Probing the early Universe with B-mode polarization

The Spider instrument, optical modelling and non-Gaussianity

Adriaan Judocus Duivenvoorden
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Abstract
One of the main goals of modern observational cosmology is to constrain or detect a stochastic background of primordial gravitational waves. The existence of such a background is a generic prediction of the inflationary paradigm: the leading explanation for the universe's initial perturbations. A detection of the gravitational wave signal would provide strong evidence for the paradigm and would amount to an indirect probe of an energy scale far beyond that of conventional physics. Several dedicated experiments search for the signal by performing highly accurate measurements of a unique probe of the primordial gravitational wave background: the \textit{B}-mode signature in the polarization of the cosmic microwave background (CMB) radiation. A part of this thesis is devoted to one of these experiments: the balloon-borne Spider instrument. The analysis of the first dataset, obtained in two (95 and 150 GHz) frequency bands during a January 2015 Antarctic flight, is described, along with details on the characterisation of systematic signal and the calibration of the instrument. The case of systematic signal due to poorly understood optical properties is treated in more detail. In the context of upcoming experiments, a study of systematic optical effects is presented as well as a numerically efficient method to consistently propagate such effects through an analysis pipeline. This is achieved by a 'beam convolution' algorithm capable of simulating the contribution from the entire sky, weighted by the optical response, to the instrument's time-ordered data. It is described how the algorithm can be employed to forecast the performance of upcoming CMB experiments. In the final part of the thesis, an additional use of upcoming B-mode data is described. Constraints on the non-Gaussian correlation between the large-angular-scale B-mode field and the CMB temperature or E-mode anisotropies on small angular scales constitute a rigorous consistency check of the inflationary paradigm. An efficient statistical estimation procedure, a generalised bispectrum estimator, is derived and the constraining power of upcoming CMB data is explored.

Keywords: cosmic microwave background, early universe, polarimetry, telescopes.

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One of the main goals of modern observational cosmology is to constrain or detect a stochastic background of primordial gravitational waves. The existence of such a background is a generic prediction of the inflationary paradigm: the leading explanation for the Universe’s initial perturbations. A detection of the gravitational wave signal would provide strong evidence for the paradigm and would amount to an indirect probe of an energy scale far beyond that of conventional physics. Several dedicated experiments search for the signal by performing highly accurate measurements of a unique probe of the primordial gravitational wave background: the $B$-mode signature in the polarization of the cosmic microwave background (CMB) radiation. A part of this thesis is devoted to one of these experiments: the balloon-borne SPIDeR instrument. The analysis of the first dataset, obtained in two (95 and 150 GHz) frequency bands during a January 2015 Antarctic flight, is described, along with details on the characterisation of systematic signal and the calibration of the instrument. The case of systematic signal due to poorly understood optical properties is treated in more detail. In the context of upcoming experiments, a study of systematic optical effects is presented as well as a numerically efficient method to consistently propagate such effects through an analysis pipeline. This is achieved by a ‘beam convolution’ algorithm capable of simulating the contribution from the entire sky, weighted by the optical response, to the instrument’s time-ordered data. It is described how the algorithm can be employed to forecast the performance of upcoming CMB experiments. In the final part of the thesis, an additional use of upcoming $B$-mode data is described. Constraints on the non-Gaussian correlation between the large-angular-scale $B$-mode field and the CMB temperature or $E$-mode anisotropies on small angular scales constitute a rigorous consistency check of the inflationary paradigm. An ef-
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Included Papers

- **Paper I**
  Full-sky beam convolution for cosmic microwave background applications
  A. J. Duivenvoorden, J. E. Gudmundsson, A. S. Rahlin
  DOI: doi.org/10.1093/mnras/stz1143

- **Paper II**
  CMB $B$-mode non-Gaussianity I: optimal bispectrum estimator and Fisher forecasts
  A. J. Duivenvoorden, P. D. Meerburg, K. Freese
  To be submitted to JCAP

- **Paper III**
  The Simons Observatory: Science goals and forecasts
  The Simons Observatory Collaboration
  *JCAP*, 2019, Vol. 1902, 56
  DOI: doi.org/10.1088/1475-7516/2019/02/056

- **Paper IV**
  A new limit on CMB circular polarization from SPIDER
  J. M. Nagy et al.
  DOI: doi.org/10.3847/1538-4357/aa7cfd
Additional Papers

- Paper V
  CMB-S4 Science Case, Reference Design, and Project Plan
  CMB-S4 Collaboration
  https://arxiv.org/abs/1907.04473
Author’s Contribution

• Paper I

I have been the main contributor to this project. I developed the code library that is presented and used to derive all results. I assisted J. E. Gudmundsson in writing and testing a suite of computer scripts that call the code library to calculate the residuals for the satellite test case. I have written the majority of the paper; I have assisted in writing sections 4 and 5. I have been responsible for the journal submission and interaction with the referee.

• Paper II

I have been the main contributor to this project. The initial idea of developing an efficient statistical framework for estimation for tensor-like non-Gaussian signals was proposed by P. D. Meerburg. I formulated and developed the statistical framework and wrote the publicly available code library that is used to calculate the Fisher forecasts presented in the paper. I calculated these forecasts, created all figures and wrote essentially all of the text. My collaborators assisted me in structuring the paper, writing and, in general, provided guidance throughout the project.

• Paper III

I used the forecasting code described in paper II to forecast the constraints on several scalar-scalar-tensor bispectrum templates. The results are summarised in Table 6. I wrote the text describing the results in Sec. 6 together with P. D. Meerburg.
AUTHOR'S CONTRIBUTION

• Paper IV
I contributed to the analysis pipeline used to derive the upper-limits presented in this paper. I derived the detector pointing offsets for each detector used in the analysis and calculated consistency checks (null tests) of the data. I contributed to the use of Planck HFI data to correct for the temperature-to-polarization leakage and investigated the impact of frequency band differences between Planck HFI and Spider. I have contributed to the writing of the paper by providing comments to drafts of the manuscript.

• Paper V
Although I am not a member of the CMB-S4 collaboration, I was granted co-authorship on this paper. I provided the CMB-S4 collaboration with forecasts on several scalar-scalar-tensor bispectrum templates using the forecasting code described in paper II. The results can be seen in Table 1-2 in Sec. 1.2.2.4 that describes the forecasts on primordial non-Gaussianity using the CMB bispectrum. I contributed to the writing but the section was primarily written by P. D. Meerburg.

Content from previous work
Chapter 4 is a reworked and summarised version of chapters 2, 3, and 4 of my licentiate thesis: Optical Modelling for the Spider Experiment, 2018 (unpublished).
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<td>ΛCDM</td>
<td>Lambda Cold Dark Matter</td>
</tr>
<tr>
<td>ACT</td>
<td>Atacama Cosmology Telescope</td>
</tr>
<tr>
<td>AIC</td>
<td>Akaike Information Criterion</td>
</tr>
<tr>
<td>CMB</td>
<td>Cosmic Microwave Background</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width at Half Maximum</td>
</tr>
<tr>
<td>HFI</td>
<td>High Frequency Instrument</td>
</tr>
<tr>
<td>HWP</td>
<td>Half-Wave Plate</td>
</tr>
<tr>
<td>IAU</td>
<td>International Astronomical Union</td>
</tr>
<tr>
<td>ISW</td>
<td>Integrated Sachs-Wolfe</td>
</tr>
<tr>
<td>KSW</td>
<td>Komatsu Spergel Wandelt</td>
</tr>
<tr>
<td>MCMC</td>
<td>Markov Chain Monte Carlo</td>
</tr>
<tr>
<td>MoM</td>
<td>Method of Moments</td>
</tr>
<tr>
<td>PO</td>
<td>Physical Optics</td>
</tr>
<tr>
<td>PSD</td>
<td>Power Spectral Density</td>
</tr>
<tr>
<td>SFSR</td>
<td>Single-Field Slow-Roll</td>
</tr>
<tr>
<td>SO</td>
<td>Simons Observatory</td>
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</table>
SPT  South Pole Telescope
SSS  Scalar Scalar Scalar
SSSS Scalar Scalar Scalar Scalar
SST  Scalar Scalar Tensor
SWSH Spin-Weighted Spherical Harmonic
TES  Transition-Edge Sensor
TOD  Time-Ordered Data
After its discovery in 1964 by Penzias and Wilson [1], the cosmic microwave background (CMB), a snapshot of the 380,000 year old Universe, has been the subject of extensive study, both from an observational and a theoretical standpoint. Following the initial discovery, there have been observations by a large number of ground-based, balloon-borne and rocket-based experiments as well as four satellite observatories.\textsuperscript{1} Data from the FIRAS instrument aboard the COBE satellite [4] convincingly measured the black-body electromagnetic spectrum of the CMB. The FIRAS data determined the CMB temperature to be [5]:

\[ T_{\text{CMB},0} = 2.72548 \pm 0.00057 \text{ K} \quad (1\sigma). \]  (1.1)

Interestingly, the FIRAS measurements, taken in 1992, still represent the most sensitive measurements of the CMB frequency spectrum. The signal observed by COBE is highly isotropic. After correcting for a dipole-like variation due to the motion of our Galaxy and Solar System, the CMB temperature is the same in all directions apart from tiny, $\Delta T/T = 10^{-5}$, deviations from isotropy.

Subsequent experiments, including the WMAP [7] and Planck [8] satellites, have concentrated on these tiny spatial variations, anisotropies, in the CMB temperature. These experiments have yielded high-resolution images of the anisotropies (see Fig. 1.1). The temperature anisotropies closely

\textsuperscript{1}See Ref. [2] for a recollection of early CMB observations and an overview of a great number of CMB experiments. Ref. [3] provides a brief overview of more modern CMB observatories, including the satellite-borne experiments.
trace the distribution of matter in the photon-baryon fluid of the early Universe. By measuring the CMB anisotropies, one indirectly probes the seeds of the structure formation that has shaped the Universe of today. The six-parameter Lambda cold dark matter ($\Lambda$CDM) model, the standard model of cosmology, dictates the preferred spatial separation and other statistical properties of the CMB anisotropies. The model predictions may be compared to the 2-point correlation function (or equivalently, the angular power spectrum) of maps such as the one depicted in Fig. 1.1. The angular power spectrum of the measured CMB anisotropies has solidified the $\Lambda$CDM model as the standard model of cosmology and has helped to establish that the current energy content of the Universe only consists of approximately 5% known, ordinary matter and radiation. The remaining 26% and 69% are taken up by an unknown dark matter component and the vacuum energy of the cosmological constant $\Lambda$, respectively [9].

The last two decades have seen a surge in measurements of the polarization of the CMB radiation. Since the first detection in 2002 [10], CMB polarization has become the main focus of experimental investigation into
the CMB. The ΛCDM model predicts that the polarization signal is sourced by the velocity gradient of the photon-baryon fluid. The polarization is now reasonably well characterised and already provides an independent check of the ΛCDM model [9]. However, more sensitive observations are still possible [11]. Fig. 1.2 provides a visualisation of the (large-angular-scale) CMB polarization measured by the Planck experiment. The polarization signal predicted by ΛCDM can be fully described as a gradient field on the sphere; the signal is referred to as $E$-mode polarization. See Fig. 1.3 for an illustration of two $E$-mode patterns with opposite sign.

CMB polarization of the curl type, the $B$-mode signal in Fig. 1.3, is only predicted to be present at a small amplitude in a ΛCDM universe. The allowed $B$-mode signal comes from an $E$-mode signal that is converted by gravitational lensing due to galaxy clusters and other structure along the line of sight. However, in a natural extension of the ΛCDM model another $B$-mode signal exists. This signal is independent from the initial scalar perturbations that cause the density and velocity gradient fluctuations in the
photon-baryon fluid. A stochastic background of gravitational waves produces this particular $B$-mode signal [12]. During the brief period in which the CMB became polarized, the gravitational waves were imprinted onto the spatial patterns of the polarization. The gravitational-wave-induced polarization patterns are not only of the $B$-mode but also of the $E$-mode type. The resulting patterns are typically correlated over $1^\circ$ angular separations.

![E-mode polarization patterns.](image1)

![B-mode polarization patterns.](image2)

Figure 1.3: Schematic depiction of $E$- and $B$-mode polarization patterns. The $E$-$B$ decomposition of the polarization field is a scalar-pseudoscalar decomposition: both types are unchanged by coordinate rotations, but a coordinate inversion will interchange the two $B$-mode patterns.

The stochastic background of gravitational waves would have originated during a period of cosmic inflation [13–15]. The $\Lambda$CDM paradigm is strongly connected to such a period. Cosmic inflation, or simply ‘inflation’, essentially serves to explain the initial conditions of the model. Inflation refers to a period directly after the Big Bang during which space is rapidly expanding. An initial phase of inflation explains the Euclidean, homogeneous and isotropic nature of our Universe. Inflation would also account for the observed statistical properties of the initial perturbations. The stochastic scalar perturbations that seed the CMB anisotropies and the late-time structure of the Universe are due to quantum fluctuations that through the rapid expansion of space during inflation turn into classical perturbations. If the energy scale associated with inflation is large ($\sim 10^{16}$ GeV), quantum gravitational fluctuations are amplified by the expansion and turn into the classical gravitational waves that source the $B$-mode polarization. The indirect observation of the gravitational wave background by the detection of a $B$-mode signal would provide a remarkable probe into the high-energy physics of inflation and would imply that inflation occurs at an enormous energy scale. Chapter 2 elaborates on the polarization of the CMB and the $B$-mode signal in particular.

The possibility of detecting the gravitational wave background through
its $B$-mode signature in the CMB has lead to the deployment of a number of dedicated polarimetric experiments. These instruments are typically small telescopes that are optimised to measure CMB polarization on degree-angular scales. In Chapter 3, one of these experiments: the balloon-borne SPIDER experiment, is introduced. The performance of $B$-mode experiments is conveniently summarised in terms of their sensitivity to the tensor-to-scalar ratio $r$. The $r$ parameter directly scales the predicted gravitational-wave-induced $B$-mode power in the CMB. The current upper limit on $r$ is obtained by combining Planck and BICEP2/Keck Array data and is set at $r < 0.064$, at 95% confidence level (CL) [9].

Recent improvements in detector technology have accelerated the search for the gravitational wave signature. As individual detector noise cannot be reduced significantly [3], the instantaneous sensitivity of experiments is increased by allowing a greater numbers of detectors per focal plane. The intrinsic noise of the polarization-sensitive bolometric detectors that are typically used today has become comparable to the photon noise (the uncertainty due to the discreteness of photon arrivals) of the sky. Photon noise from the atmosphere mostly limits ground-based observatories. Satellite and balloon-borne experiments are largely limited by the CMB itself [3]. Ground-based CMB experiments are often classified by number of detectors. Currently, there is a transition from stage-II experiments with $O(10^3)$ detectors to stage-III experiments with $O(10^4)$ detectors. Examples of stage-II experiments are BICEP2 and the Keck Array. As mentioned above, these experiments obtained a sensitivity that allowed for $r$-values below 0.064 (at 95% CL). Stage-III $B$-mode experiments are BICEP3 [16] and the upcoming Simons Observatory (SO) experiment [17]. These experiments aim to improve the sensitivity on $r$ by a factor of approximately ten. A fourth stage with $O(10^5)$ detectors will be presented by the proposed CMB-S4 experiment [18, 19], aiming at $r < 0.001$. Similar sensitivity to $r$ might also come from satellite observatories such as the proposed LiteBIRD [20] or PICO [21] experiments.

It should be noted that the above mentioned uncertainties affecting the $r$ parameter are already subdominant to the systematic uncertainty caused by modelling the polarized Galactic foregrounds [22]. Besides these Galactic foregrounds, the spurious $B$-mode signal created by imperfections in the optics of $B$-mode instruments constitutes a second source of systematic error that has the potential to dominate over the statistical uncertainty on $r$. A method to simulate this type of systematic bias is presented in Chapter 4.
CHAPTER 1. INTRODUCTION

The method is implemented in the form of a publicly available code library (beamconv) that is described in Paper I. In Chapter 5, the beamconv code is used to construct the systematic error budget of the SPIDER instrument. Chapter 5 also presents a description of the post-flight calibration and instrument characterisation of the SPIDER instrument. In addition to the application to SPIDER that is described in this thesis, the beamconv code is currently also employed to forecast the systematic bias due to optical imperfections of the B-mode telescopes used by the SO experiment. In a similar way, this code will be applied to the LiteBIRD experiment.

In Chapter 6 it is explained how the expected wealth of future B-mode data may be used to go beyond constraints on the angular power spectrum of B-mode polarization. As explained in Ref. [23], B-mode data will be able to place meaningful constraints on certain 3-point correlation functions between the $B$-mode, temperature and $E$-mode anisotropies of the CMB. Such correlations are essentially unconstrained at the moment. The most simple models of inflation do not allow such non-Gaussian correlations to be present at an observable level [24, 25]. By detecting a violation of this rather robust prediction, one would rule out a large class of inflation models [26]. A dedicated statistical estimation procedure for this type of non-Gaussian correlations is described in Paper II. Forecasts for the SO and CMB-S4 experiments are presented in Paper III and V.

Conventions and notation Throughout this document we will work in units with $c = \hbar = k_B = 1$ unless SI units are explicitly mentioned. We will make use of the Einstein summation convention: repeated (upper and lower) indices are implicitly summed over. Greek indices run from 0 to 3, latin indices $i, j, \ldots, z$ run from 1 to 3 and latin indices $a, b, \ldots, h$ run from 1 to 2.
Chapter 2

The Cosmic Microwave Background

It is safe to say that the CMB and its anisotropies have yielded the most convincing observational evidence for the ΛCDM model. The aspect that sets the CMB apart from many other cosmological probes is the relative simplicity of the relevant physics. The formation of the CMB is well understood and has at this point become a textbook subject. Examples of cosmology textbooks that have a relatively strong focus on the CMB are the books by Dodelson [27], Weinberg [28], Lyth and Liddle [29], Mukhanov [30] and Durrer [31]. In this chapter we will make no attempt at rigour in our description of the CMB but will instead mainly focus on aspects that are relevant for the later chapters. We will explain how the initial perturbations, scalar or tensor, can be probed with CMB data and how the perturbations are connected to the theory of cosmic inflation. As this thesis largely revolves around CMB polarization, we include a general introduction to the concept of polarized radiation and its mathematical description.

2.1 The expanding Universe

Cosmology is fundamentally based on the assumption that the theory of general relativity can be applied to the Universe as a whole. In addition there is the cosmological principle: the assumption that there is no preferred location and directionality to the Universe. Clearly, a universe that
fulfils this principle can only be used to describe the background geometry and content of our Universe; the observed structure has to be described in terms of perturbations that violate the principle. An observer that sees the (unperturbed) Universe as isotropic is called a comoving observer. In coordinates \((t, \mathbf{x})\) where such an observer sits at constant \(\mathbf{x}\), the spacetime interval \(ds^2\) may be represented as follows \([32, 33]\):

\[
\begin{align*}
\frac{ds^2}{g_{\mu\nu} dx^\mu dx^\nu} &= -dt^2 + a^2(t) \tilde{g}_{ij} dx^i dx^j. \\
&= -dt^2 + a^2(t) \tilde{g}_{ij} dx^i dx^j.
\end{align*}
\]

Here \(g_{\mu\nu}\) is the spacetime metric. The coordinates are referred to as comoving coordinates; the ‘time’ coordinate \(t\) is said to slice up (foliate) the four-dimensional spacetime into a series of non-intersecting three-dimensional spacelike hypersurfaces. The spatial metric \(\tilde{g}_{ij}\) describes the geometry of the \(t = \text{constant}\) spatial hypersurfaces. The Robinson-Walker scale factor \(a(t)\) is a yet unspecified dimensionless function of \(t\) that scales the spatial hypersurfaces.

The cosmological principle limits the spatial metric \(\tilde{g}_{ij}\) to be described by a single parameter \(\kappa\). The hypersurfaces can be Euclidean \((\kappa = 0)\) or are allowed to have either constant positive curvature \((\kappa > 0)\) or constant negative curvature \((\kappa = -1)\). Using spherical coordinates, the resulting Friedmann-Lemaître-Robertson-Walker (FLRW) metric is expressed as:

\[
\frac{ds^2}{-dt^2 + a^2(t) \left( \frac{dr^2}{1 - \kappa r^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right)}.
\]

In this form, the parameter \(r\) has dimensions of length. The dimensionless scale factor is normalised such that \(a(t_0) = 1\), where \(t_0\) is the current time. CMB observations were the first to suggest that the \(\kappa = 0\) case seems to describe our Universe \([34, 35]\). Current observations constrain the Universe to be Euclidean to 0.2% \([9]\). The \(\Lambda\)CDM model assumes that \(\kappa = 0\); in the rest of this thesis we will do the same.

