z_i}{\sigma} \right) \right] \right\}. \quad (\text{D.1})$$

This parametrization preserves the same parameters z_i and w_i of the discontinuous case, while adding one extra parameter σ controlling the width of this transition. The smaller the widths are the closer this model is to the original binned $w(z)$ model. We have post-processed the binned $w(z)$ MCMC samples with this new model, assessing the difference in χ^2 between both cases. We have chosen to fix the σ parameter to three values of $\sigma = 0.01$, $\sigma = 0.03$ and $\sigma = 0.05$.

Figure D.2 shows the constraints on Ω_m , σ_8 , w_0 , w_1 and w_2 for the discontinuous case and the three continuous cases. We observe almost perfect agreement between all cases.

A histogram of χ^2 differences is shown in Figure D.3 for the three σ values. For $\sigma = 0.01$ and $\sigma = 0.03$, the percentage of points with $|\Delta\chi^2| < 1$ is 96%, falling to 94% for $\sigma = 0.05$. The percentages of points within a threshold of $|\Delta\chi^2| < 0.5$ are 81%, 79% and 71% for the respective σ values.

D.3 Appendix: Transition Model: Varying σ

In this Appendix, we show parameter constraints for the transition model described in Section 7.2.1, but now varying the σ parameter with a prior $\mathcal{U}[0.01, 0.5]$. The results are shown in Figure D.4.

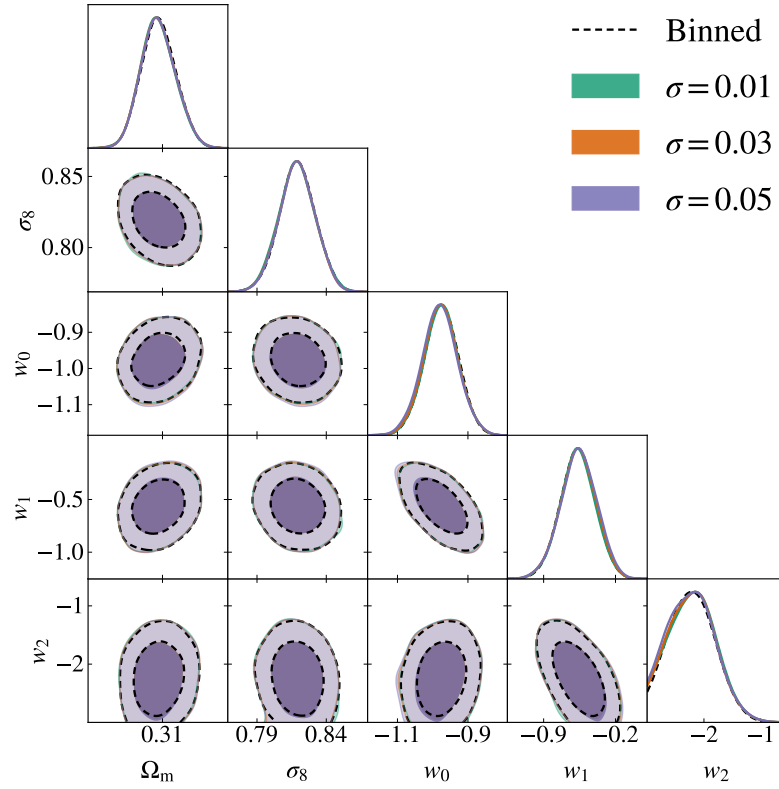


Figure D.2: 2D parameter constraints for the binned $w(z)$ model and the continuous version with three values of $\sigma = 0.01, 0.03$ and 0.05 . We observe no significant differences between the constraints.

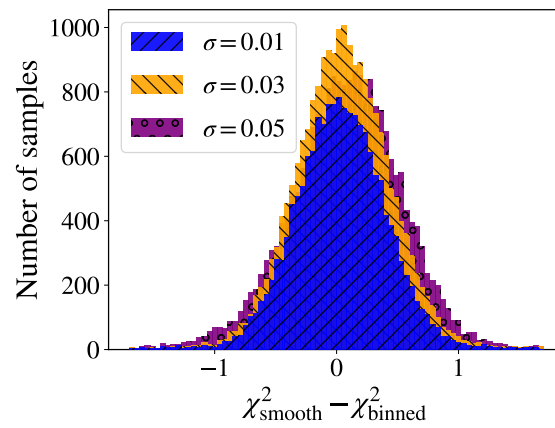


Figure D.3: Histogram of χ^2 differences between the binned $w(z)$ model described in Section 7.2.2 and the continuous version in Equation D.1

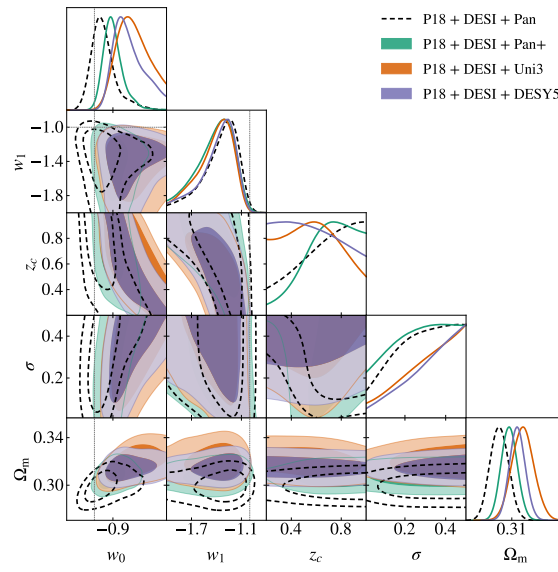


Figura D.4: Parameter constraints for the transition model described in Section 7.2.1. Here, we vary the σ parameter with a prior $\mathcal{U}[0.01, 0.5]$.

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