The cosmological principle implies that the energy-momentum tensor, the other ingredient of Einstein’s equation besides the metric, determined by a comoving observer is given by that of a perfect fluid:

\[
T^\mu_\nu = \text{diag}(\rho, p, p, p) \, .
\]

where \(\rho\) and \(p\) denote the energy density and pressure of the fluid. From observations of the CMB it can be concluded that we are almost comoving
observers. A true comoving observer would observe an isotropic CMB. We see a small dipole variation in the CMB temperature. The CMB dipole implies that we are moving with respect to the comoving frame. The latest Planck High Frequency Instrument (HFI) data [36], using the temperature from Eq. (1.1) as a fixed quantity, find the following ratio:

$$\left( \frac{T_{\text{dipole},0}}{T_{\text{CMB},0}} \right) = (1.23357 \pm 0.0003) \times 10^{-3}. \quad (2.5)$$

When interpreted as a relativistic doppler shift, the dipole perturbation implies a motion of $369.816 \pm 0.0010$ km s$^{-1}$ with respect to the frame in which the dipole vanishes.

With the energy-momentum tensor specified, one has the necessary ingredients for the Einstein equation:

$$R_{\mu \nu} - \frac{1}{2} R g_{\mu \nu} + \Lambda g_{\mu \nu} = 8\pi G T_{\mu \nu}. \quad (2.6)$$

The Ricci tensor $R_{\mu \nu}$ and its trace $R = R^{\mu}_{\mu}$ are fully specified by the metric $g_{\mu \nu}$. The cosmological constant is denoted by $\Lambda$ and $G$ is the gravitational constant. In principle, the Einstein equation comprises ten equations. However, the FLRW metric only produces two independent equations: one for the purely temporal $(\mu \nu = 00)$ case and one for the spatial $(\mu \nu = ij)$ case. From these, one can derive the two famous Friedmann equations. The first is given by:

$$H^2(t) = \frac{8\pi G}{3} \rho(t) - \frac{\kappa}{a^2(t)} + \Lambda. \quad (2.7)$$

We have briefly reintroduced the $\kappa$ parameter. The Hubble parameter $H$ is defined as follows:

$$H(t) \equiv \frac{\dot{a}}{a}, \quad (2.8)$$

where $\dot{} \equiv \partial / \partial t$. The first Friedmann equation thus describes how energy density is responsible for the expansion rate of space and vice versa. The second Friedmann equation relates the acceleration of space to the cosmological constant and the energy density and pressure of the fluid:

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3} [\rho(t) + 3p(t)] + \frac{\Lambda}{3}. \quad (2.9)$$
The observed recession of distant galaxies, first observed by Hubble [37], implies that the Universe is currently expanding, i.e. $\dot{a}(t_0) > 0$. In order to use this information together with Eq. (2.7) to solve for the expansion history of the Universe, the time dependence of the energy density $\rho(t)$ has to be known. The dependence may be found by first noting that the energy-momentum tensor in Eq. (2.6) can be written as a sum with terms representing different components of the fluid. One may assume that $\rho = \sum_X \rho_X$ and $\rho = \sum_X \rho_X$, where $X$ labels the different components: (dark) matter, radiation and neutrinos. The energy density and pressure are related by constant ‘equation of state’ parameters:

$$p_X = w_X \rho_X .$$

Conservation of the energy-momentum tensor yields the continuity equation. Combined with the above parametrisation, the continuity equation shows that energy density changes as follows with the expansion of space:

$$\rho_X(t) \propto a(t)^{-3(1+w_X)} .$$

Components with distinct equations of state thus scale differently. Recall that 69% of the current energy density of the Universe is given by $\Lambda$. The energy density of the cosmological constant $\Lambda$ stays constant with expansion. This implies that the matter ($w = 0$) and radiation ($w = 1/3$) components dominated the energy density and dynamics of the Universe at earlier times. It is natural to divide the cosmological history into radiation-, matter- and dark-energy-dominated eras. In terms of cosmological redshift:

$$z(t) \equiv \frac{1}{a(t)} ,$$

the radiation-dominated era turned into the matter-dominated era at $z \approx 3600$. The $\Lambda$-dominated era started at $z \approx 0.4$. The neutrino component of the Universe counts as radiation at early times, but starts to behave as non-relativistic matter during the matter-dominated era [29].

The expansion history of the Universe implies that during the radiation- and early matter-dominated eras the photon and baryonic matter components were in thermal equilibrium. To a rough approximation, the non-dark (baryonic) matter in the early Universe consists of hydrogen that is kept in an ionised state due to constant interactions with photons. The thermal equilibrium between the two components in this ‘photon-baryon fluid’ results in a black-body spectrum for the distribution of photon frequencies.
2.2. INHOMOGENEITIES AND ANISOTROPIES

The black-body nature of the spectrum is unchanged by expansion of space. However, the temperature that describes the distribution is inversely proportional to the scale factor and thus drops with the expansion. At the epoch of recombination, at $z \approx 1100$, the temperature of the photon fluid drops to the point where hydrogen seizes to be ionised; there are not enough interactions with energetic photons anymore. With no free electrons, the Universe becomes transparent. The released photons that make up the CMB are able to propagate largely unperturbed. Their spectrum remains that of a black body with a temperature that scales inversely with the expansion of space [28].

2.2 Inhomogeneities and anisotropies

Structure, or inhomogeneity, in the Universe is described in terms of perturbations to the FLRW background. To describe the CMB anisotropies, one may treat the perturbations as small; first order perturbation theory is sufficient. The most general first-order perturbed form of the $\kappa = 0$ FLRW metric in Eq. (2.3) is given by [38]:

$$
\begin{align*}
\begin{aligned}
 ds^2 &= -(1 + 2\Phi)dt^2 + 2a(t)w_1dtdx^i \\
 &+ a^2(t)[(1 - 2\Psi)\delta_{ij} + 2\gamma_{ij}]dx^i dx^j.
\end{aligned}
\end{align*}
$$

(2.13)

Note that Cartesian coordinates are used instead of spherical coordinates. The $\Phi$ and $\Psi$ fields are scalar fields, while the $w_i$ perturbation is a 3-vector field and $\gamma_{ij}$ is a symmetric, traceless 3-tensor. Together, the $\Phi$, $\Psi$, $w_i$, and $\gamma_{ij}$ perturbations thus constitute $1 + 1 + 3 + 5$ degrees of freedom.

The metric perturbations are related to perturbations in the energy-momentum tensor through the Einstein equation. The symmetries of the FLRW metric are such that the first-order perturbed Einstein equation can be separated into three uncoupled differential equations: one for fields that are ‘scalar’, one for fields that are ‘vector’ and one for fields that are ‘tensor’.\(^1\) The equations of motion for the fields in each class are independent from the other equations of motion. The $\Phi$ and $\Psi$ potentials are already scalars, but $w_i$ and $\gamma_{ij}$ can still be decomposed into scalar ($\parallel$), vector ($\perp$) and tensor $h_{ij}$ components [38]. The $w_i$ perturbation can be decomposed as follows:

$$
 w = w_\parallel + w_\perp.
$$

(2.14)

\(^1\)Less ambiguous names are ‘longitudinal’, ‘solenoidal’ and ‘transverse’.
The fields have vanishing curl and gradient, respectively:
\[
\nabla \times \mathbf{w}_\parallel = \nabla \cdot \mathbf{w}_\perp = 0.
\] (2.15)

The \(\gamma_{ij}\) perturbation is decomposed as:
\[
\gamma_{ij} = \gamma_{\parallel,ij} + \gamma_{\perp,ij} + h_{ij},
\] (2.16)
with \(\nabla_i h^i = 0\). The scalar \(\gamma_{\parallel,ij}\) and vector part \(\gamma_{\perp,ij}\) may be expressed in terms of a scalar field \(h\) and a vector field \(h_i\) (with \(\nabla_i h^i = 0\)), respectively:
\[
\gamma_{\parallel,ij} = \left( \nabla_i \nabla_j - \frac{1}{3} \delta_{ij} \nabla^2 \right) h, \quad \gamma_{\perp,ij} = \frac{1}{2} (\nabla_i h_j + \nabla_j h_i).
\] (2.17)

The two degrees of freedom of the tensor perturbation \(h_{ij}\) describe the gravitational waves mentioned in Chapter 1. We will come back to \(h_{ij}\) in Sec. 2.3.2. The vector perturbations are not used to describe the initial perturbations in the \(\Lambda\)CDM model; only the scalar perturbations are required [29].

The comoving coordinates specify the preferred slicing of the four-dimensional spacetime of an unperturbed FLRW universe; the coordinates are such that each \(t = \) constant hypersurface is isotropic and homogeneous. When the FLRW background is perturbed, the choice of slicing becomes ambiguous. The general covariance of general relativity implies that one may always pick a coordinate transformation of \(x^\mu\) (a ‘gauge transformation’), to cancel out the effects of four metric perturbations; only six are physical. Note that the tensor perturbation \(h_{ij}\) is gauge invariant to first order [29]; only the eight scalar and vector degrees are affected by the gauge transformations. One can avoid the complications of the gauge freedom by defining the gauge-invariant curvature perturbation \(\zeta(x, t)\) [39]:
\[
\zeta \equiv -\Psi - \frac{H}{\dot{\rho}} \delta \rho.
\] (2.18)

The \(\zeta\) perturbation is also referred to as the ‘curvature perturbation on uniform-density hypersurfaces’. It is defined in terms of the metric perturbation \(\Psi\), the Hubble parameter \(H\), the time-derivative of the energy density and the linear perturbation to the energy density. Although \(\zeta\) is referred to as the curvature perturbation, it does not necessarily describe perturbations to the curvature. For example, in a gauge where \(\Psi\) disappears, \(\zeta\) only...
describes the perturbation to the energy density. Calculations with different gauge choices should agree on the value of $\zeta$, but not necessarily on its physical interpretation.

A description of the initial scalar perturbations in terms of $\zeta$ is convenient because the perturbations that source the observed CMB anisotropies seem to be purely adiabatic scalar perturbations. Adiabaticity refers to the fact that all components of the cosmic fluid (dark matter, baryonic matter, photons, neutrinos) are perturbed in the same way, specified by a single field.\footnote{The opposite case, where each component has a unique starting value: isocurvature, turns out to have a very distinct signature on the power spectra of CMB anisotropies. If present, isocurvature perturbations have to be small; the telltale sign of adiabatic initial conditions: a negative correlation between temperature and $E$-mode anisotropies, was first observed in the WMAP data\cite{40, 41}.} For the scalar perturbations, $\zeta$ may serve as that field\cite{42}.

To describe the initial adiabatic perturbations we use $\zeta_k$: the Fourier coefficient of the $\zeta$ field on some initial hypersurface at $t_i$ during the early radiation-dominated era:

$$\zeta_k \equiv \int d^3x \, \zeta(x, t_i) e^{-ik \cdot x}.$$  

(2.19)

Note that $k$ denotes a comoving wave vector. The perturbations sourced by $\zeta_k$ are evolved from $t_i$ until today using numerical Einstein-Boltzmann solvers such as the CAMB\cite{43, 44} or CLASS\cite{45} codes.\footnote{See \url{https://camb.info} and \url{http://class-code.net}.}

As the Boltzmann solution is linear in the perturbations, it can be summarised in a set of transfer functions: linear transformations that transform the amplitude $\zeta_k$ to the CMB observed today.

The observed CMB temperature as function of direction $\mathbf{n}$ may be expanded into spherical harmonics $Y_{\ell m}$:

$$T(\mathbf{n}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{T, \ell m} Y_{\ell m}(\mathbf{n}),$$  

(2.20)

with $\mathbf{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ in spherical coordinates. The above transformation is referred to as the inverse transformation. The forward transformation is given by:

$$a_{T, \ell m} = \int_{S^2} d\Omega(\mathbf{n}) \, T(\mathbf{n}) \, Y^{*}_{\ell m}(\mathbf{n}).$$  

(2.21)
The transfer functions relate a Fourier mode of $\zeta$ with comoving wave vector $k$ to a spherical harmonic mode on the sky with multipole order $\ell$ and azimuthal number $m$. As a consequence of the rotational invariance of the Boltzmann solutions, the transfer functions only depend on the comoving wavenumber $k \equiv |k|$ and the multipole order $\ell$. The observable $a_{T,\ell m}$ relates to $\zeta_k$ as follows:

$$a_{T,\ell m} = 4\pi (-i)^\ell \int \frac{d^3k}{(2\pi)^3} \zeta_k T_{T,\ell}^{(\zeta)}(k) Y_{\ell m}^*(\hat{k}) ,$$

(2.22)

where the complex phase is a convention and $\hat{k} \equiv k/k$. The transfer function for the CMB temperature anisotropies is denoted by $T_{T,\ell}^{(\zeta)}(k)$.

To reasonable approximation, the CMB anisotropies were created during the epoch of recombination. The CMB thus allows one to probe $\zeta$ in a thin spherical shell at a comoving distance $r_{\text{rec}}$ that is equal to the comoving distance traveled by a photon since the epoch of recombination; $r_{\text{rec}}$ is roughly 14100 Mpc. A mode in the CMB anisotropy with multipole order $\ell$ is then predominantly sourced by a $\zeta$ perturbation with comoving wavenumber $k$ that obeys:

$$\ell \approx kr_{\text{rec}},$$

(2.23)

or put differently: $T_{T,\ell}^{(\zeta)}$ is, to a good approximation, only nonzero around $k = \ell/r_{\text{rec}}$.

### 2.2.1 Polarization of the microwave background

In addition to the temperature anisotropies, there is another CMB observable: the CMB is weakly polarized. The polarization is generated by Thomson scattering, the interaction that coupled the photons and free electrons in the photon-baryon fluid before the epoch of recombination. Thomson scattering will produce polarized radiation when the incident radiation before scattering has a net quadrupole moment as seen from the perspective of the electron. Before recombination the scattering rate is too high for any appreciable quadrupole moment to be formed by velocity gradients in the photon-baryon fluid. As a result, polarization will be predominantly created during the small period during recombination in which the scattering rate is low enough for a quadrupole moment to form but high enough for scattering to still occur. The polarization of the CMB is therefore rather weak compared to the unpolarized CMB anisotropies [46].
Polarization is introduced with some rigour in this section as the mathematical description is also needed for the later chapters. We will see how the linear polarization of the CMB can be described in the $Q(\hat{n})$ and $U(\hat{n})$ Stokes parameters or in terms of the $E$- and $B$-mode patterns that were illustrated in Fig 1.3. Both descriptions will be important; measurements are usually expressed in terms of the Stokes parameters while cosmological predictions are formulated in $E$ and $B$. The scalar perturbations introduced in the previous section are unable to produce the $B$-mode signal in linear perturbation theory. The velocity gradients mentioned in the previous paragraph are ultimately sourced by the initial scalar perturbation $\zeta$ and therefore only produce $E$-mode polarization. In this section we first introduce several ways to quantify polarization before coming back to the $E$-$B$ decomposition at the end.

**Polarization formalism**

The CMB radiation incident on a telescope today can be described in terms of an electric field vector $E$ that oscillates transverse to its direction of propagation $-\hat{n}$. For computational ease, we express the (real-valued) electric field as the real part of a complex representation:

$$
E(x,t) = \text{Re} \left\{ \epsilon_{\perp}(x,t)e^{-i(\bar{\omega}t-\bar{k}r)} \right\}, 
$$

with radial distance $r$ and $x = r\hat{n}$. The mean angular frequency $\bar{\omega}$ is related to the wavenumber as $\bar{\omega} = c\bar{k}$. $\epsilon_{\perp}$ is a complex vector field transverse to $\hat{n}$. We described the radiation as quasi-monochromatic. Effectively, the field is treated as monochromatic but with a ‘slow’ time-dependence to $\epsilon_{\perp}$ implying that the phase and amplitude of the electric field are stable over a large number of wave periods [47, 48].

When the time-dependence of $\epsilon_{\perp}$ is neglected, the transverse components of the electric field in Eq. (2.24) at fixed radius $r$ describe an ellipse parameterised by $t$. Writing the components of the fields on the orthogonal basis vectors $\hat{e}(\theta)$ and $\hat{e}(\phi)$ of the spherical coordinate system as $E_\theta$ and $E_\phi$ yields:

$$
E_\theta = |\epsilon_{\perp,\theta}| \cos(\omega t + \delta_{\theta}),
E_\phi = |\epsilon_{\perp,\phi}| \cos(\omega t + \delta_{\phi}),
$$

(2.25)

\[^4\text{http://healpix.sourceforge.net}\]
CHAPTER 2. THE COSMIC MICROWAVE BACKGROUND

Figure 2.1: The coordinate convention used throughout this document whenever the standard coordinate spherical coordinates \((\theta, \phi)\) or \((zyz)\) Euler angles \((\psi, \theta, \phi)\) are used. Note that the X and Y axes are aligned with \(\hat{e}_\theta\) and \(\hat{e}_\phi\) respectively. This convention is traditionally used in the CMB literature and corresponds to the COSMO convention in the HEALPix package [49]. The convention differs from the convention used by the International Astronomical Union (IAU); the important difference is a sign change of Stokes \(U\).

Figure adapted from Ref. [50]. See also Ref. [51] for more details on the two polarization conventions.

where we have expressed the transverse components of \(\epsilon_\perp\) as \(\epsilon_{\perp,\theta} = |\epsilon_{\perp,\theta}| e^{i\delta_\theta}\) and \(\epsilon_{\perp,\phi} = |\epsilon_{\perp,\phi}| e^{i\delta_\phi}\). With time, the tip of the electric field vector will trace out an ellipse in the space transverse to \(r\hat{n}\) with a shape that depends on the components of \(\epsilon_\perp\). Linear and circular polarized light correspond to the limiting configurations in which the ellipse becomes a line and circle. In all other cases, the state is said to describe elliptical polarization.

Without loss of generality, we can treat the complex vector \(\epsilon_\perp\) as a vector field on the sphere. Let us refer to its components as \(\epsilon^a(\hat{n}, t)\) with

---

5 The vector field is defined on the tangent space of the sphere, i.e. the plane spanned by X and Y in fig 2.1. The tangent space is a two-dimensional vector space on which we can pick two basis vectors: \(\hat{e}_i\) with \(i \in \{1, 2\}\), to describe vector or tensor fields on the sphere.
a ∈ \{1, 2\}. All information about the shape of the ellipse, or polarization state, is contained in the complex vector \( e^a(\hat{n}, t) \). When \( e \) is defined with respect to an orthogonal basis on the sphere and its time-dependence is neglected, the resulting vector field is referred to as a Jones vector field in the optics and radio astronomy literature [48, 52, 53].

By definition, the Jones vectors describe fully polarized radiation: the type of radiation for which the orthogonal complex components of the analytic signal differ by a constant phase. Equivalently, one can interpret a fully polarized signal as one that has transverse components of \( E \) that are fully correlated in time [54]. Signals with a time-varying relative phase are either partially polarized or unpolarized. Unpolarized light has a vanishing temporal cross-correlation between the orthogonal components, while partially polarized light sits in between the two extreme cases. The Jones vectors are thus not appropriate to describe the partially polarized CMB radiation; we require a formalism that describes the correlation between the components of \( e \).

To quantify the correlation between different components of the complex \( e \) vector, we follow [54] and define the density matrix, i.e. the following tensor field on the sphere:

\[
W_{ab}(\hat{n}, \omega) \equiv \int_0^\infty d\tau \Gamma_{ab}(\hat{n}, \tau) e^{i\omega \tau},
\]

(2.26)

where

\[
\Gamma_{ab}(\hat{n}, \tau) = \langle e^a(\hat{n}, t) e^*_b(\hat{n}, t + \tau) \rangle,
\]

(2.27)

is the cross-spectral density of the Jones vector. The signal is assumed to be stationary so only the time lag \( \tau \) is required to describe \( \Gamma \). The angled brackets denote an ensemble average which in reality would be replaced with a time average over a sufficiently long measurement period [54].

**Stokes parameters**

In the CMB literature, polarized signal is expressed in terms of the elements of the density matrix in Eq. (2.26): the real-valued Stokes parameters \( I, Q, U \) and \( V \). When using the standard spherical coordinates \( \theta, \phi \) with metric \( g_{ab} = \text{diag}(1, \sin^2 \theta) \), the density matrix is expressed as [55, 56]:

\[
W_{ab}(\hat{n}, \omega) = \frac{1}{2} \begin{pmatrix}
I + Q & (U - iV) \sin \theta \\
(U + iV) \sin \theta & (I - Q) \sin^2 \theta
\end{pmatrix}
(\hat{n}, \omega).
\]

(2.28)
Stokes $Q$ and $U$ represent linear polarization and will be our main focus. Stokes $V$ represents circular polarization and is not produced by Thomson scattering. The total intensity of the signal is given by $I$. For CMB radiation, $I$ is proportional to the temperature $T$ of the black-body radiation.

The density matrix is a covariance matrix and must thus be positive-semi-definite, i.e. $\det W \geq 0$. In terms of the Stokes parameters, this means that:

$$I^2 \geq Q^2 + U^2 + V^2.$$  \hfill (2.29)

When the two sides of the equation are equal, the signal is fully polarized. When the r.h.s. vanishes, the signal is unpolarized [47]. Note that $I \geq 0$.

### Spin-weighted functions

Eq. (2.28) demonstrates that the polarization of the CMB is fundamentally a tensor-like observable. When using the Stokes parameters as scalar-valued fields on the sphere it should be kept in mind that the $Q$, $U$ and $V$ parameters are not true scalar fields under coordinate transformations; their transformation properties reflect the transformation of the underlying density matrix. $Q$ and $U$ mix under coordinate rotations; $U$ and $V$ change their sign under the parity operation. Due to the underlying tensor-like behaviour of $Q$ and $U$, it is often convenient to describe linear polarization in terms of so-called spin-weighted representations of the density matrix.

We start by defining two complex orthonormal vectors as linear combinations of two orthonormal coordinate basis vectors that describe the coordinates used on the sphere [57–59]:

$$m = \frac{1}{\sqrt{2}} (\hat{e}_{(1)} + i \hat{e}_{(2)}) ,$$  \hfill (2.30)

$$m^* = \frac{1}{\sqrt{2}} (\hat{e}_{(1)} - i \hat{e}_{(2)}) .$$  \hfill (2.31)

We have $m^a m_a = 0$, $m^a m^*_{a'} = 1$ and $m^a m^*_{b} + m^*_{a} m_b = \delta^a_b$. For a right-handed rotation of the coordinates around the point $\hat{n} \in S^2$ of angle $\psi$ (see fig 2.1), we have:

$$m(\hat{n}) \mapsto e^{-i\psi} m(\hat{n}) ,$$  \hfill (2.32)

$$m^*(\hat{n}) \mapsto e^{i\psi} m^*(\hat{n}) .$$  \hfill (2.33)
Simultaneously, following [57], we define a set of complex spin-weighted functions on the tangent space that are defined by their transformation properties under the same right-handed rotation:

\[(s)f(\hat{n}) \rightarrow e^{-is\psi}(s)f(\hat{n})\],

(2.34)

with integer spin weight \(s\). With the vectors \(m\) and \(m^*\), we may decompose any tensor on the sphere into spin-weighted functions writing down all possible contractions with \(m\) and \(m^*\). For example, a vector \(v\) contracted with \(m\), i.e. \(v^a m_a\), yields an \(s = 1\) function, while the same vector contracted with \(m^*\) yields an \(s = -1\) function.

Using the \(m\) and \(m^*\) vectors, we may construct the spin-weighted representation of the density matrix in Eq. (2.28). The representation consists of two spin-0 fields:

\[I = W_{ab} (m^a m^b + m^{*a} m^b) / 2,\]

(2.35)

\[V = W_{ab} (m^{*a} m^b - m^{*a} m^b) / 2,\]

(2.36)

and a spin-\(\pm 2\) combination:

\[(Q + iU) = W_{ab} m^a m^b,\]

(2.37)

\[(Q - iU) = W_{ab} m^{*a} m^{*b}.\]

(2.38)

For this reason, it is often more natural to work with the following quantities:

\[(2)^P(\hat{n}) \equiv (Q + iU)(\hat{n}),\]

(2.39)

\[(-2)^P(\hat{n}) \equiv (Q - iU)(\hat{n}),\]

(2.40)

to describe linear polarization; \(2^P\) and \((-2)^P\) do not mix under coordinate rotations. It should be noted that since the Stokes parameters are necessary real, \(\pm 2^P\) fulfils the ‘reality’ condition: \((2^P)^* = (-2)^P\).

**Spin-weighted spherical harmonics**

The harmonic decomposition is highly useful in describing fields on the sphere. The spherical harmonic decomposition was already introduced in

---

\(^6\)Our convention for the sign of \(s\) follows the one used in the CMB literature [60].

\(^7\)For a general spin-\(s\) function \((s)f\) the condition \((s)f^* = (-s)f\) does not need to hold. The condition is really a statement about the reality of the elements of the underlying tensor, or equivalently: the existence of a rotational frame in which \((s)f\) is real. Following Ref. [61], we refer to this condition as the reality condition.
Eq. (2.21). A harmonic decomposition of the spin-$\pm 2$ polarization fields $\pm 2\mathcal{P}$ into regular spherical harmonics suffers from a coordinate dependence: the spin-weighed fields are coordinate dependent (see Eq. (2.34)) but the spherical harmonics are not. A set of basis functions with the same coordinate dependence as $\pm 2\mathcal{P}$ is needed in order for the coordinate dependence to cancel out. These are the spin-weighed spherical harmonics (SWSHs) [57, 58]. The SWSHs were introduced to the CMB literature in Ref. [60], but were already used in e.g. the gravitational wave literature [62]. We give a brief overview.\(^8\)

The SWSH are denoted by $sY_{\ell m}$, where $s$ denotes the spin-weight. The $s = 1$ and $s = 2$ SWSHs are defined in terms of the regular spherical harmonics as follows:

$$1Y_{\ell m}(\hat{n}) = 2 \sqrt{\frac{(\ell - 1)!}{(\ell + 1)!}} m^a(\hat{n}) \nabla_a Y_{\ell m}(\hat{n}) ,$$

$$2Y_{\ell m}(\hat{n}) = 2 \sqrt{\frac{(\ell - 2)!}{(\ell + 2)!}} m^a(\hat{n}) m^b(\hat{n}) \nabla_a \nabla_b Y_{\ell m}(\hat{n}) ,$$

where $m^a$ is defined in Eq. (2.30) and where $\nabla_i$ is the covariant derivative on the sphere, distinguished from the three-dimensional derivative by the tilde. The covariant derivatives reduce to regular angular derivatives when operated on scalar fields such as $Y_{\ell m}$, but introduce corrections in the form of the Christoffel symbols when operated on vector or tensor fields [32, 63]. The contractions with $m$ mean that $1Y_{\ell m}$ and $2Y_{\ell m}$ are spin-$1$ and -$2$ respectively. A second useful parametrisation comes from the insight that the SWSHs in the standard spherical basis can be expressed in terms of the Wigner $D$-matrices [57, 58]. In terms of the spherical coordinates and the Euler angles illustrated in Fig. 2.1 the relation is:

$$sY_{\ell m}(\theta, \phi) = (-1)^m \sqrt{\frac{2\ell + 1}{4\pi}} D^\ell_{-ms}(\phi, \theta, \psi) \bigg|_{\psi=0} .$$

For equal spin-weights the SWSHs form a complete and orthonormal basis on the sphere. The orthonormality relation is given by:

$$\int_{S^2} d\Omega(\hat{n}) sY_{\ell m}(\hat{n}) s'Y^*_{\ell' m'}(\hat{n}) = \delta_{\ell \ell'} \delta_{mm'} .$$

\(^8\)It should be noted that a part of the CMB literature makes use of the so-called ‘tensor spherical harmonics’ [63] as opposed to the SWSHs. The tensor spherical harmonics provide a somewhat more explicit description, but both serve the exact same purpose.
We thus define:
\[ \pm 2a_{\ell m} = \int_{S^2} d\Omega(\hat{n}) (\pm 2)P(\hat{n}) \pm 2 Y_{\ell m}^*(\hat{n}). \] (2.45)

The $2a_{\ell m}$ coefficients have now lost the coordinate dependence that $(\pm 2)P$ has. This implies that under a coordinate rotation specified by Euler angles $\psi$, $\theta$, and $\phi$ the coefficients transform among themselves as follows:
\[ \pm 2a_{\ell m} \mapsto \sum_{m'} \pm 2a_{\ell m'} D_\ell^{m'}(\phi, \theta, \psi). \] (2.46)

This relation holds in general for harmonic coefficients $s f_{\ell m}$ that were obtained by transforming a spin-$s$ function with $s Y_{\ell m}$. We then have:
\[ s f_{\ell m} \mapsto \sum_{m'} s f_{\ell m'} D_\ell^{m'}(\phi, \theta, \psi). \] (2.47)

Under the parity transformation $2a_{\ell m}$ and $-2a_{\ell m}$ do mix into each other. The parity transformation $x \mapsto -x$ expressed in spherical coordinates becomes the following mapping of the $(r, \theta, \phi)$ coordinates:
\[ \hat{e}_{(r)} \mapsto \hat{e}_{(r)}, \]
\[ \hat{e}_{(\theta)} \mapsto \pi - \hat{e}_{(\theta)}, \]
\[ \hat{e}_{(\phi)} \mapsto \hat{e}_{(\phi)} + \pi. \] (2.48)

The SWSHs transform as follows under parity:
\[ s Y_{\ell m} \mapsto -s Y_{\ell m}(-1)^{\ell+s}, \] (2.49)

which results in the following mixing of the $\pm 2a_{\ell m}$ coefficients under parity:
\[ \pm 2a_{\ell m} \mapsto \pm 2a_{\ell m}(-1)^\ell. \] (2.50)

**E-B decomposition of CMB polarization**

We now describe the $E$- and $B$-mode patterns that were already sketched in Fig. 1.3 more formally. The importance of the $E$-$B$ decomposition is that $E$ and $B$ do not mix under parity. In terms of the spin-$\pm 2$ harmonic coefficients used to decompose $Q \pm iU$ defined in Eq. (2.45), the $E$- and $B$-mode harmonic coefficients are given by:
\[ a_{E, \ell m} = -\frac{1}{2}(+2a_{\ell m} + -2a_{\ell m}), \] (2.51)
\[ a_{B, \ell m} = -\frac{1}{2i}(+2a_{\ell m} - -2a_{\ell m}). \] (2.52)
Figure 2.2: Four $20^\circ \times 20^\circ$ patches of the sky depicting random Gaussian linear polarization fields with spatial correlations as predicted by the $\Lambda$CDM+$r$ model with $r = 0.03$. The patches are centred on the equator ($\theta = \pi/2$) at $\phi = 0$. The top row shows the Stokes $Q$ and $U$ signal sourced by the $E$-mode component of the polarization field: signal that is predominantly sourced by the scalar perturbations. The bottom row shows Stokes $Q$ and $U$ sourced by the $B$-mode component. Spatial correlations on scales of a degree and larger in the bottom figures are sourced by the primordial tensor field, smaller correlations are caused by scalar-sourced $E$-mode signal converted by gravitational lensing. $Q$ and $U$ in the bottom figures have been multiplied by a factor ten to allow comparison with the same colour scale.
From Eq. (2.50) one can derive the behaviour under parity for each of the three types of spherical harmonic coefficients commonly used to describe the CMB and its polarization field:

\[
\begin{align*}
a_I,\ell m &\mapsto (-1)^\ell a_I,\ell m , \\
a_E,\ell m &\mapsto (-1)^\ell a_E,\ell m , \\
a_B,\ell m &\mapsto (-1)^{\ell+1} a_B,\ell m .
\end{align*}
\] (2.53)

The parity-even and parity-odd behaviour of \( E \) and \( B \) is illustrated in Fig. 2.2. Shown are Stokes \( Q \) and \( U \) for both a purely \( E \)-mode and purely \( B \)-mode polarization field. Only a small patch around the equator is plotted such that the \((\theta,\phi)\) coordinates closely resemble Cartesian coordinates. It can be seen how a purely \( E \)-mode polarization field yields patterns in \( Q \) that are aligned with \( \hat{e}_\theta \) and \( \hat{e}_\phi \) and patterns in \( U \) that are at a 45° angle with \( \hat{e}_\theta \) and \( \hat{e}_\phi \). The exact opposite behaviour is seen for the purely \( B \)-mode polarization field.

In addition to the definitions in Eq. (2.51) and Eq. (2.52), it is instructive to directly relate the \( E-B \) decomposition to the Stokes \( Q \) and \( U \) parameters in coordinate space. Linear polarization is described by the symmetric, traceless part of the full density matrix \( W \), i.e. Eq. (2.28) with \( I = V = 0 \), let us refer to it as \( \tilde{W} \). Instead of decomposing the two degrees of freedom of \( \tilde{W}(\hat{n}) \) into Stokes \( Q \) and \( U \), we may equally well describe linear polarization with two other scalar fields that are constructed by contracting \( \tilde{W} \) with two covariant derivatives [55, 60]:

\[
\begin{align*}
\tilde{E}(\hat{n}) &= \bar{\nabla}^a \bar{\nabla}^b W_{ab}(\hat{n}) , \\
\tilde{B}(\hat{n}) &= \epsilon_{bc} \bar{\nabla}^a \bar{\nabla}^c W_{ab}^b(\hat{n}) .
\end{align*}
\] (2.54)

\[\tilde{E} \] and \( \tilde{B} \) are scalar under coordinate rotations, i.e. spin-0. The antisymmetric tensor \( \epsilon \), the two-dimensional Levi-Civita symbol, should not be confused with the Jones vector. The symbol is defined as follows in terms of \( g \): the determinant of metric on the sphere [63]:

\[
\epsilon_{ab} \equiv \sqrt{g} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \sin \theta \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} ,
\] (2.56)

where the second equality holds for the standard \((\theta,\phi)\) coordinates. The presence of \( \epsilon \) means that \( \tilde{B} \) is a pseudoscalar field that changes sign under inversion of the spatial coordinates (a parity transformation). The \( \tilde{E} \) field is invariant under parity.
\( \tilde{E} \) and \( \tilde{B} \) are sometimes referred to as the real space or causal representations of \( E \) and \( B \) \cite{60,64}. The relation between \( \tilde{E} \) and \( \tilde{B} \) and the true \( E \) and \( B \) definition is most easily understood by decomposing \( \tilde{E} \) and \( \tilde{B} \) into spherical harmonic coefficients:

\[
\tilde{E}(\hat{n}) = \sum_{\ell,m} \sqrt{\frac{(\ell+2)!}{(\ell-2)!}} a_{E,\ell m} Y_{\ell m}(\hat{n}),
\]

(2.57)

and defining the \( E \) and \( B \)-mode fields as follows:

\[
E(\hat{n}) = \sum_{\ell,m} a_{E,\ell m} Y_{\ell m}(\hat{n}),
\]

(2.59)

\[
B(\hat{n}) = \sum_{\ell,m} a_{B,\ell m} Y_{\ell m}(\hat{n}).
\]

(2.60)

The harmonic coefficients of \( \tilde{E} \) and \( \tilde{B} \) are thus related to those of \( E \) and \( B \) by a factor \( \sqrt{\frac{(\ell+2)!}{(\ell-2)!}} \). In coordinate space, this factor translates to a somewhat complicated differential operator \cite{60}. To provide some intuition: the operator reduces to the two-dimensional laplacian \( \nabla^2 \) in the flat-sky approximation. The following relations thus hold on the flat sky: \( \nabla^2 E = \tilde{E} \) and \( \nabla^2 B = \tilde{B} \). The presence of the laplacian (or equivalently, the \( \sqrt{\frac{(\ell+2)!}{(\ell-2)!}} \) factor) is of consequence: it means that the \( E-B \) decomposition depends non-locally on the Stokes parameters; an unambiguous determination of both \( E \) and \( B \) at a given location on the sky formally requires measurements of \( Q \) and \( U \) over the entire sky \cite{64}.

We now return to the polarization of the CMB. Explaining why the scalar perturbation is unable to source the \( B \)-mode polarization in a satisfactory way is beyond the scope of this section. See the review in Ref. \cite{65} for a pedagogical introduction. Taking for granted that the \( \zeta \) perturbations to first order only source \( E \)-mode polarization, we may introduce the transfer function \( T^{(\zeta)}_{E,\ell} \) that relates the initial \( \zeta_k \) perturbation to the \( E \)-mode spherical harmonic modes observable today. Let us thus extend our summary of the
linear relation between $\zeta$ and the CMB anisotropies in Eq. (2.22) with $E$-mode polarization:

$$a_{X,\ell m} = 4\pi(-i)^\ell \int \frac{d^3k}{(2\pi)^3} \zeta_k T_{X,\ell}^{(C)}(k) Y_{\ell m}^*(\hat{k}),$$  \hspace{1cm} (2.61)

for $X \in \{T,E\}$.

### 2.2.2 Angular power spectra

As we will see in the next section, the initial scalar perturbations $\zeta$ are thought to be generated by a stochastic process. Exactly reconstructing the perturbations is thus of limited interest; in order to learn about the responsible process, the statistical properties of $\zeta$ have to be reconstructed. There is strong observational evidence that $\zeta$ is governed by a Gaussian distribution [66]. In this case all statistical information is contained in the 2-point correlation function of the super-horizon Fourier modes introduced in Eq. (2.19). The 2-point correlation function is parametrised as follows:

$$\langle \zeta_k \zeta_{k'}^* \rangle = (2\pi)^3 \delta^{(3)}(k - k') P_\zeta(k),$$  \hspace{1cm} (2.62)

where $P_\zeta(k)$ is the power spectrum. The fact that the power spectrum only depends on $k = |k|$ is due to the assumed isotropy of the correlation. Similarly, the delta function is a consequence of the assumed homogeneity of the correlation.

Gaussian initial conditions lead to highly Gaussian-distributed CMB anisotropies because (almost) all responsible physics is captured by the linear transfer functions. A linear transformation of a Gaussian random field does not change its Gaussian nature. The isotropy and homogeneity of the 2-point correlation function of $\zeta$ and the rotational invariance of the transfer functions result in an isotropic 2-point correlation function of the CMB anisotropies. The angular power spectrum $C^{XX'}_\ell$ is defined in terms of the 2-point correlation of the $a_{X,\ell m}$ harmonic modes:

$$\langle a_{X,\ell m} a_{X',\ell'm'}^* \rangle = \delta_{\ell\ell'} \delta_{mm'} C^{XX'}_\ell.$$

Using Eq. (2.61), the angular power spectrum can be related to the primordial power spectrum:

$$C^{XX'}_\ell = \frac{2}{\pi} \int_0^\infty k^2 dk P_\zeta(k) T_{X,\ell}^{(C)}(k) T_{X',\ell'}^{(C)}(k),$$  \hspace{1cm} (2.64)
Figure 2.3: Compilation of CMB data from recent experiments. From top to bottom: the temperature, $E$-mode and lensing-induced $B$-mode power spectra, the cross-correlation between temperature and $E$-mode polarization and the lensing power spectrum. The dashed lines give the best-fitting $\Lambda$CDM predictions based on the Planck data (the dark blue dots). The $TT$, $EE$, $BB$, and $IE$ spectra are in units of $D_\ell \equiv \ell(\ell+1)C_\ell/(2\pi)$. The lensing power spectrum $C_\ell^{\phi\phi}$ will be briefly discussed in Sec. 2.4. Image credit: ESA and the Planck Collaboration, see Ref. [8].
for $XX' \in \{TT, EE, TE\}$. There is a correlation between $T$ and $E$ as both are sourced by $\zeta$.

Fig. 2.3 shows a compilation of recent CMB power spectrum measurements. The $C_{\ell}^{TT}$, $C_{\ell}^{EE}$ and $C_{\ell}^{TE}$ power spectra have been measured over a wide range of angular scales and are all in excellent agreement with predictions from the six-parameter $\Lambda$CDM model. The regular peaks and troughs seen the spectra are a direct consequence of a pattern of standing waves, the baryon acoustic oscillations, in the photon-baryon fluid before recombination. Having access to the $C_{\ell}^{TT}$, $C_{\ell}^{EE}$ and $C_{\ell}^{TE}$ spectra removes a number of degeneracies in the parameters of the $\Lambda$CDM model; it is possible to jointly fit for the parameters governing the power spectrum $P(k)$ and the parameters of the transfer functions governing the dynamics of the photon-baryon fluid. With the addition of weak gravitational lensing measurements (the other two spectra in Fig. 2.3) or external measurements of the large-scale structure of the Universe more degeneracies are removed. Combining complementary measurements in order to break parameter degeneracies has become an important aspect of modern cosmology.

We have ignored the initial power spectrum $P_\zeta(k)$ in Eq. (2.64) up to now. The structure seen in the CMB angular power spectra is not due to $P_\zeta(k)$ in the $\Lambda$CDM model. The power spectrum $P_\zeta(k)$ is given by a completely featureless power law that is parameterised with an amplitude $A_s$ and a spectral tilt $n_s - 1$:

$$P_\zeta(k) = 2\pi^2 \frac{A_s(k_0)}{k^3} \left( \frac{k}{k_0} \right)^{n_s(k_0)-1}. \quad (2.65)$$

The amplitude $A_s$ and the $n_s$ parameter are constrained to [9]:

$$A_s = (2.105 \pm 0.1014) \cdot 10^{-9}, \quad (2.66)$$

$$n_s = 0.9665 \pm 0.0038. \quad (2.67)$$

We see that $n_s$ is smaller than one in a statistically significant manner. The power spectrum is therefore referred to as a nearly scale-invariant power spectrum.\(^9\) The nonzero spectral tilt $n_s - 1$ breaks the scale invariance; the power spectrum is slightly ‘red’: it has more power on large scales.

\(^9\)A spectrum proportional to $k^{-3}$ is perfectly scale-invariant in the sense that the associated coordinate-space version of the 2-point correlation function is invariant under a constant rescaling $\mathbf{x} \mapsto \lambda \mathbf{x}$ of the comoving coordinates.
2.3 Connection to primordial physics

2.3.1 Cosmic inflation

The theory of cosmic inflation was originally invented to explain the Euclidean and isotropic nature of our Universe [67, 68]. Cosmic inflation has become rather compelling because of its role as a generation mechanism for the initial $\zeta$ perturbations [69–71]. Cosmic inflation is a framework; a wide range of models that implement the general idea of an inflationary phase in the early Universe. Models of inflation range from highly phenomenological models to string-theory inspired models [29, 72]. Single-field slow-roll (SFSR) models [73, 74] are arguably the simplest implementations that are consistent with current data.

In SFSR models one postulates a single homogeneous scalar field, the inflaton field, with an almost flat potential. The energy-density of the field is assumed to dominate the total energy of the Universe. The resulting energy-momentum tensor describing the matter and energy of the Universe becomes that of a perfect fluid with negative pressure. Through the Einstein equation, the resulting exponential expansion of space drives the spatial hypersurfaces towards flat Euclidean geometry and moves previously connected points to spacelike separations. Both of these effects serve to explain the characteristics of our Universe on the largest observable scales. Roughly 60 $e$-foldings of exponential expansion are needed to produce the observed flat geometry and isotropy [29].

The mechanism for the creation of the initial $\zeta$ perturbations revolves around the small, spatially varying vacuum fluctuations of the inflaton field during inflation. Fluctuations at a physical wavenumber $k/a(t)$ that initially behave as a quantum harmonic oscillator lose their time dependence when $k/a(t)$ becomes comparable to the expansion (Hubble) rate $H$. When the wavenumber becomes smaller than the Hubble rate, or equivalently as $k \ll aH$, the fluctuation is said to have left the horizon and is converted to a classical curvature perturbation $\zeta$ that remains constant with time. The power spectrum of the resulting super-horizon $\zeta_k$ perturbations is of the nearly scale-invariant form like Eq. (2.65).

Inflation has to end at some point so there has to be a ‘clock’ that tells each part of the Universe to eventually stop accelerating. The role of clock is taken by the field value of the inflaton field; once the inflaton field starts to evolve significantly with time, inflation ends and a phase of reheating
2.3. CONNECTION TO PRIMORDIAL PHYSICS

Figure 2.4: CMB angular power spectra calculated using CAMB for the best-fitting Planck 2018 ΛCDM parameters [9] sourced by scalar perturbations (left) and tensor perturbations with $r = 0.03$ (right), slightly below the current $r < 0.064$ (95% CL) upper limit [9]. The shaded regions denote 1σ cosmic variance. By comparing the two panels it can be seen how the $\ell \lesssim 100$ $B$-mode power spectrum is the only observable of tensor-induced signal for which scalar-induced cosmic variance does not prohibit a statistically significant detection given currently allowed values of $r$.

occurs. During reheating the enormous potential energy of the inflaton field is (indirectly) transferred to the constituents of the Universe. For inflation models driven by a single inflaton field, the conservation of $\zeta$ on super-horizon scales allows one to effectively ignore most of the unknown physics of reheating: the statistical properties of $\zeta_k$ are unaffected [42].

2.3.2 $B$-modes and tensor perturbations

Similar to how the vacuum fluctuations of the inflation field produce the $\zeta$ perturbation, vacuum fluctuations in the gravitational field during inflation become classical perturbations when the wavenumber of the fluctuations exits the horizon. The resulting classical perturbation are given by the tensor perturbation $h_{ij}$ in Eq. (2.16). Just like $\zeta$, the super-horizon tensor perturbations are constant with time. A nearly-scale invariant power spectrum of tensor perturbations is a rather generic prediction of inflation.
The amplitude of the gravitational waves is model dependent [13–15, 75].

It is convenient to describe the two degrees of freedom of $h_{ij}$ on superhorizon scales in terms of two helicity states with Fourier coefficients given by:

$$ (\pm 2)h_k \equiv \frac{e_{\pm 2}^{ij}(\hat{k})}{2} \int d^3x \, h_{ij}(x, t_i) e^{-i\hat{k}\cdot x} \,. \quad (2.68) $$

The time $t_i$ again specifies an initial hypersurface during the early radiation-dominated era. The polarization tensors $e_{\pm 2}$ are two symmetric, traceless and transverse tensor fields with the following properties:

$$ (e_{\pm 2}^{ij}(\hat{k}))^* = e_{\mp 2}^{ij}(\hat{k}) \,, \quad (2.69) $$

$$ e_{\lambda}^{ij}(\hat{k}) e_{\lambda'}^{ij}(\hat{k}) = 2\delta_{\lambda,\lambda'} \quad (\lambda \in \pm 2) \,. \quad (2.70) $$

In terms of the helicity states, the 2-point function of the tensor perturbations is given by:

$$ \langle (\lambda)h_{k}(\lambda')h_{k'}^* \rangle = (2\pi)^3\delta^{(3)}(k - k')\delta_{\lambda,\lambda'} \frac{P_h(k)}{2} \,. \quad (2.71) $$

The tensor power spectrum is assumed to be of the nearly scale-invariant form:

$$ P_h(k) = 2\pi^2 \frac{A_t(k_0)}{k^3} \left( \frac{k}{k_0} \right)^{n_t(k_0)} \,. \quad (2.72) $$

The tensor amplitude $A_t$ is related to the amplitude of the scalar perturbations in Eq. (2.65) through the tensor-to-scalar ratio $r$:

$$ r_k = \frac{A_t(k)}{A_s(k)} \,. \quad (2.73) $$

The connection between the primordial tensor perturbations and CMB polarization was first pointed out by Ref. [12]. The notion that the $B$-mode signal provides a probe of the tensor perturbation was formulated in Ref. [55, 60]. The three CMB fields ($X \in \{T, E, B\}$) sourced by the two helicity components of the tensor perturbation are given by [28]:

$$ a_{X,\ell m}^{(h)} = 4\pi(-i)^\ell \int \frac{d^3k}{(2\pi)^3} T_X^{(h)}(\hat{k}) \sum_{\lambda \in \pm 2} \text{sgn}(\lambda)^\ell (-\lambda)h_k - \lambda Y_{\ell m}^*(\hat{k}) \,. \quad (2.74) $$
with \( x = 1 \) for \( X = B \) and 0 otherwise. As the transfer function are invariant under parity, the parity-even \( T \) and \( E \) fields are solely sourced by the parity-even combination:

\[
a_{T/E,\ell m}^{(h)} \sim (-2)h_{k-2}Y_{\ell m}^* + (2)h_{k+2}Y_{\ell m}^*,
\]

while the parity-odd \( B \) field is sourced by the parity-odd combination:

\[
a_{B,\ell m}^{(h)} \sim (-2)h_{k-2}Y_{\ell m}^* - (2)h_{k+2}Y_{\ell m}^*.
\]

The per-multipole cosmic variance on a measurement of an angular power spectrum \( C_{XY}^\ell \), with \( X, Y \in \{ T, E, B \} \), is approximately given by [76]:

\[
\sigma^2(C_{XY}^\ell) \approx \frac{2}{2\ell + 1}(C_{XY}^\ell)^2.
\]

This assumes that all \( 2\ell + 1 \) modes are measured per \( \ell \), i.e. a full-sky measurement. The variance increases inversely proportional to the fraction of the sky measured. Recall that the scalar perturbations do not source \( B \)-mode polarization (neglecting the \( B \)-mode power due to gravitational lensing). By measuring the \( B \)-mode angular power spectrum \( C_{BB}^\ell \) on large (\( \gtrsim 1 \degree \)) angular scales, the tensor-to-scalar ratio \( r \) can thus be constrained in a manner that is insensitive to the cosmic variance induced by the scalar perturbations; see Fig. 2.4.

A detection of nonzero \( r \) would fix the energy scale of the potential \( V(\phi) \) of the inflaton field \( \phi \) in slow-roll inflation:

\[
V^{1/4} \sim \left( \frac{r}{0.01} \right)^{1/4} 10^{16} \text{ GeV}.
\]

A detection of \( r \) in the foreseeable future would therefore imply that inflation occurs at an enormous energy scale [29]. The recently improved upper-limits on \( r \) already disfavour a number of inflation models; see Fig. 2.5. A detection of \( r \) would also serve as an indication that inflation is described by a ‘large-field’ model.\(^\text{10}\)

\(^{10}\)For slow-roll inflation, the distance traveled through field space \( \Delta \phi \) is related to \( r \) as follows:

\[
\Delta \phi \sim \left( \frac{r}{0.01} \right)^{1/2} M_{\text{pl}},
\]

where \( M_{\text{pl}} \approx 2.435 \times 10^{18} \text{ GeV} \) represents the reduced Planck mass. This relation, the Lyth bound [77], implies that any detection of \( r \) in the foreseeable future, i.e. \( r \gtrsim 10^{-3} \) [18], will place \( \Delta \phi \) roughly at the Planck scale [78, 79].
Figure 2.5: Planck 2018 joint constraints (at 95% CL) on the tensor-to-scalar ratio \( r \) and the spectral tilt \( n_s \) of the primordial power spectrum. It can be observed that the addition of the BiCeP2/Keck Array \( B \)-mode power spectrum data (BK14) constrains \( r \) more efficiently than temperature and \( E \)-mode data (TT, TE, EE+lowE+lensing) can. The predictions of several inflation models, either denoted by name or by potential \( V \), are plotted for two choices \( (N_\star = 50, 60) \) of the number of e-foldings of exponential expansion during inflation. The separation into convex and concave refers to a model-independent prediction on the second derivative of the inflaton potential \( (\partial^2 V / \partial \phi^2) \) during slow-roll inflation [80]. Image credit: ESA and the Planck Collaboration, see Ref. [66].

### 2.4 The microwave sky

On the large-angular scales that are relevant for the primordial \( B \)-mode signal, the polarized signal from the Galaxy is bright compared to the CMB polarization. Current data are well described by modelling the polarized foreground signal with just two components: a thermal dust component that dominates at frequencies above 70 GHz and a synchrotron component that dominates at lower frequencies [6]. The frequency dependence of the components is described by a power law and a modified black-body spectrum, respectively. The two components are illustrated in Fig. 2.6 and 2.7. Polarized Galactic foregrounds are constrained with data from the Planck...
and WMAP satellite experiments spanning 30-400 GHz. Unfortunately, those data do not provide high sensitivity to the polarized foregrounds in the low-foreground regions at high and low Galactic latitude that B-mode experiments observe. Still, it is now established that there are no patches of sky without significant foreground contamination [6].

Weak gravitational lensing by the Universe’s large-scale structure along the line of sight contributes to $C^{BB}_\ell$ by converting $E$-mode polarization to a $B$-mode signal [81]. The lensed $B$-mode signal was initially detected indirectly with the use of tracers of the large-scale structure [82–84], but has since been detected directly through measurements of $C^{BB}_\ell$ [85]. Besides contributing to the $B$-mode power spectrum, lensing effectively flattens the peaks and troughs of the $C^{TT}_\ell$, $C^{TE}_\ell$, and $C^{EE}_\ell$ power spectra. However, the real, discriminating property of lensing is its non-Gaussian contribution to the CMB. By measuring the (connected, i.e. non-Gaussian) 4-point function of the CMB temperature or polarization, the angular power spectrum of the lensing potential ($C^{\phi\phi}_\ell$ in Fig. 2.3) can be reconstructed. Roughly speaking, the lensing potential is the gravitational potential integrated along the line of sight. The first detection of the lensing-induced 4-point function and thus the lensing power spectrum was presented in Ref. [86]. Measurements of the lensing potential have since been much improved as is evident from
Figure 2.7: The amplitude \((\sqrt{Q^2 + U^2})\) of polarized dust emission evaluated at 353 GHz in Galactic coordinates estimated with Planck data. Image credit: ESA and the Planck Collaboration, see Ref. [6].

Fig. 2.3. See Ref. [87] for a comprehensive review on gravitational lensing of the CMB.

Below \(\ell \approx 500\), the \(B\)-mode power spectrum due to lensing is similar to a (constant) white noise spectrum with a 5 \(\mu\)K arcmin\(^{-1}\) amplitude. The cosmic variance due to the lensing contamination seemingly prohibits inference on low values of \(r\). However, with knowledge of the lensing potential the effect of lensing can be effectively undone in a process referred to as delensing [88–90]. Inference on \(r\) is currently not limited by the lensing signal, but this is expected to change with more sensitive experiments. As an example, the proposed CMB-S4 experiment would require \(C_{\ell}^{BB}\) to be delensed by a factor of ten in order to reach its goal of \(r < 0.001\) at 95% CL [19].
Chapter 3

The SPIDER Experiment

3.1 Overview

SPIDER is a balloon-borne experiment designed to study the polarization signal of the CMB with a special focus on a degree-scale $B$-mode signal [91–93]. The instrument launched from the McMurdo Station on the Antarctic coast for its first long-duration balloon flight on January 1, 2015 and deployed six cryogenically cooled refractor telescopes. During the 16-day flight, these telescopes mapped approximately 10% of the southern sky at 94 and 150 GHz.

The main science goal of SPIDER is to measure the primordial $B$-mode polarization of the CMB. In terms of constraints on the tensor-to-scalar ratio $r$, the expected sensitivity and control over systematic errors result in a forecasted constraint of $r < 0.03$ (at 99% CL) in the absence of an primordial contribution but in the presence of expected polarized foregrounds [92]. This limit is based on two flights, with the second flight adding a 280 GHz band described in Ref. [101]. The expected statistical sensitivity to the $B$-mode power spectrum is depicted in Fig. 3.1. The 280 GHz band will be sensitive to Galactic dust and is designed to fill the frequency coverage gap between the 217 GHz and 353 GHz bands of the Planck HFI instrument. In addition to the $B$-mode power spectrum, the experiment will produce high-fidelity sky maps of the southern polarized sky at 94, 150 and 280 GHz.

Compared to existing ground-based experiments dedicated to the $B$-mode signature, SPIDER observed a relatively large patch of sky. This is
Figure 3.1: Projected statistical sensitivity per multipole for the three SPIDER frequency bands after two flights. The curves for the 94 GHz and 150 GHz bands are based on measured noise levels during the first flight. Shown in black are theoretical $E$- and $B$-mode power spectra that include a primordial tensor contribution at the $r = 0.03$ level, the amplitude SPIDER is designed to constrain. Bicep2 data are those from the initial degree-scale $B$-mode detection described in Ref. [94], the uncertainty on these measurements have since been improved [22]. The shaded area shows the spread in sensitivity between the 100 and 217 GHz Planck HFI bands and serves as a comparison to the SPIDER sensitivity. The different $E$-mode power spectrum detections are described in Ref. [95–100]. When comparing the per-multipole SPIDER curves to the binned data points, the SPIDER values should be divided by the square root of the bin width for a fair comparison. Figure courtesy of A. S. Rahlin.
3.1. OVERVIEW

Figure 3.2: The sky region observed by SPIDER (green) in equatorial coordinates. The region lies in the southern hemisphere and is approximately centred on (RA, DEC) = (50°, −35°). The outlines of regions observed by three other experiments are shown, emphasising the large sky fraction observed by SPIDER. Outlines are projected over the polarization amplitude of the Commander polarized dust model [102] from Fig. 2.7 evaluated at 150 GHz. Not shown is a second 2000 deg$^2$ region, roughly centred on the star cluster RCW 38 at (RA, DEC) = (135°, −47°), that was briefly observed by SPIDER for calibration purposes. Figure courtesy of A. S. Rahlin.
illustrated in Fig. 3.2. The increased sky coverage allows measurements of
a larger number of independent degree-scale angular modes and provides
the experiment with sensitivity to $C_\ell^{BB}$ at relatively low multipole $\ell$, which
provides useful sensitivity to the polarized Galactic signal. The drawback
of the large sky patch is that the instrument’s sensitivity is diluted over a
large region. The high-altitude (36 km) observations provided by the bal-
loon platform suffer significantly less from atmospheric contamination than
ground-based observations. As a result, the SPIDER detectors have a large
instantaneous sensitivity to the CMB, comparable to detectors on a satel-
lite platform. The reduced atmospheric contamination enables the use of
less aggressive filtering of the data and allows for more efficient use of high
frequency bands like the upcoming 280 GHz band.

The preparation for the second flight is currently underway and a series
of papers describing the first flight are in preparation. In this chapter a
brief overview of the instrument is given as well as a summary of the data
analysis. An overview of the experiment is given in Ref. [103–105]. We will
briefly introduce Paper IV, which constitutes the first published result from
the SPIDER data.

3.2 The SPIDER instrument

Figure 3.3 shows the fully assembled SPIDER payload a few hours before
launch. The instrument employs six monochromatic refracting telescopes in
a single cryostat that is described [106, 107]. The telescopes are indexed as
X1 through X6; the telescopes with even index house a 94 GHz focal plane,
odd indices house the 150 GHz focal planes. Each telescope is composed of
two high-density polyethylene lenses that are cooled to 4 K. A schematic
view of one of the telescopes is given in Fig. 3.4. The objective lens has a
diameter of 290 mm. As a result, the SPIDER telescopes have an angular
resolution of about 1° for the mm-wavelength radiation of the CMB. The
SPIDER telescopes are outfitted with reflective forebaffles to reduce contam-
ination from Galactic emission or signals from the ground or balloon outside
the telescope’s roughly 20° field of view.

The lenses focus radiation onto a 300 mK focal plane that is populated
with 288 (512) polarization-sensitive detectors at 94 (150) GHz. Fig. 3.5
shows one of the 150 GHz focal planes. The detectors on each focal plane
are placed on four detector tiles. Each tile houses a square grid of either $6 \times 6$
94 GHz detector pairs or $8 \times 8$ 150 GHz detector pairs. Each detector pair
3.2. **THE SPIDER INSTRUMENT**

Figure 3.3: The fully integrated SPIDER payload just before the January 2015 Antarctic flight from McMurdo Station. The reflective baffles of each of the six telescopes, X1 to X6, can be seen extending from the vacuum vessel. The vacuum vessel and ancillary components are shielded from the (continuous) sun-light by the reflective housing. Photo courtesy of J. A. Shariff.

consists of two orthogonally polarized detectors. The detectors are antenna-coupled transition-edge sensor (TES) bolometers: polarization sensitive bolometers that are described in Ref. [108]. The 94 GHz and 150 GHz detectors do not make use of feedhorns. Instead, the beam-forming elements are arrays of slot dipole antennas that are directly lithographed into the silicon wafer, seen in Fig. 3.5, that also contains the bolometers. SPIDER serves, together with the balloon-borne EBEX experiment [109], as a testbed for the space performance of the TES detector technology for proposed $B$-mode satellite missions as LiteBIRD [110] or PICO [21].

A polarization modulator, a half-wave plate (HWP), is placed in front
Figure 3.4: Drawing of the main components (with name and operating temperature indicated) of a single SPIDER telescope. Of special interest to this work are the reflective forebaffles designed to prevent direct illumination of the vacuum window by spurious signal, the half-wave plate (HWP), designed to modulate the linearly polarized component of the sky signal, the two lenses and the focal plane. Figure courtesy of J. E. Gudmundsson.

(skywards) of the objective lens, as seen in Fig. 3.4. By rotating the HWP the polarized part of the sky signal is modulated in a controlled fashion. The HWP and the HWP rotation mechanism are described in Ref. [111] and [112] respectively. The HWPs are constructed out of a birefringent material that, for radiation of a predetermined wavelength and incidence angle, introduces a phase difference of \( \pi \) between the radiation component aligned along a direction intrinsic to the material and the orthogonal component. The HWP is placed skywards of the objective lens in order to (almost) be the first optical element; the only elements in front of the HWP are a set of filters, a vacuum window and the baffles. The HWP modulation plays an integral part in the way SPIDER reconstructs the polarized sky signal, and due its placement as the first optical element allows mitigation of spurious polarized signal from within the telescope.

The in-flight pointing of the telescope is determined by a variety of sensors [113]. During flight, three star cameras and a 3-axis gyroscope gather
3.3. DATASET AND ANALYSIS

Figure 3.5: One of the 150 GHz SPIDER focal planes. The detector pairs are visible in $8 \times 8$ grids on each of four detector tiles. The combined area of the four tiles is approximately $14 \times 14$ cm$^2$. Photo courtesy of M. A. Runyan.

data that is used to determine the post-flight pointing of the telescope.

3.3 Dataset and analysis

The 2015 flight produced a 1.56 TB dataset. The 2400 SPIDER detectors sampled the sky at a rate of 119 Hz. Before the data are used to reconstruct the sky signal several steps were taken. The low-level analysis is described in e.g. Ref. [103, 114, 115].

The first step in the analysis is the identification of glitches in the time-ordered data and flagging the contaminated periods. The SPIDER time-streams had to be corrected for a large number of spurious ‘steps’ in the average amplitude of the data. Following the low-level analysis, the noise characteristics of each detector are determined. Roughly speaking, three sources of non-white noise are identified. There is the characteristic TES $1/f$ correlated noise [108] that is roughly stationary during the flight, and two non-stationary components. The first non-stationary source is attributed to
interference between the detectors and the reaction wheel that is used to point the payload with azimuth during flight. The second source is less well understood but well correlated with the azimuth direction of the telescope. Especially the latter noise component necessitates the use of relatively aggressive filtering of the data.

After the cleaned data are filtered, the sky signal is reconstructed using a map-making approach that will be explained in more detail in the next section and Sec. 4.1.2. After reconstruction of the sky, the different angular power spectra are determined. The uncertainty in the noise modelling motivates the choice of a cross-spectrum based analysis that relies less heavily on accurate noise modelling at the expense of some statistical optimality. The cosmological analysis makes use of the \texttt{xFaster} code [116] that jointly solves for the best-fitting cosmological signal and Galactic foreground signal using the \texttt{SPIDER} data together with the \textit{Planck} data. Independently from this cross-spectrum based analysis several map-based foreground estimating methods are being explored. The analysis of the $B$-mode power spectrum is only unblinded after a range of predetermined consistency checks (null tests) are passed [114].

### 3.3.1 Reconstructing linear polarization

In order to provide context for the discussion the modelling of optical systematics in Chapters 4 and 5, we briefly discuss how \texttt{SPIDER} reconstructs the polarized signal on the sky. The HWP installed on each telescope allows \texttt{SPIDER} to use a technique that does not rely on differencing the signal from the orthogonally polarized detectors in a pair (although that option is available given the architecture of the \texttt{SPIDER} focal planes). Each of the approximately 2000 \texttt{SPIDER} detectors reconstructs both the $Q$ and $U$ parameters of the sky. The single-detector technique provides better rejection of certain systematic effects that are prone to occur with the ‘pair-differencing’ technique [117].

Given that the \texttt{SPIDER} detectors are, individually, only sensitive to a single linear polarization state, the $\psi$ dependence of Stokes $Q$ and $U$ in Eq. (2.34) has to be exploited. By rotating the instrument around $\hat{n}$, $Q$ and $U$ are modulated in a controlled fashion. The \texttt{SPIDER} scan strategy is described in Ref. [93, 113]. During its flight, \texttt{SPIDER} floats relatively close to the south pole at an average latitude of $-77^\circ$. With no possibility to rotate the telescopes about their optical axes, the position angle $\psi$, see Fig. 2.1,
describing the orientation angle of the instrument only changes by approximately 20° as the sky rotates relative to the instrument. A 20° variation is not ideal for the joint determination of $Q$ and $U$. HWP modulation is thus employed to construct information about $Q$ and $U$ on the sky.

A HWP, with its fast axis oriented with angle $\alpha$ relative to a meridian fixed on the sky, modulates the Stokes parameters $I$, $Q$, $U$ and $V$ that describe the sky signal as follows:

$$
\begin{pmatrix}
    I' \\
    Q' \\
    U' \\
    V'
\end{pmatrix} =
\begin{pmatrix}
    1 & 0 & 0 & 0 \\
    0 & \cos 4\alpha & \sin 4\alpha & 0 \\
    0 & \sin 4\alpha & -\cos 4\alpha & 0 \\
    0 & 0 & 0 & -1
\end{pmatrix}
\begin{pmatrix}
    I \\
    Q \\
    U \\
    V
\end{pmatrix}. 
$$

(3.1)

Assume for simplicity that the telescope stares at a fixed point on the sky while the HWP is rotated. Schematically, the time stream $d_t$ measured by a detector behind the HWP that is oriented to be only sensitive to incoming $Q'$ radiation is then:

$$
d_t = I'(\alpha_t) + Q'(\alpha_t),
$$

(3.2)

where $\alpha_t$ denotes the time-dependent HWP angle. By taking into account the modulation of the sky signal due to the HWP, the signal can be expressed as:

$$
d_t = I + Q \cos 4\alpha_t + U \sin 4\alpha_t.
$$

(3.3)

This represents a linear problem with three unknown parameters ($I$, $Q$ and $U$); measurements of the same point on the sky at three or more distinct HWP angles thus provide the necessary information to solve for the unknown sky signal. During the flight, eight discrete (22.5°) HWP angles are used. The HWP s are stepped through these angles once every 12 hours. The HWP angles are determined pre-flight [105].

### 3.3.2 Constraining circular polarization

In Paper IV it is described how the method for jointly determining $Q$ and $U$ from the previous section is extended to estimate the Stokes $V$ sky signal. By doing so, the first SPIDER dataset improves upon the exiting upper-limits on the Stokes $V$ sky signal. In Sec. 2.2.1, $V$ was briefly introduced; the quantity specifies circular polarization. The Thomson scattering that is
responsible for the linear polarization of the CMB does not produce a Stokes $V$ signal. There are several other mechanisms that could produce a $V$ signal that is correlated over the large angular scales that SPIDER is sensitive to, although it is not expected that the resulting signals should be observable given the SPIDER sensitivity. The $V$ analysis deviates from the main science goal of SPIDER but still relies on the main analysis pipeline, including the instrument characterisation that is presented in Chapter 5.

The polarization sensitive bolometers employed by SPIDER have no sensitivity to circular polarization. By transforming the $V$ sky signal to a spurious $Q'$ or $U'$ signal the circular polarization of the sky can be determined. The formalism presented in [118] is used. The (Mueller) matrix describing the ideal HWP in Eq. (3.1) is replaced with that of a non-ideal HWP. For $\alpha = 0$, the matrix is given by:

$$
\begin{pmatrix}
I' \\
Q' \\
U' \\
V'
\end{pmatrix} =
\begin{pmatrix}
T & \rho & 0 & 0 \\
\rho & T & 0 & 0 \\
0 & 0 & c & -s \\
0 & 0 & s & c
\end{pmatrix}
\begin{pmatrix}
I \\
Q \\
U \\
V
\end{pmatrix}.
$$

(3.4)

An ideal HWP corresponds to $T = -c = 1$ and $\rho = s = 0$. Because the HWPs are well characterised pre flight, there is evidence for a nonzero $s$ parameter for three of the six HWPs. The measured $s$ coupling is approximately 10%. Given the above expression, the nonzero $s$ parameter introduces a coupling of $V$ to $U'$ (or $V$ to $Q'$ in a rotated configuration) that is modulated as $\sin 2\alpha$ by the HWP angle $\alpha$.

The $\sin 2\alpha$ modulation of the $V$ signal is used to update the method for reconstructing the sky (the map-maker). The updated method jointy solves for $I$, $Q$, $U$ and $V$. After reconstruction of the $V$ sky signal, the angular power spectrum of $V$ is determined. It is a testament to the sensitivity of SPIDER instrument that the small $s$ coupling allows for meaningful constraints. The limits set by Paper IV improve over the previous limits on large-scale circular polarization at microwave frequencies by several orders of magnitude.
Chapter 4

Simulating Optical Systematics

4.1 Introduction

Optical systematics, spurious signals due to imperfect telescopes, are a concern for CMB $B$-mode experiments. Compared to, for instance, visible frequencies, there is a lack of suitable astrophysical calibration sources in the microwave frequency domain. As a result, a significant part of the error budget of a $B$-mode experiment is typically taken up by the uncertainty in the instrument’s sensitivity to the sky, i.e. its optical response. Through a combination of optical design, calibration and consequent corrections to the data model, the effects of optical systematics have to be controlled to acceptable levels. In light of this effort, Paper I describes the development of a numerical tool that is able to simulate realistic optical systematic signal. This main goal of this chapter is to provide background and intuition for the numerical method presented in the paper.

The main focus of the results presented in Paper I are unaccounted systematic optical effects that transform a part of the sky signal into a spurious $B$-mode signal. Such signal is especially worrisome due to the smallness of the primordial $B$-mode signal compared to the unpolarized and $E$-mode sky signal. For instance, for current inference on the tensor-to-scalar $r$ at the $r = 0.03$ level, a rough estimates of the required level of systematic control can be made by comparing amplitudes of the power
spectra in Fig. 2.4. By taking the ratio of power spectra at the relevant angular scales ($\ell \approx 80$), one can infer the required control over temperature-to-$B$ leakage and $E$-to-$B$ leakage. In terms of the power spectrum, they need to be understood at the $10^{-6}$ and $10^{-2}$ level, respectively.

The approach taken in this chapter can be illustrated with the elementary data model of a CMB experiment in matrix notation:

$$d = As + n. \quad (4.1)$$

The experiment’s time-ordered data $d$ is related to the sky signal $s$ through the linear transformation $A$. Additive noise in the time domain is represented by $n$. After the data are taken, a noisy, pixelized estimate $\hat{s}$ of the sky signal is produced by solving the inverse problem $d \mapsto \hat{s}$ in a process referred to as ‘map-making’ [119]:

$$\hat{s} = \left(A^\top N^{-1}A\right)^{-1} A^\top N^{-1} d. \quad (4.2)$$

The $N^{-1}$ matrix is the inverse of the noise autocorrelation matrix: $N \equiv \langle nn^\top \rangle$. Under the assumption that the noise $n$ is purely Gaussian with zero mean, the noise of the sky estimate $\hat{s}$ is described as a mean zero random Gaussian field described by the noise covariance matrix $N$ transformed to the pixel basis:

$$C = \left(A^\top N^{-1}A\right)^{-1}. \quad (4.3)$$

We are interested in the part of $A$ that describes how the optics of the instrument transform the sky signal before it is absorbed by the instrument’s detectors. In a regularised manner, the map-making procedure effectively undoes the transformation $A$ applied to the sky signal. From this perspective, optical systematics are caused by an incomplete description of $A$ during map-making. Uncertainties in optical calibration and numerical limitations generally force CMB analyses to employ rather crude descriptions of their instrument’s optical response. Simplified versions of $A$ are thus generally used to calculate Eq. (4.2) and Eq (4.3). To quantify the resulting bias in

---

1The estimate is noisy not just because of the additive noise component $n$ but also because the linear system in Eq. (4.1) is ill-conditioned: the transformation destroys a part of the information contained in the sky signal $s$. For example, the finite resolution of the experiment removes the signal on small angular scales, while signal on large angular scales might for example be removed by high-pass filters applied to the time-ordered data.
the inferred sky signal and the derived power spectra, our approach will be
to simulate the forward process $s \mapsto d$ as realistically as possible while using
the standard simplified map-making techniques to perform $d \mapsto \hat{s}$.

In the remainder of this introduction we will expand on the data model
in Eq. (4.1) and briefly discuss calibration schemes. In Sec. 4.2 we intro-
duce two complementairy formalisms used to describe the manipulation of
polarized light and describe how to model the optical response of a CMB
experiment. In Sec 4.3 we demonstrate how we may efficiently calculate
the process of ‘beam convolution’: the convolution of the optical response
and the sky. We then describe an implementation of this beam convolution
algorithm in Sec. 4.4 and, finally, in Sec. 4.5 we summarise the results from
Paper I.

4.1.1 Limited angular resolution

The angular resolution of a telescope is fundamentally limited by diffrac-
tion of the incoming radiation on the telescope’s aperture. To illustrate this
effect, consider a single detector in the focal point of a telescope with a
circular aperture with diameter $D$. We assume, for now, that light is de-
scribed by longitudinal (scalar) waves. In the time-reversed sense, wherein
the detector emits light of wavelength $\lambda$, the resulting diffraction pattern
at a distance $d$ (with $d \gg 2D^2/\lambda$) can be found by using the Fraunhofer
diffraction equation \[47\]. The squared absolute value of the pattern gives
the intensity of the resulting radiation as a function of angular distance $\theta$
away from the pattern centre:

$$\tilde{I}(\theta) = |E(\theta)|^2 \propto \left| \frac{J_1(ka \sin \theta)}{ka \sin \theta} \right|^2,$$

(4.4)

where $k = 2\pi/\lambda$, $a = D/2$ and $J_1$ is a Bessel function of the first kind of
order one. The intensity reaches a maximum at the centre of the pattern
($\theta = 0$) and decreases towards the first minimum at $\theta \approx 1.22\lambda/D$ in a way
that closely resembles a Gaussian fall-off. At larger angular distances, a
characteristic diffraction pattern emerges. The intensity pattern in Eq. (4.4)
is referred to as the Airy pattern. The Airy pattern and the Gaussian
approximation are plotted in Fig. 4.1.

We now introduce the optical response of the instrument by consider-
ing the reverse situation wherein the telescope scans over a point source at
distance $d$. It turns out that the signal received by the detector as func-
Figure 4.1: Airy intensity patterns from a 25 cm circular aperture for three different frequencies around 100 GHz. The dashed black line shows a Gaussian pattern fitted to the main lobe of the central frequency pattern. left—Intensity pattern as function of opening angle $\theta$, normalised to peak amplitude. right—Legendre transforms of the intensity patterns.

The optical response of the telescope to such a point source is referred to as the beam or the point spread function. As a practical measure of the resolution of the instrument one may either use the first null of the Airy pattern for the central frequency observed by the instrument or, as is more common in the CMB literature, quote the full width at half maximum (FWHM) parameter of a Gaussian function fitted to the Airy pattern. The above description does not take into account the transverse-vector-like or stochastic behaviour of radiation and neglects the fact that the effective aperture will generally not be circular for all detectors on a focal plane. Still, the resulting beam pattern in Eq. (4.4) tends to come remarkable close to a more complete description. For this reason experiments often start by approximating the detector beams as azimuthally-symmetric Gaussian.

Similar to how the sky signal is expanded in spherical harmonics in Eq. (2.21), we may expand an azimuthally-symmetric beam $\tilde{I}(\theta)$ in Legendre
polynomials $P_\ell$ [3, 120]:

$$B_\ell^I = 2\pi \int_{-1}^{1} d\cos\theta \, \tilde{I}(\theta) P_\ell(\cos\theta).$$

(4.5)

As an example, in Fig. 4.1, the Legendre coefficients of the Gaussian and Airy intensity patterns are plotted. The Legendre coefficients of the Gaussian beam with unit response to the sky are [120]:

$$B_\ell^I(\sigma) = e^{-\frac{1}{2}\ell(\ell+1)\sigma^2},$$

(4.6)

where $\sigma$ is related to the FWHM parameter as: $\sigma = \text{FWHM}/\sqrt{8\ln 2}$.

The signal received by the instrument is given by the sky signal convolved with the instrumental beam. As a convolution between two functions is equivalent to the multiplication of the harmonic representations of the functions, it is generally simpler to treat beam effects in the harmonic domain. The beam-convolved sky is described as the product of the beam and sky harmonic coefficients:

$$I_{\text{eff}}(\hat{n}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} B_\ell^I a_{I,\ell m} Y_{\ell m}(\hat{n}),$$

(4.7)

where the harmonic coefficients $a_{I,\ell m}$ of the sky intensity are given by Eq. (2.21).

The finite resolution imposed by the beam corresponds to the fact that the Legendre coefficients $B_\ell^I$ will truncate the sum over multipole order $\ell$ at some harmonic band-limit $\ell_{\text{max}}$. Sky signal on scales smaller than the corresponding angular scale does not contribute to $I_{\text{eff}}$. The $B_\ell^I$ coefficients provide a useful measure of the sensitivity of an experiment to the angular power spectrum of the CMB. To a rough approximation, the angular power spectrum $\hat{C}_{\ell,\text{eff}}^{II}$ inferred from $I_{\text{eff}}$ will be related to an unbiased estimate of the angular power spectrum $\hat{C}_{\ell}^{II}$ as:

$$\hat{C}_{\ell,\text{eff}}^{II} = (B_\ell^I)^2 \hat{C}_{\ell}^{II}.$$

(4.8)

The relation also approximately holds for the $E$- and $B$-mode power spectra. Fig. 4.2 shows the window function $(B_\ell^I)^2$ for Gaussian approximations to the beams of SPIDER (25-cm aperture), Planck (1.5-m aperture) and the Atacama Cosmology Telescope (ACT) (6-m aperture) for radiation at 150 GHz. The 25-cm apertures of the SPIDER telescopes dictate that the
instrument is only sensitive to $\ell \gtrsim 300$. Clearly, the optics are tailored towards the expected primordial $B$-mode signal; higher angular resolution is simply not needed. The 6-m aperture of the ACT allows the experiment to probe the small-scale damping tail of the CMB as well as small-scale signal from extragalactic sources that are not depicted in the figure.

### 4.1.2 Nominal data model for a CMB detector

Before introducing more complexity to the description of the optical response, it is useful to inspect the data model, i.e. $d = As$ in Eq. (4.1), appropriate for the description up to now. We consider a sky signal $s$ that consists of Stokes $I$, $Q$, and $U$. As an extension to the definition of $I_{\text{eff}}$ in Eq. (4.7) let us defined the following shorthand for $Q$ and $U$ convolved by
4.1. INTRODUCTION

the same symmetric beam:

\[(Q_{\text{eff}} + iU_{\text{eff}}) (\hat{n}) = \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} B \tilde{I}_{\ell} 2a_{\ell m} 2Y_{\ell m}(\hat{n}), \tag{4.9}\]

where \(2a_{\ell m}\) is defined in Eq. (2.45). As we will see later, the situation in which the optical response is completely determined by the \(\tilde{I}\) beam corresponds to the assumption of a purely ‘co-polarized’ beam. The time-ordered data \(d = \{d_t\}\) for an polarization-sensitive detector receiving monochromatic radiation from \(\hat{n}_t \in S^2\) is then given by \[117\]:

\[d_t = I_{\text{eff}}(\hat{n}_t) + Q_{\text{eff}}(\hat{n}_t) \cos(2\psi_t + 2\gamma) + U_{\text{eff}}(\hat{n}_t) \sin(2\psi_t + 2\gamma). \tag{4.10}\]

The angle \(\psi_t\) is the position angle that describes the (right-handed) orientation, or attitude, of the instrument about \(\hat{n}_t\) measured with respect to the southern part of the meridian passing through \(\hat{n}_t\), as illustrated in Fig. 2.1. The spin-2 nature of linear polarization is responsible for the modulation of Stokes \(Q\) and \(U\) as the orientation of the instrument \(\psi_t\) changes between time samples. The angle \(\gamma\) is the polarization angle: an instrumental parameter that is constant with time and describes the orientation of the polarization-sensitive device, e.g. antenna, coupled to the detector. The polarization angle will generally also include a contribution from the telescope optics.\(^2\)

Eq. (4.10) forms the basis for various map-making schemes \[117\], e.g. the one used for SPIDER and Planck HFI analysis \[36\]. It is important to realise that these map-making schemes do not correct for the optical response and thus produce a beam-convolved estimate of the sky signal \(I_{\text{eff}}, Q_{\text{eff}}, U_{\text{eff}}\) instead of the true sky. Assuming a discretised (pixelized) sky signal, we may express Eq. (4.10) as follows:

\[d_t = \sum_{p,i} A_{t,p,i} s_{\text{eff},p,i}, \tag{4.11}\]

where the \(p\) index runs over the pixels and where \(i \in \{1, 2, 3\}\) runs over the three beam-convolved Stokes fields: \(s_{\text{eff},p} = \{I_{\text{eff},p}, Q_{\text{eff},p}, U_{\text{eff},p}\}\). The transformation \(A\) used for Eq. (4.2) and Eq. (4.3) is then given by:

\[A_{t,p} \propto \{1, \cos(2\psi_t + 2\gamma), \sin(2\psi_t + 2\gamma)\} 1_p(t), \tag{4.12}\]

\(^2\)The addition of a rotating HWP as described in Eq. (3.3) would amount to replacing \(\gamma\) with \(\gamma + 2\alpha_t\), where \(\alpha_t\) is the HWP angle for a given time sample \(t\).
where the indicator function $1_P(t)$ is one for time samples $t$ in the set $P$ of samples that hit pixel $p$ and zero otherwise:

$$1_P(t) \equiv \begin{cases} 1 & \text{if } t \in P \\ 0 & \text{if } t \notin P \end{cases}. \quad (4.13)$$

Eq. (4.12) describes a sparse multivariate array: for each time sample $t$ only the single pixel the telescope pointed towards is considered. This ‘pencil beam approximation’ is common among map-making schemes due to its numerical efficiency but also because the resulting beam-convolved sky estimates can always be related to the true sky signal with knowledge of the beam window function and Eq. (4.7), Eq. (4.9), and Eq. (4.8). Importantly, these relations will only hold for azimuthally symmetric beams. In case of azimuthally asymmetric beams, the pencil-beam approach will produce an estimate of the sky that is biased in a non-trivial way.

### 4.1.3 Calibration of the optical response

The optical response, or beam, of an instrument has to be carefully calibrated. From the simplified data model in Eq. (4.10) it is clear that one, at minimum, will have to measure the beam harmonic modes $B_\ell^I$ and the polarization angle $\gamma$. Miscalibration of $B_\ell^I$ will directly bias the inferred angular power spectra while a miscalibrated $\gamma$ will mix $Q$ and $U$ and thus also the inferred $E$- and $B$-mode power spectra. An ideal beam-calibration source would consist of a bright, polarized point source with perfectly known properties. As a point source is perfectly localised, its harmonic modes have infinite support and may thus be used to reconstruct all harmonic modes of the beam. By performing repeated scans over such a source, one gradually reconstructs the optical response to the required sensitivity. A polarized calibration source is needed to measure the absolute polarization angle\(^3\) (more generally, the optical response to the polarized components of the sky). Beam calibration can be performed with astrophysical (or cosmological) sources, artificial sources, or, indirectly, with the use of numerical

\(^3\)Absolute calibration of the polarization angle is challenging. A common alternative approach is to ‘self-calibrate’ the polarization angle [121]. A miscalibrated polarization angle will partially convert $IE$, $EE$ and $BB$ power spectra into spurious $IB$ and $EB$ spectra. As the $\Lambda$CDM model does not allow $TB$ and $EB$ correlations, one can calibrate the polarization angle. Of course, Galactic signal [122] or new physics that does allow for $IB$ and $EB$ complicate the approach.
simulations. In reality, experiments often rely on a combination of methods. Beam calibration is not the focus of this chapter but we will briefly introduce each method.

Calibration data from a calibration source on the sky are easy to interpret as they are taken under similar conditions as the main dataset. For CMB experiments, suitable unpolarized astrophysical sources are the planets [123–126] and the moon [127]. Polarized astrophysical calibration sources are rare; the most suitable polarized source is the Crab Nebula (Tau A) which provides polarization angle measurements up to roughly $0.5^\circ$ systematic uncertainty, but is not visible from the south pole. [128–131]. The sky maps from *WMAP* and *Planck* are also used to calibrate the beams of *B*-mode polarization experiments [132]. The satellite data have a significant signal-to-noise ratio over the range of angular scales probed by the low-resolution *B*-mode experiments. Therefore, they serve as a replacement of an unpolarized point source calibrator. The full-sky coverage of the data means that the beam is calibrated on the same patch of sky that is observed for the cosmological analysis. The *WMAP* or *Planck* *Q* and *U* sky maps are generally not used to calibrate the polarized beam: the data have a lower signal-to-noise ratio compared to the temperature data, imposing a larger risk for systematic contamination.

Beam calibration by scanning over an artificial microwave source is another possibility. See Ref. [133] for an overview of methods used by different experiments. The calibration source is ideally placed in the far-field of the telescope. The far-field (Fraunhofer distance) defines the minimum distance at which a calibration source has to be placed to allow accurate reconstruction of the optical response to an astrophysical source. It is defined as the distance:

$$d_{\text{far}} = \frac{2D^2}{\lambda},$$

where $D$ is the diameter of the instrument’s aperture and $\lambda$ is the wavelength under consideration. For small-aperture telescopes such as *SPIDER*, with an aperture diameter of about 25 cm, the far-field is only about 100 m. In the case of a 5 m aperture telescope, the far-field lies at around 15 km, thus requiring a balloon, or satellite platform with a bright calibration source. Both ideas have been proposed [134, 135], but have not yet matured. Especially the $< 0.01^\circ$ accuracy in polarization angle obtainable from such platforms would be a significant improvement over the approximately $0.5^\circ$ uncertainties that are currently obtained on absolute polarization angle measure-
ments. Upcoming \( B \)-mode measurements will require uncertainty control at the \( 0.1^\circ - 0.01^\circ \) level \[136\]. In principle, a calibration source in the near-field of a telescope can still be used to reconstruct the far-field beam, but this requires sophisticated optical modelling and is not common.

Finally, the spatial response of a telescope can be simulated using numerical methods with varying degrees of sophistication. A common technique is known as ray-tracing. This technique neglects the wave-like properties of light, but the polarized nature of light can, to some extent, be included in the method. More advanced approaches incorporate material properties such as surface conduction of the modelled objects in an attempt to incorporate wave-like phenomena such as diffraction. Such approaches are usually more numerically intensive than the ray-tracing variants, but may provide more detailed information on systematics. We will make use of beam simulations of the latter type later in this chapter and in Sec 5.2.

### 4.2 The optical response

Having established the nominal data model for a CMB detector in Sec. 4.1.2, we would like to formulate a more complete model. We would like to incorporate the \( I \to P \) leakage due to beam asymmetry: a description of the beam not just in terms of an opening angle \( \theta \), but also with a dependence on the azimuthal angle \( \phi \) around the beam centre. Beam asymmetry is commonly described in terms of ‘beam ellipticity’ which implies the use of an elliptical Gaussian beam parametrisation \[56, 132\]. The elliptical Gaussian beam parametrisation is convenient, but not strictly physically motivated. With a more complete description one is able to capture other types of \( \phi \)-dependence including non-Gaussian, asymmetric shapes due to beam sidelobes. Furthermore, we aim to include the \( E \to B \) leakage due to miscalibration of the polarized beam response in a more sophisticated way than the common approach that uses the \( \bar{I} \) beam corrected with scalar correction due to the polarization angle, polarization efficiency or cross-polar components \[117\].

#### 4.2.1 Polarimetry on the sphere

Describing the optical response to polarized or partially polarized sources requires one to go beyond the scalar description of the instrumental beam, i.e. \( \bar{I} \), that was used up to now. This section summarises two formalisms used to describe the manipulation of polarized light: the Jones calculus and
4.2. THE OPTICAL RESPONSE

the Mueller calculus. See Ref. [52] for an extensive overview and Ref. [48, 53] for a more pedagogical introduction to (radio) polarimetry.

Jones formalism

The Jones vectors, introduced in Sec. 2.2.1, are of limited use as they are unable to describe partially- or unpolarized light. However, the transformations that transform Jones vectors into different Jones vectors, the Jones matrices, still play an important role in our case. The Jones matrices represent transformations or media with no stochastic behaviour. As such, the matrices are unable to transform a fully-polarized (pure) state with $I = \sqrt{Q^2 + U^2 + V^2}$ into a partially-polarized (mixed) state [48]. As telescopes are designed to work in this regime, one can generally accurately describe their optical components with Jones matrices.

Recall that the polarization state of fully-polarized radiation traveling along $\hat{n}$ through vacuum is described by the transverse vector field $\epsilon$, introduced in Eq. (2.24). A change of medium may be described as the linear map:

$$\epsilon^a \mapsto J^a_{\ b} \epsilon^b,$$

as long as the medium responds linearly on the incident electric field and is non-depolarizing, or equivalently, deterministic. $J$ is a $(1,1)$-tensor field on the sphere, i.e. transverse to $\hat{n}$, with a possible dependence on $\omega$.

The corresponding $2 \times 2$ matrix representations of $J$ in an orthonormal basis are referred to as Jones matrices. For given $\hat{n} \in S^2$, the matrix has four independent complex degrees of freedom. There is no restriction on the non-singularity of the matrix. For instance, perfect absorption is described by the zero matrix. The subset of unitary Jones matrices describe non-absorbing media that leave the radiation intensity invariant [137]. The Jones matrices are tensor fields so they transform as follows under coordinate rotations around $\hat{n}$:

$$J^a_{\ b} \mapsto R^a_{\ c} R^d_{\ b} J^c_{\ d}.$$

The representation of $R$ as a two-dimensional rotation matrix constitutes a valid Jones matrix itself. The orthogonal subset of matrices are equivalent to rotations or reflections around $\hat{n}$. 
Mueller formalism

Recall that partially or unpolarized radiation is described by the density matrix in Eq. (2.28) or, equivalently, the Stokes parameters $S^\mu = \{I, Q, U, V\}$. In the presence of a linear, deterministic medium described by a Jones matrix $J$, we may describe the corresponding transformation of the density matrix as:

$$W_{ab} \mapsto W'_{ab} = J^a_c J^d_b W_{cd}.$$  \hfill (4.17)

We can relate the density matrix to the Stokes parameters as follows:

$$S^\mu = W_{ab} \sigma^{(\mu)ab},$$ \hfill (4.18)

where $\sigma^{(\mu)}_{ab}$ with $\mu \in \{0, 1, 2, 3\}$ and $a, b \in \{1, 2\}$ are the Pauli matrices with the appropriate inserted powers of $\sin \theta$ given Eq. (2.28).\footnote{The powers of $\sin \theta$ have to be inserted to make sure that $\sigma^{(0)}_{ab} g^{ab} = 2$ and $\sigma^{(i)}_{ab} g^{ab} = 0$ still hold on the sphere with metric $g_{ab} = \text{diag}(1, \sin^2 \theta)$ and negative unit determinants: $\epsilon_{ab} \sigma^{(i)ab} = -1$. The two-dimensional Levi-Civita symbol is defined in Eq. (2.56). The order of the Pauli matrices differs from the convention used in particle physics: in terms of the particle-physics convention $\mu$ runs over $\{0,3,1,2\}$.}

Eq. (4.17) and Eq. (4.18) imply that a medium described by a Jones matrix $J$ transforms the Stokes vector as:

$$S^\mu \mapsto S'^\nu = M^\mu_\nu S^\nu,$$ \hfill (4.19)

with the Mueller-Jones matrix:

$$M^\mu_\nu = \frac{1}{2} \sigma^{(\mu)ab} j^c_a (J^*)^d_b \sigma^{(\nu)cd}.$$ \hfill (4.20)

There is a Mueller-Jones matrix for each Jones matrix $J$.

When operating on a fully polarized (or pure) signal, a Mueller-Jones transformation can be shown to leave the condition $I^2 = Q^2 + U^2 + V^2$ unchanged. Mueller-Jones matrices cannot transform fully polarized signal into partially polarized signal [48]. The reason is evident: the Mueller-Jones matrices contain the same information as the corresponding Jones matrices, the transformations describe deterministic effects that are unable to depolarize the signal. Such deterministic transformations do not involve any randomness (on top of the possible stochastic behaviour of the electric field). In contrast, a depolarizing operation does introduce another
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stochastic element. This element does not need to be truly random, e.g.
quantum random. A pseudo-depolarizing operation relies on the ignorance
of an observer with respect to a deterministic process. See Ref. [53] for some
illustrative examples.

In order to describe both non- and depolarizing transformations, we con-
sider the set of operations that describe transformations between Stokes
vectors. As we have seen, we may not naively assign 16 independent scalar
variables to each of these transformations. Strictly speaking, the set of
Stokes vectors is not a vector space. The structure is analogous to one,
but has to confirm to the restriction in Eq. (2.29). To check whether a
transformation qualifies as a Mueller operator (the Stokes criterium), one
constructs the following hermitian (2, 2) tensor field from the Mueller matrix
in question [52]:

\[ H_{ab}^{\mu \nu} = \frac{1}{4} M_{\mu \nu}^{\mu \nu} \sigma_{\mu \nu} \sigma_{\mu \nu} \cdots \cdots(4.21) \]

The ‘coherency matrix’ \( H \) represents a correlation matrix and thus has non-
negative and real eigenvalues. Physically, this corresponds to the decom-
position theorem that states that every linear optical element can be repres-
ented by, at most, four deterministic (non-depolarizing) elements [138–140].
As a result, the coherency matrix corresponding to a Mueller-Jones matrix
will only have a single unique nonzero eigenvalue, while a general Mueller
matrix can have up to four. Negative eigenvalues correspond to unphysical
transformation resulting in Stokes vectors that do not obey Eq. (2.29).

4.2.2 Optical response of incoherent receiver

We generalise the simple data model in Eq. (4.10) to one that includes a
realistic optical response. We start by imposing that the type of detectors on
the focal plane we consider are ‘incoherent’. Unlike coherent detectors that
are capable of measuring the amplitude and phase of incoming radiation,
incoherent detectors only measure the time-averaged intensity of a signal.
Let us use \( I' \) to denote the signal absorbed the detector after having been
transformed by the optics of the instrument and the polarization sensitive
device coupled to the detector. In terms of the Stokes vector of the sky
\( S \) and the time-dependent Mueller matrix of the instrument \( M_t \), we may
express the data model as [117]:

\[ d_t \propto \int_{S^2} d\Omega(\hat{n}) \, I'_t(\hat{n}), \quad (4.22) \]

\[ = \int_{S^2} d\Omega(\hat{n}) \left( M_t \right)_\mu^0(\hat{n}) \, S^\mu(\hat{n}), \quad (4.23) \]

where the constant of proportionality is overall calibration of the instrument. For convenience, we denote the elements of the row: \( (M_t)_\mu^0 \) by \( \{\tilde{I}, \tilde{Q}, \tilde{U}, \tilde{V}\} \).

By virtue of the incoherent receiver at the end of the optical chain all other elements of \( M_t \) must be zero. Note that we have neglected to include an overall integral over the electromagnetic frequency in Eq. (4.23). This is not the focus of the chapter. It should be understood that the optical response is not constant over the frequency bandpass of the instrument and thus couples differently to sources with distinct electromagnetic spectra.

Knowing the general shape of the instrument’s Mueller matrix, we may now compute the eigenvalues of the associated coherency matrix in Eq. (4.21). One may check that the resulting spectrum only contains two distinct eigenvalues. As they must be non-negative for a physical system, we obtain:

\[ \tilde{I} \pm \sqrt{\tilde{Q}^2 + \tilde{U}^2 + \tilde{V}^2} \geq 0. \quad (4.24) \]

Due to the reality of the elements of the Mueller matrix, these two conditions demand that:

\[ \tilde{I} \geq \sqrt{\tilde{Q}^2 + \tilde{U}^2 + \tilde{V}^2}. \quad (4.25) \]

Of course, this is exactly the condition needed to regard the row \( M^0_\mu \) as a valid Stokes (dual) vector. Intuitively, this is not surprising; if one considers the situation in which the detectors radiate unpolarized light, the resulting radiation in the far-field of the telescope should constitute a valid Stokes vector. See Ref. [120] for similar reasoning. We can expand the expression for the data into two more useful equations:

\[ d_t \propto \int_{S^2} d\Omega(\hat{n}) \left( \tilde{I}_t I + \tilde{Q}_t Q + \tilde{U}_t U + \tilde{V}_t V \right)(\hat{n}), \quad (4.26) \]

\[ = \int_{S^2} d\Omega(\hat{n}) \left( \tilde{I}_t I + \text{Re} \left\{ \tilde{P}_t^* P \right\} + \tilde{V}_t V \right)(\hat{n}). \quad (4.27) \]

With \( P = (Q + iU) \) and \( \tilde{P}_t = (\tilde{Q}_t + i\tilde{U}_t) \). Although the inequality in Eq. (4.25) is always saturated for non-depolarizing instrumental setup, it
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provides a sanity check (or a statistical prior) on measured Mueller matrix elements during calibration.

There exist a completely equivalent expression for the data model in the harmonic domain. It can be found by expressing the elements of the instrument’s Mueller matrix in Eq. (4.27) in terms of SWSH coefficients:

\[ b_{I}^{\ell m, t} = \int_{S^2} d\Omega(\hat{n}) \hat{I}_t(\hat{n}) Y_{\ell m}^*(\hat{n}), \quad (4.28) \]

\[ 2b_{P}^{\ell m, t} = \int_{S^2} d\Omega(\hat{n}) \hat{P}_t(\hat{n}) 2Y_{\ell m}^*(\hat{n}), \quad (4.29) \]

\[ b_{V}^{\ell m, t} = \int_{S^2} d\Omega(\hat{n}) \hat{V}_t(\hat{n}) Y_{\ell m}^*(\hat{n}). \quad (4.30) \]

Doing the same for the Stokes parameters of the sky and making use of the orthonormality of the SWSH in Eq. (2.44) allows one to rewrite Eq. (4.27) as:

\[ d_t \propto \sum_{\ell, m} \left[ (b_{I}^{\ell m, t})^* a_{\ell m}^I + \text{Re} \left\{ (2b_{P}^{\ell m, t})^* 2a_{\ell m}^P \right\} + (b_{V}^{\ell m, t})^* a_{\ell m}^V \right]. \quad (4.31) \]

4.2.3 Co- and cross-polarized beams

The general data model in Eq. (4.27) allows the polarized beam to be independent from the intensity beam as long as Eq. (4.25) is respected. However, the \( \hat{I} \) and \( \hat{P} \) beams are not independent as they are the result from the same optical system. For non-depolarizing instrumental setups, the relation between the \( \hat{I} \) and \( \hat{P} \) beams is fully described in terms of the so-called co- and cross-polarized beam components. It is often convenient to describe a beam as perfectly co-polarized. Intuitively, a linearly polarized detector with a perfectly co-polarized beam, is one that does not pick up incident linearly polarized signal in a state that is orthogonal to the polarization sensitivity of the detector. Any deviation from this behaviour is referred to as cross-polar leakage. Detectors are designed to have small amounts of cross-polar leakage, hence, the co-polarized approximation is often quite appropriate.

At the beam centre, the above explanation of co- and cross-polar components is sufficient. However, to describe co-polarization across the angular extent of the beam we need a slightly more formal definition. In terms of the Jones matrices on the sphere, a perfectly co-polarized detector corresponds
to a (rotated) perfect linear polarizer \[117\]:

\[
J \propto R(\gamma) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} R(-\gamma).
\]

(4.32)

Here, \(R\) is a rotation matrix and \(\gamma\) is the polarization angle. Clearly, the above definition is not invariant under a change of coordinates. By convention, the co- and cross-polar components are defined with respect to a particular coordinate system described in Ref. \[141\] (Ludwig's third definition) (see Fig. 4.3). In terms of the standard spherical coordinates, the unit vectors of this frame are given by:

\[
\hat{e}_{(\text{co})} = \sin(\phi) \hat{e}_\theta + \cos(\phi) \hat{e}_\phi,
\]

(4.33)

\[
\hat{e}_{(\text{cx})} = \cos(\phi) \hat{e}_\theta - \sin(\phi) \hat{e}_\phi.
\]

(4.34)

We may convert the Jones matrix \(J\) of the perfectly co-polarized detector to a Mueller-Jones matrix by using Eq. (4.20). One can check that the top row of this Mueller-Jones matrix has elements that obey:

\[
\tilde{I}_\ell(\hat{n})e^{\pm 2i\gamma} = (\tilde{Q}_\ell \pm i\tilde{U}_\ell)(\hat{n}), \quad \text{(co-pol. approx.)}
\]

(4.35)

where the subscript reminds us that the Stokes parameters are defined with respect to Ludwig's coordinate system. This illustrates why an unpolarized calibration source is sufficient to fully characterise the instrument's response (up to \(\gamma\)) if the co-polar approximation holds.

To get a more practical understanding of the above, imagine placing the centre of the beam in the positive \(\hat{z}\) direction in Fig. 4.3. Imagine that the width of the beam is small compared to the curvature of the sphere. The co-polarized approximation can then be understood as the requirement that the polarization direction of the beam is the same everywhere inside the beam. The polarization angle \(\gamma\) can then be interpreted as the rotation angle of the linearly polarized detector around the \(z\) axis.

Although Ludwig's coordinate system is convenient for purely optics related work, we have to make the connection with the sky signal defined with respect to the standard \((\theta, \phi)\) spherical coordinate system. We thus relate the Stokes parameters defined on the \((\hat{e}_{(\text{co})}, \hat{e}_{(\text{cx})})\) basis to the ones on the standard coordinate system. Clearly, the first Stokes parameter remains

\[\text{http://www.ticra.com/software/grasp/}\]. Note that the linear polarization definition in \textsc{grasp} interchanges \(\hat{e}_{(\text{co})}\) and \(\hat{e}_{(\text{cx})}\) compared to the original definition from Ref. \[141\] that we use in this document.
invariant. Using Eq. (4.33) and Eq. (4.34), one can check that the others transform as [120]:

\[
(Q \pm iU)(\hat{n}) = (\hat{Q}_L \pm i\hat{U}_L)(\hat{n})e^{\mp 2i\phi},
\]

\[
\hat{V}(\hat{n}) = -\hat{V}_L(\hat{n}).
\]

The co-polarized approximation in Eq. (4.35) can be approximated into a simple relation between the harmonic coefficients of \(\tilde{T}\): \(b_{\ell m}\), and those of the linearly polarized part of the response: \(\pm 2\hat{P}_{\ell m}\). Converting to the Ludwig grid using Eq. (4.36) and using the co-polarized approximation in Eq. (4.35)
Figure 4.4: Linearly polarized beam defined with respect to the $(\theta, \phi)$ coordinate system placed on the equator ($\theta = \pi/2$) along the $\phi = 0$ meridian. Shown is the simulated far-field response from a square-aperture pixel (detector) centred on the focal plane illuminating the two lenses and the baffles seen in Fig. 3.4. The addition of a baffle in the simulation results in the annulus-shaped sidelobe profile. The dot left from the main beam at the centre of the figure is a $4.5^\circ$ offset copy of the beam at 1% amplitude representing a ghost beam due to an internal reflection in the telescope. *top*—Total intensity $\tilde{I}$. *middle*—Absolute value of $\tilde{Q}$ component. Sourced by the co-polar component of the beam. *bottom*—Absolute value of $\tilde{U}$ component. Sourced by the cross-polar component of the beam, note the change in colour scale. Original **GRASP** output courtesy of J. E. Gudmundsson.
Figure 4.5: Zoomed-in version of Fig. 4.4, concentrating on the main beam and the 4.5° offset ghost beam. *top*—Total intensity of the beam $\tilde{I}$. *middle*—Absolute value of the $\tilde{Q}$ component. *bottom*—Absolute value of the $\tilde{U}$ component, note the change in colour scale. The ghost beam has been given a significant cross-polarized component compared to the main beam, resulting in a relatively prominent $\tilde{U}$ ghost beam. Original GRASP output courtesy of J. E. Gudmundsson.
yields:
\[ \pm 2 b_{\ell m}^P = e^{\pm 2i \gamma} \int_{S^2} d\Omega(\hat{n}) \, \hat{I}(\hat{n}) e^{\pm 2i \phi} \pm 2 Y^*_{\ell m}(x) , \]  
(4.38)

where we neglect to write the \( L \) subscript of \( \hat{I} \) since it is coordinate-invariant. Expressing the above as a convolution in the harmonic domain yields the following expression:
\[ \pm 2 b_{\ell m}^P = e^{\pm 2i \gamma} \sum_{\ell'} b_{\ell'(m\pm 2)}^I K_{\ell,\ell',m} , \]  
(4.39)

in terms of a harmonic kernel \( K \). As as long as the beam is relatively localised on the sphere the kernel can be approximated as diagonal per azimuthal mode \( m \) \cite{142}, resulting in:
\[ \pm 2 b_{\ell m}^P \approx e^{\pm 2i \gamma} b_{\ell (m\pm 2)}^I . \]  
(4.40)

A realistic beam is plotted in Fig. 4.4 and 4.5. Shown are the \( \hat{I}, \hat{Q}, \) and \( \hat{U} \) components defined relative to the standard \((\theta, \phi)\) coordinates. In Appendix B of Paper I it is described how to convert the output of an optical simulation to such Stokes fields. Here we give a brief summary. The optical simulation outputs a vector field on the sphere defined with respect to \( \hat{e}_{(co)} \) and \( \hat{e}_{(cx)} \). The components of the vector field can be related to the elements of a Jones vector that represents the (non-depolarizing) beam. The Jones matrix is then converted to a Mueller-Jones matrix using Eq. (4.20). The elements in the top row of that matrix are the \( \hat{I}_L, \hat{Q}_L, \hat{U}_L \) and \( \hat{V}_L \) elements of the beam. Using Eq. (4.36) and Eq. (4.37) the Stokes parameters are then transformed to the \((\theta, \phi)\) coordinate system. As the beams are centred on the north pole of the sphere, the \( \exp(\mp 2i \phi) \) terms in the conversion for \( \hat{Q} \) and \( \hat{U} \) results in a ‘clover-leaf’ pattern aligned with \( \phi = 0 \) in \( \hat{Q} \) and a similar pattern rotated by 45° in \( \hat{U} \). To obtain Fig 4.4 and 4.5, the beams are then rotated along the \( \phi = 0 \) meridian towards the equator; the beams lose their clover-leaf shape. The resulting \( \hat{Q} \) field is sourced by the co-polarized component of the original vector field while \( \hat{U} \) is sourced by the cross-polarized component. The beams in Fig 4.4 are produced by a detector polarized in the \( \hat{e}_{co} \) direction. The faint, but nonzero \( \hat{U} \) field (as well as a faint \( \hat{V} \) field that is not shown) is thus the result of non-idealities in the telescope.
4.3 Beam convolution

As mentioned in the introduction, we aim to simulate the beam convolution operation in Eq. (4.27) as faithfully as possible in order to ‘forward propagate’ optical systematics into simulated time-ordered data. Ideally, we would like to use realistic optical simulations or calibration measurements of the instrumental beam in this process without any ad hoc simplifications.

4.3.1 Overview of methods

Beam convolution is numerically challenging primarily due to the azimuthal asymmetry of realistic beams. Roughly speaking, there are three approaches to convolution with azimuthally asymmetric beams:

Pixel-domain convolution This method describes the effects on the time-ordered data by calculating the beam convolution directly on pixelized sky maps. One notable example is the FEBeCoP code [145], that was also used in the Planck analysis [146, 147]. Essentially, the method directly calculates Eq. (4.27). To do so, one truncates the angular extent of the assumed beam and precomputes the ‘effective beam’ per pixel on the sky. The effective beam is a weighted average of all beam orientations that hit the pixel. Computing the effective beams is numerically intensive, but once precomputed and stored, the convolution operation is relatively fast as the actual convolution operation only has to be done once per pixel and not per time-sample. As a result, the main use of the method is to quickly convolve different sky realisations with the same beam, e.g. in a Monte Carlo analysis approach. Unlike the two methods below, the effective-beam method may account for the apparent elongation of the beams in the scanning direction due to the finite detector time-response and other time-varying beam effects. The method is not well suited to describe off-axis sidelobes due to the required angular truncation of the beam.

Power spectrum based Codes that directly simulate the effects of optical systematics on the inferred power spectra of the sky. The main example is quickpol [142], but see also [148]. quickpol was developed

\textsuperscript{6}In Paper I it is argued why this approach is taken over the opposite approach in which the beam is deconvolved during the map-making stage [143, 144].
for and used in the *Planck* analysis [147]. It expands on the analytic description of the effects of asymmetric beams on the pseudo-$C_\ell$ statistic [149, 150] as formulated by e.g. [151]. Roughly speaking, the method works by (analytically) inserting the expression for the beam-convolved time-ordered data in Eq. (4.31) into the standard mapmaking equation [117]. The resulting expression is used to directly calculate the mixing of the $II$, $EE$, $BB$, $IB$ and $EB$ angular power spectra. The method is numerically efficient due to its analytic nature. However, as the method works in the power spectrum domain, it is unable to describe the systematic effects on the time-ordered data or the sky maps produced by an experiment.

Harmonic-domain convolution This method describes the effects on the time-ordered data by calculating the beam convolution in the harmonic domain [120, 152]. The main implementations are the `conviqt` code [153] and the `totalconvolver` code [154]. Both codes have seen use in the *Planck* analysis [147, 155]. The `conviqt` code has been used for various forecasting efforts, e.g. [156]. The method is well-suited to handle beams that possess an approximate azimuthal symmetry around the beam centre. Including off-axis sidelobes comes with no numerical penalty as long as they do not break the approximate symmetry. In many ways this method and the previous pixel-based method are optimal in opposite regimes (diffuse versus localised beams), as one would expect from a comparison between coordinate- and Fourier space methods.

We will describe the third method as it seems the most natural method for $B$-mode experiments. An important goal is to quantify the potential bias of sidelobe signal on the (map domain-based) foreground cleaning/component separation efforts. The combination of far-sidelobes and map-based analysis already drives us away from the first two methods mentioned above. The relatively symmetric and low resolution beams of $B$-mode experiments make the harmonic (Fourier) approach particularly well-suited. Furthermore, by using a time-domain method instead of the power spectrum based method, incorporating time-domain filtering operations to the simulations is straightforward. The forward-propagated, beam-convolved data are simply passed to the standard analysis pipeline to correctly apply the same transformations that the real data are subjected to.
4.3.2 Beam convolution in the harmonic domain

In Eq. (4.27), the data model is expressed in terms of a constant sky signal and a time-varying instrumental response that reflects the telescope scanning the sky. At first sight, evaluation of the data model requires an integral over sphere per time sample. An enormous leap in computational efficiency can be made by making use of the fact that the intrinsic properties of the beam are independent of time. This means that in a coordinate frame fixed to the telescope, the instrumental response does not change between time samples. We may exploit this by formulating the appropriate basis transformation, as detailed in [120, 152, 157], such that we may interpret the data as a convolution of a constant beam and sky signal.

We now impose that the optical response at a time sample $t$ and a later time sample $t'$ are related by a rotation of the telescope. As a result, the SWSH coefficients of the beam transform among themselves as Eq. (2.47) under a coordinate rotation $g^{-1} \in SO(3)$. We may thus compute the harmonic coefficients of the beam in some fiducial reference frame, and use Eq. (2.47) to transform them between samples:

$$d_t \propto \sum_{\ell,m,s} \left[ b_{\ell s}^{I} a_{\ell m}^{I} + \frac{1}{2} \left\{ -2b_{\ell s}^{P} 2a_{\ell m}^{P} + 2b_{\ell s}^{P} - 2a_{\ell m}^{P} \right\} + b_{\ell s}^{V} a_{\ell m}^{V} \right] \times (-1)^m D_{-m}^{\ell} (g_t), \quad (4.41)$$

where $-2b_{\ell s}^{P} = (2b_{\ell s}^{P})*(-1)^s$. Using the relation between the Wigner $D$-matrices and the spin-weighted spherical harmonics on the standard spherical basis from Eq. (2.43), we arrive at the final expression:

$$d_t \propto \sum_{\ell,m,s} \left[ b_{\ell s}^{I} a_{\ell m}^{I} + \frac{1}{2} \left\{ -2b_{\ell s}^{P} 2a_{\ell m}^{P} + 2b_{\ell s}^{P} - 2a_{\ell m}^{P} \right\} + b_{\ell s}^{V} a_{\ell m}^{V} \right] \times q_{\ell} e^{-i\psi_s} Y_{\ell m}(\hat{n}_t), \quad (4.42)$$

where $(\psi_t, \theta_t, \phi_t)$ are the Euler angles in Fig. 2.1 that describe the rotation $g_t$. We used the following shorthand:

$$q_{\ell} \equiv \sqrt{\frac{4\pi}{2\ell + 1}}. \quad (4.43)$$

We take a moment to consider the benefit of using Eq. (4.42) over the expressions in Eq. (4.27) or Eq. (4.31). By having factored the optical
response into a constant and time-varying piece, we have the outline for an efficient beam-convolution algorithm. One first calculates the following quantities:

\[ I_{\text{conv},s}(\hat{n}) = \sum_{\ell,m} b_{\ell s}^I \ell a_{\ell m} \ell g_{\ell s} Y_{\ell m}(\hat{n}) \quad \forall s \in \{0, \ldots, s_{\text{max}}\}, \]  
\[ P_{\text{conv},s}(\hat{n}) = \frac{1}{2} \sum_{\ell,m} \left\{ -2 b_{\ell s}^P 2a_{\ell m}^P + 2 b_{\ell s}^P - 2 a_{\ell m}^P \right\} q_{\ell s} Y_{\ell m}(\hat{n}) \quad \forall s \in \{-s_{\text{max}}, \ldots, s_{\text{max}}\}, \]  
\[ V_{\text{conv},s}(\hat{n}) = \sum_{\ell,m} b_{\ell s}^V \ell a_{\ell m} \ell g_{\ell s} Y_{\ell m}(\hat{n}) \quad \forall s \in \{0, \ldots, s_{\text{max}}\}. \]

The required computations will (asymptotically) scale as \( O(\ell_{\text{max}}^3 s_{\text{max}}) \). This is due to the \( O(\ell_{\text{max}}^3) \) scaling of the algorithms used to compute the SWSHs for each value of \( s \) [61, 158]. The \( s_{\text{max}} \) band-limit refers to the value of \(|s|\) above which the beam coefficients become zero. It can be understood as the highest frequency harmonic mode in the \( \phi \) direction required to describe the beam. The maximum value of \( s \) is given by \( \ell_{\text{max}} \), but is typically significantly lower. For instance, an azimuthally-symmetric beam can be described using only \( s = 0 \) modes when placed on the north pole of the standard spherical basis. Small deviations from the symmetric case will generally only significantly excite low \( s \) modes [142, 151]. After the \( I_{\text{conv},s}, P_{\text{conv},s} \) and \( V_{\text{conv},s} \) maps have been computed for the required values of \( s \), the pointing information in the form of \( \hat{n}_t \) and \( \psi_t \) is used to create the time-ordered data (TOD) \( d_t \) by sampling or interpolating from the pixels and modulating the time sample by the appropriate factor of \( \exp(-is\psi_t) \).

As an example of how the algorithm handles an (exaggerated) asymmetric beam, we take the beam depicted in Fig. 4.4 and 4.5 and increase the amplitude of the ghost beam to equal that of the main beam. This creates a highly asymmetric beam. When centred on the north pole of the (\( \theta, \phi \)) coordinate system the corresponding harmonic coefficients will have their power distributed over the \( s \) modes. This is demonstrated in Fig. 4.6 for the case.

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7This is normally not how one should incorporate ghost beams, the proper way is described in Paper I.
Figure 4.6: Absolute value of the spherical harmonic coefficients of the intensity beam in Fig. 4.4 and 4.5 but with a ghost beam with the same amplitude as the main beam in order to exaggerate the effect of beam asymmetry. Shown are the absolute values of the first five azimuthal modes. A symmetric beam would only have a nonzero $s = 0$ mode.

Figure 4.7: Random realisation of the CMB temperature field with spatial correlations as predicted by the best-fitting $\Lambda$CDM model. The map represents the sky before beam convolution is performed. Note that only a $50^\circ \times 50^\circ$ patch is depicted here, but that the full-sky map is used for the beam convolution.
Figure 4.8: The CMB temperature map from Fig. 4.7 convolved with the $s = 1, 2, 3$ azimuthal modes of the asymmetric beam shown in Fig. 4.4. 

*left*—Real part.  
*right*—Imaginary part.  
*top to bottom*—Contribution from the $s = 1, 2, 3$ azimuthal modes of the beam.
4.4. CODE IMPLEMENTATION

intensity beam. We then compute the $I_{\text{conv}, s}$ maps using the harmonic coefficients in Fig. 4.6 and the temperature map Fig. 4.7 as input. The resulting $I_{\text{conv}, s}$ maps are shown for $s = 1, 2, 3$ in Fig. 4.8. Comparing the maps for $s = 2$ with the two $Q$ fields in Fig. 2.2 provides a nice illustration why the $s = 2$ modes of the beam are responsible for $I \rightarrow P$ leakage and how the real and imaginary parts of $b_{\ell s}^I$ are responsible for $I \rightarrow E$ and $I \rightarrow B$ leakage respectively [56, 159].

As a sanity check, we combine the co-polarized approximation with the assumption that the optical response is azimuthally symmetric to demonstrate that the full expression for the beam-convolved TOD reduces to the nominal model in Eq. (4.10). We start by inserting the co-polarized approximation from Eq. (4.40) into Eq. (4.42):

$$d_t \propto \sum_{\ell, m, s} \left[ b_{\ell s}^I a_{\ell m}^I \frac{1}{2} \left\{ b_{\ell (s-2)}^I 2a_{\ell m}^P e^{-2i\gamma} + b_{\ell (s+2)}^I -2a_{\ell m}^P e^{2i\gamma} \right\} \right] \times q_\ell e^{-is\psi_t} Y_{\ell m}(\hat{n}_t).$$

(4.46)

The assumed azimuthal symmetry of the beam means that only $b_{\ell 0}^I$ is nonzero. Performing the sum over $s$ thus simplifies the expression to:

$$d_t \propto \sum_{\ell, m} \left[ b_{\ell 0}^I a_{\ell m}^P q_\ell Y_{\ell m}(\hat{n}_t) + \text{Re} \left( b_{\ell 0}^I 2a_{\ell m}^P q_\ell 2 Y_{\ell m}(\hat{n}_t)e^{-2i(\psi_t+\gamma)} \right) \right].$$

(4.47)

One may insert the shorthands $I_{\text{eff}}, Q_{\text{eff}},$ and $U_{\text{eff}}$ defined in Eq. (4.7) and Eq. (4.9) while noting that the Legendre coefficients of the beam are related to the spherical harmonic coefficients as:

$$B_{\ell}^I = \sqrt{\frac{4\pi}{2\ell + 1}} b_{\ell 0}^I = q_\ell b_{\ell 0}^I.$$

(4.48)

By doing so, it can be verified that the expression indeed reduces to the desired form in Eq. (4.10).

4.4 Code implementation

The beam-convolution algorithm based on Eq. (4.42) is implemented in the form of beamconv: a lightweight open source python package. The primary

https://github.com/AdriJD/beamconv
purpose of the code is to compute time-ordered data that include contributions from optical non-idealities such as asymmetric and cross-polarized beams. The `beamconv` code is described in Paper I. We provide a summary here.

The `beamconv` code was initially developed to quantify optical systematics for the SPIDER experiment. The code was designed as a lightweight addition to the experiment’s analysis pipeline. The code now exist independently from the SPIDER codebase. An important reason for the development of a dedicated code package was the lack of a publicly available beam-convolution algorithm. Although the publicly-available Toast code\(^9\) was able to perform such calculations, it relied on a precompiled version of the conviqt code. Furthermore, the Toast framework was not easily adaptable to the SPIDER analysis pipeline. It should be noted that since the development of the `beamconv` code, a publicly available version of the conviqt code has been released.\(^10\)

The code requires three types of input: a scan strategy for the telescope, the beams of a number of detectors and an input sky. As the beam convolution is performed in the harmonic domain, the user needs to provide the spin-weighted spherical harmonic (SWSH) coefficients of both the sky and the beams. The SWSH coefficients of the beams may correspond to independent \(\bar{I}, \bar{Q}\) and \(\bar{U}\) beams. Nonzero \(\bar{V}\) is currently not supported. The beam convolution described by Eq. (4.42) is evaluated in several steps. First, using the SWSH coefficients of the beam and sky, the quantities in Eq. (4.44) and Eq. (4.45) are computed for the user-specified number of azimuthal modes of the beam. For all beams considered in this thesis \(s_{\text{max}} = 4\) is sufficient. The required inverse SWSH transformations are done by the highly optimised libsharp library [158] that is part of the healpy\(^11\) library. The beam-convolved TOD are obtained by combining the boresight pointing with the detector pointing offsets and possible instrument rotation. The polarization angle can be included in the beam coefficients following Eq. (4.40). With the pointing \(\hat{n}_t\) and \(\psi_t\) specified, the TOD are either sampled directly from the standard HEALPix [49] pixels or after bi-linear interpolation of the pixel values. To calculate the final TOD, each time sample is modulated by the appropriate phase, i.e. \(\exp(is\psi_t)\) or \(\exp(is\psi_t + 4i\alpha_t)\) when HWP modulation is included. Both continuously spinning HWP modulation and

\(^9\)http://hpc4cmb.github.io/toast/
\(^10\)https://github.com/hpc4cmb/libconviqt
\(^11\)https://github.com/healpy
stepped modulation is possible. The boresight pointing data can either be computed in realtime by the code using one of a few implemented scanning models, or loaded from an external file or function. All pointing-related operations are handled by the external qpoint\textsuperscript{12} code using quaternion algebra to efficiently calculate pointing-related rotations in real-time. The generated T0D can be binned into a sky map using a pencil-beam map-maker provided by qpoint.

The python package includes a suite of unit tests, example scripts and notebooks. No comparisons between the code and the conviqt code have been made at this point, but the beamconv package includes a number of internal consistency checks. The code has also been tested against the main SPIDER analysis pipeline. Besides healpy and qpoint, the code only depends on the standard Numpy and Matplotlib python packages. The main code consists of about 4000 python lines. Parallel computations are supported through the Message Passing Interface (MPI) protocol. Given multiple processors, the code will distribute the computational load related to the boresight pointing calculations and will assign a subset of the detectors to each processor. Although the code is written in python, all performance critical parts are performed by calling fast compiled code in the external libsharp or qpoint libraries or in the standard numpy routines. The serial performance of the code seems to be consistent with published results obtained with the conviqt code\textsuperscript{[153]}. Paper I includes a more detailed benchmark. As an indication of actual use: the realistic year-long datasets with 200 detectors described in Paper I are computed in a $O(1)$ hour on a node with 72 Xeon E5-2697 v2 processors clocked at 2.7 GHz. For small-aperture experiments such as the instrument considered in Paper I or SPIDER, $\ell_{\text{max}}$ is low enough such that the $O(\ell_{\text{max}}^2 s_{\text{max}})$ part of the algorithm does not dominate the overall computation time.

## 4.5 Satellite test-case

In this section we summarise the results of Paper I. Besides introducing the beamconv code, the paper considers a hypothetical CMB satellite experiment designed to constrain the primordial $B$-mode signal on degree-angular scales. The experiment uses a two-lens refracting telescope design that is comparable to telescope designs used by dedicated $B$-mode experiments.

\textsuperscript{12}https://github.com/arahlin/qpoint
The hypothetical satellite mission serves as a proof of concept; the beamconv code is used to simulate full-sized datasets. Additionally, the setup allows the investigation of several relatively unexplored types of optical systematics.

Several possibilities for the optical response of the instrument are explored. One of the choices involves realistic beams that are calculated for each detector using numerical simulations of the optical system. The beamconv code is used to simulate year-long datasets for 200 detector pairs for each choice of optical response. The resulting data are binned on the sphere using a pencil-beam map-making approach that does not take the beam into account (see Sec. 4.1.2). As the beam is not corrected for, spurious systematic signal is thus injected into the maps. The systematic $B$-mode signal is estimated for each choice of the optical response by calculating the $B$-mode angular power spectrum.

It is found that an elliptical Gaussian parameterisation of the (per-detector) beam results in a significant underestimation of the systematic $B$-mode signal on degree-angular scales. The fact that this holds true even for the simple telescope design used in this work implies that the elliptical Gaussian parameterisation should be used with caution for more involved optical systems. A range of systematic effects that cause $E$-mode-to-$B$-mode leakage is explored; it is found that these effects are under control for the telescope design. Even with a conservative sidelobe model, there is significant sidelobe coupling to polarized foregrounds near the Galactic plane. This is the largest systematic effect in our study. It emphasises the need for sidelobe characterisation and the importance of including the Galaxy in simulations. We expect that the sidelobe-induced bias will be significantly worse when the frequency dependences of the sidelobe and Galactic signal are taken into account. Overall, the systematic residuals are relatively small. It is expected that some of this is due to the idealised model for the, already simple, instrument.
Chapter 5

Data Analysis for SPIDER

In this chapter a part of the analysis of the first SPIDER dataset is described. In Sec. 5.1, the characterisation of the instrument with flight data is reported. The main focus is the determination of the pointing offset for each of the approximately 2000 SPIDER detectors. In Sec. 5.2 it is described how the systematic effects of certain expected optical non-idealities are modelled and an assessment of their impact on the main science case is made.

5.1 Instrument characterisation

In this section we focus on those aspects of the instrument characterisation that were done using the flight data, the data gathered during SPIDER’s first flight. In general, the majority of the instrument characterisation is performed before the actual flight. For SPIDER, the HWP properties and detector polarization angles are examples of instrumental parameters that were determined pre flight [105]. However, for particular aspects of the characterisation, the use of flight data is ideal. We will cover the three main instrumental properties that were determined after the flight: the detector pointing offsets, the detector calibration and the beam transfer functions. The post-flight analysis relies heavily on the publicly available Planck HFI temperature sky maps as a calibration source. The similarity between the frequency bandpasses of the 100 and 143 GHz Planck HFI bands and the 94 and 150 GHz SPIDER bands allows for (almost) direct comparisons.

In term of the optical response, the HFI data are a rather natural calibra-
tion source. The apertures of the SPIDER telescopes are significantly smaller than that of the Planck instrument (~25 cm versus ~1.5 m); residual optical systematic effects in the HFI data are therefore expected at smaller angular scales than those relevant for the characterisation of the SPIDER telescopes. See the discussion on optical calibration in Sec. 4.1.3.\footnote{Note that a comparable calibration scheme has been successfully used for the BICEP2 and Keck Array instruments [132], both of which have telescopes that are comparable to the SPIDER telescopes.}

### 5.1.1 Detector pointing offsets

In this section we describe the characterisation of the detector pointing offsets, or ‘centroids’ for SPIDER. Roughly speaking, the pointing offsets quantify the direction of incoming light before it is focussed onto a particular detector, i.e. the direction a detector ‘points’ towards. The offsets are measured relative to the direction the telescope points to as a whole. Miscalibrated pointing offsets result in $I \rightarrow P$ leakage. As an example of the effect, the closely related ‘differential pointing’ systematic was determined to be the main source of $I \rightarrow P$ leakage in the BICEP2/Keck Array analysis [132, 160]. By its design, SPIDER is less susceptible to pointing offset systematics, but the analysis still requires accurately determined offset values.

We explore how comparing the SPIDER CMB data to the Planck HFI data can improve the calibration of the detector pointing offsets. Three different approaches are presented; the same results are reached regardless of the method. Before this effort, the analysis pipeline relied on pointing offsets derived from the observations of the RCW 38 star-forming region. Although the (sub-degree) uncertainty on the inferred offsets constituted a significant improvement over the accuracy of pre-flight measurements, the RCW 38 data provides limited statistical power. SPIDER obtains its most sensitive measurements in its main CMB sky region. Given that the cosmological analysis would benefit from more accurate pointing offsets, these data are explored. We indeed see a strong improvement in accuracy with the CMB data. We comment on the advantages and disadvantages of each of the three presented methods.
Systematic errors due to miscalibrated pointing offsets

The pointing offset quantifies the angular distance between the detector’s beam centre and the boresight. For SPIDER, the boresight simply refers to a vector pointing at the sky along the symmetry axis of the telescope. The pointing offsets are a consequence of the optics: a detector in the centre of the focal plane (in line with the symmetry axis) has no pointing offset, while a detector on the edge of the focal plane has a large offset. See Fig. 5.1 for an example: only horizontal incoming rays converge in the centre of the focal plane. For a SPIDER telescope, the beams of detectors in the corners of the focal plane are offset by approximately $10^\circ$. The conversion factor between length on the focal plane and angular separation on the sky: the plate scale, is approximately $0.098^\circ \text{mm}^{-1}$. This means that the approximate $14 \times 14 \text{ cm}^2$ area of the focal planes correspond to fields-of-view of about $14^\circ \times 14^\circ$. A rough indication of the detector offsets can thus be made using the location of the detectors on the focal plane.

![Figure 5.1: A (to scale) schematic depiction of the two-lens refractive optical configuration used for SPIDER, demonstrating the relative simplicity of the system. The coloured lines are ray-traced representations of the reciprocal light path of several detectors on the focal plane (left side). It is clear how sets of parallel incoming rays focus on different locations on the focal plane, or, put differently, different detectors on the focal plane are sensitive to different parts of the sky. Figure courtesy of J. E. Gudmundsson.](image)

Any deviation from a detector’s true pointing offset will distort the reconstruction of the sky and introduce $I \rightarrow P$ leakage. Heuristically, the fact that this leakage occurs can be understood by going back to Sec. 4.3.2. There it was illustrated how $I \rightarrow P$ leakage is introduced when beam asymmetry is ignored during the map-making stage. A miscalibrated pointing
offset can be completely understood in terms of a beam asymmetry. For instance, consider an intrinsically azimuthally symmetric $\tilde{I}$ beam that is placed on the north pole. Such a beam only has $m = 0$ spherical harmonic coefficients and will therefore not produce $I \rightarrow P$ leakage. An error in the pointing offset is then understood as a small rotation away from the north pole. The rotated beam will gain a dependence on $\phi$. To formulate this in a more formal way, we may use Eq. (2.47) to describe the spherical harmonic coefficients of the beam after the rotation: the original, unprimed, coefficients change as follows under a rotation $g \in SO(3)$ of the beam itself:

$$b_{\ell m}^\tilde{I} \rightarrow b_{\ell m}' = \sum_{m=-\ell}^{\ell} b_{\ell m}^\tilde{I} D_{\ell m}(g).$$  \hspace{1cm} (5.1)

The beam function thus receives a contribution from $m \neq 0$ modes after the rotation.

In Paper I it is demonstrated how $m \neq 0$ modes of the $\tilde{I}$ beam result in leakage when not accounted for. Leakage due to the $m \neq \pm 2$ modes will be suppressed by sky- or instrument rotation with a map-making approach like SPIDER uses. HWP modulation will suppress $I \rightarrow P$ leakage from all $m$ modes. The same does not apply exactly to a pair-differencing map-maker as for example used by the Bicep2/Keck Array analysis. In these cases, differential pointing, i.e. a difference in the detector offset between the two detectors in a pair, will introduce $I \rightarrow P$ leakage that is not suppressed by sky- or instrument rotation. Detector pointing offsets become crucial instrumental parameter in these cases. This is reflected in the analysis of the Bicep2/Keck Array instruments. The bulk of the $I \rightarrow P$ leakage is due to differential pointing [132, 160]. Because the SPIDER analysis does not use a pair-differencing map-maker and incorporates HWP modulation, there is slightly less worry about detector pointing offsets.

### Map-based analysis

In the map-based approach, SPIDER data are binned on the sphere using different choices for the detector offsets.\(^2\) The resulting maps are directly

\(^2\)The choice for a map-domain analysis might seem odd. Due to the equivalence between detector offset errors and beam asymmetry, an analysis in the time domain should be statistically optimal. During map-making, the unique feature of a beam asymmetry (the $\psi$-dependence) is averaged over and thus suppressed. In the presence of a uniform sampling of $\psi$, due to e.g. sky rotation, the systematic effects from detector offsets on the
compared to an estimate of the sky signal given by the Planck HFI data. More specifically, we use the publicly available 100 and 143 GHz full-mission sky maps from the 2015 data release. The analysis does not rely on $Q$ or $U$ data in order to avoid a dependence on the HFI polarization data. The derived pointing offsets for the intensity beams should closely match those for the polarized beams, so an intensity-only analysis is expected to be sufficient.

A simple map-making scheme is used. The algorithm completely neglects the $\psi$-dependence in the data model and thus only solves for the intensity $I$. Besides the fact that $Q$ and $U$ estimates are not needed, the main argument for an $I$-only map-maker is the use of sky regions that would be too poorly conditioned for a full polarization solution. This is a rather important consideration for single-detector data; for data taken over short time scales (shorter than the 12-hour HWP periods, see Sec. 3.2) or for data that are heavily flagged, there might not be a joint $I, Q, U$ solution.\footnote{In general, data that are poorly conditioned for the polarized map-making solution include the most suitable data for this analysis: it requires data with an almost constant $\psi$ sampling.} Besides neglecting polarization, the map-maker and time-domain processing are identical to the default analysis.

We may formally phrase the search for the detector offsets as a Bayesian inference problem. We are interested in the posterior distribution of the two angles that determine the detector offset: $\Theta = \{\delta_{\text{az}}, \delta_{\text{el}}\}$, defined in local azimuth and elevation relative to the boresight. Using Bayes’ theorem, we may express the posterior in terms of the likelihood $\Pr(d|\Theta)$ and prior $\Pr(\Theta)$ as follows:

$$\Pr(\Theta|d) = \frac{\Pr(d|\Theta)\Pr(\Theta)}{\Pr(d)}.$$ 

(5.2)

As we are only interested in the relative probability of different parameters here, we neglect the ‘evidence’ $\Pr(d)$ and replace the equal sign in the above with a proportionality sign.

As a prior on the detector offset, we use a 2-dimensional uniform distribution over a $10 \times 10$ arcmin$^2$ section of the $\delta_{\text{az}} \times \delta_{\text{el}}$ parameter space map are degenerate with an isotropic smoothing. However, as the effects of sky-rotation are relatively minor for SPIDER\footnote{\cite{92}}, this degeneracy is largely absent. The actual reason for choosing a map-based approach over a time-domain approach came from the idea that the noise covariance would behave better after map-making. The results from the time domain analysis below seem to disprove this idea, but in any case, a map-based approach was first explored.
that is centred on the old value of the offset. We expect relatively small (few arcmin) deviations from the old offset values, so this prior range quantifies that belief. It is verified that broadening the uniform distribution does not change the results. With the prior distribution specified, we may now characterise the shape of the posterior distribution by sampling from the likelihood of the data. Due to the low dimensionality of the model, we do not require a specialised sampling technique, e.g. a Markov Chain Monte Carlo (MCMC) method; we perform a brute-force exploration of the parameter space. We divide the $10 \times 10$ arcmin$^2$ parameter space allowed by the prior into 121 discrete samples and evaluate the likelihood for each sample.

The model for the likelihood considers all SPIDER detectors as independent. The noise level in the full-mission Planck maps is negligible compared to that of a single SPIDER detector, so we only model the SPIDER noise. Under the assumption that the noise is Gaussian distributed, the joint log likelihood for the $n_{\text{pix}}$ pixels of the binned data $\hat{I} = \{\hat{I}_1, \hat{I}_2, \ldots, \hat{I}_{n_{\text{pix}}}\}$ from a single detector with pointing offsets $\Theta = \{\delta_{\text{az}}, \delta_{\text{el}}\}$ is given by:

$$
\log \Pr(\hat{I}|\Theta) = -\frac{1}{2} \sum_{i,j=1}^{n_{\text{pix}}} \left( \hat{I}(\Theta) - \bar{I} \right)_i C_{N,i,j}^{-1}(\Theta) \left( \hat{I}(\Theta) - \bar{I} \right)_j - \log \left[ (2\pi)^{n_{\text{pix}}/2} \sqrt{\det C_N(\Theta)} \right].
$$

(5.3)

Here, $I$ represents an HFI map that is reprocessed identically to the data, i.e. including the same filtering and flagging. Before processing, the HFI maps are convolved with the best-fitting Gaussian beam window function derived for the specific SPIDER detector (see Sec. 5.1.2); the appropriate Planck beam is deconvolved. $C_N(\Theta)$ and $C_N^{-1}(\Theta)$ are the $n_{\text{pix}} \times n_{\text{pix}}$ noise covariance matrix and its inverse. They describe the statistical properties of the detector noise after the binning process, so they depend on the detector pointing offsets.

We now make some assumptions that simplify Eq. (5.5) significantly. The pixel-pixel noise covariance matrix $C_N$ is assumed to be independent between pixels and thus becomes diagonal. As mentioned in Sec. 3.3, this

---

4 The detector offsets are used when the time streams are sampled from the HFI maps, but they are again used when the data are binned on the sphere to form $I$. The dependence on $\delta_{\text{az}}$ and $\delta_{\text{el}}$ thus drops out.

5 The inferred detector offsets do not depend significantly on the smoothing scale; the map-based approach yields the same results when all detectors are smoothed with the same Gaussian beam window function.
approximation is expected to hold relatively well after the time-domain filtering has been applied. Furthermore, we assume that the pixel-to-pixel variance only differs by the number of data samples $n_{\text{hit}}$ that are binned into a pixel. To suppress the statistical weight of regions at the edges of the map where the smallness of $n_{\text{hit}}$ might invalidate this approximation, we convolve $n_{\text{hit},i}$ with a two-dimensional symmetric Gaussian apodization function ($7^\circ$ FWHM), schematically: $n_{\text{hit}} \rightarrow \tilde{n}_{\text{hit}}$. We thus assume the following to hold:

$$N_{ij}(\Theta) = \delta_{ij} \sigma_i^2(\Theta) = \delta_{ij} \frac{\sigma^2}{n_{\text{hit},i}(\Theta)},$$

where $\sigma^2$ is the (constant) variance of the Gaussian white noise in the detector time stream. With this assumption, the second line in Eq. (5.5) simplifies significantly. The part dependent on $\Theta$ becomes equal to the trace over the diagonal covariance matrix: $\text{Tr} \ C_N$, which simply yields the total number of hits in the map. As a change in the detector pointing offset leaves the total number of hits unchanged, we see how the whole term looses its dependence on $\Theta$. The relevant parts of the likelihood are reduced to:

$$\log \Pr(\hat{I}|\Theta) \propto \sum_{i=1}^N \tilde{n}_{\text{hit},i}(\Theta) \left( \hat{I}_i(\Theta) - I_i \right)^2.$$  \hspace{1cm} (5.5)

Note that the actual value of the noise variance can be absorbed in the proportionality sign, the only relevant quantity is $\tilde{n}_{\text{hit}}$. We use the HEALPix pixelization scheme with an $N_{\text{side}} = 256$ pixel size; smaller pixels do not improve the optimality by a significant amount, this is seen as a consequence of the SPIDER beam scale. A visualisation of the grid search method is shown in Fig. 5.2.

We run a number of simulations in order to verify the validity of the approximate likelihood function. For each simulation, we replace the time-ordered SPIDER data by HFI data. The time-ordered HFI data are sampled from the (beam-convolved) map using a known value of the detector offset. This allows us to check whether the inferred posterior distribution is biased. The simulated data are processed in the same way as the real data, but only after an appropriate amount of Gaussian noise is added in the time domain. We assume the noise to be statistically stationary and periodic, but relax the assumption of a constant power spectral density (PSD). Instead, we use an $1/f$ PSD profile that best describes the noise of the SPIDER detector. This
Figure 5.2: Visualisation of a typical result of the brute-force exploration of the detector pointing offset posterior. The colour denotes the unnormalised value of the log likelihood for different choices of centroid offset (in azimuth and elevation) for a randomly selected detector (x1r01c15). The maximum a posteriori offset is denoted with the larger dot. The white contour lines denote an elliptical Gaussian fitted to the grid, the mean of the elliptical Gaussian is denoted with the smaller dot.

Type of time stream noise invalidates the assumption in Eq. (5.4): the noise covariance matrix $C_N$ ceases to be diagonal. After processing and binning the simulated data on the sphere, Eq. (5.5) is evaluated as normal.

We perform a set of 31 simulations for two randomly selected detectors on each of the six focal planes. The small number of simulations is mainly due to numerical cost: for each iteration we have to simulate a detector’s entire dataset 121 times. With only 31 simulated posterior distributions we can already be confident that the non-trivial noise covariances do not bias the estimate in any significant way. The widths of the simulated posteriors closely match those inferred from the data. We conclude that for full-flight data the detector noise is a subdominant contribution to the overall uncertainty. The main uncertainty is inherent to an analysis in the map-domain. The sub-optimality of the method means that even with noiseless simulations a similar uncertainty is reached. Still, we estimate that the method is capable of detecting 1 arcmin changes in the pointing offsets at a $1\sigma$ CL,
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which is enough for our purpose.\textsuperscript{6}

In Fig. 5.3 we show results from the map-based analysis. The updated pointing offsets show coherent shifts away from the offset values derived from the RCW 38 data. We interpret the coherent patterns as a clear sign that the results are physical. The patterns differ per detector tile: some tiles seem to be rotated, others are translated or prefer a different plate scale. We have not investigated whether we are actually probing the orientation of the tiles with respect to the telescopes or whether we are partly undoing errors that were introduced by the pointing offsets inferred from the RCW 38 data.

With the results in hand, we look for significant differential pointing and quantify whether or not the effect is coherent across the detector tiles or focal planes. Recall that differential pointing is defined as the difference in pointing offset between the two orthogonally polarized detectors (A and B) that make up a detector pair. Systematic differential pointing is a physical phenomenon that was clearly observed in e.g. the BICEP2 analysis \cite{132}. In Fig. 5.4 we plot the estimated differential pointing. We see a typical deviation of roughly 0.5 arcmin, but no strong spatial coherence.

In order to make the statement about the weak spatial coherence slightly more precise, we compare a model for the pointing offsets that allows for nonzero differential pointing to a model without differential pointing. To start, we parameterise the grid of pointing offsets per detector tile using nine linear models with increasing complexity. We find that a model with eight parameters per tile fits the offset data best based on the reduced $\chi^2$ statistic and the Akaike information criterion (AIC). Six out of the eight parameters specify the location, spacing and orientation of the grid, while the two remaining parameters allow for non-linear grid spacing. The model is shown as the red lines in Fig. 5.3. We then test whether the reduced $\chi^2$ and AIC statistics improve when we allow for differential pointing in the model. We see that the model fit improves at $3\sigma$ or higher confidence for nine out of 24 detector tiles located on five different focal planes. When we perform the same test at the focal plane level, only two focal planes, X1

\textsuperscript{6}In retrospect, the $1 \times 1$ arcmin$^2$ resolution of the grid search is suboptimal, given that the estimated 1$\sigma$ uncertainty is 1 arcmin. As an approximate solution that does not involve a finer grid, we fit an elliptical Gaussian to each posterior and effectively use the tails of the distributions to slightly increase the precision of the estimate of the posterior mean. Of course, this assumes the posteriors are well described by an elliptical Gaussian. The sub-arcmin agreement between these estimates and the results from the optimal time-domain analysis (presented later) suggest that this assumptions is valid.
Figure 5.3: The updated pointing offsets as arrows projected on the sky (exaggerated by a factor 10) away from the RCW-38 derived grids. The six focal planes (X1-X6) are shown. Grey arrows denote the inferred posterior means, red arrows the best-fitting per-detector-tile model. The boresight pointing direction of each telescope is denoted with a black dot.
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Figure 5.4: Differential pointing (from detector B to detector A) for each complete pair on SPIDERS focal planes (X1-X6). The vectors are multiplied by a factor 25. The boresight pointing direction of each telescope is denoted with a black dot.
and X6, show significant coherence. We conclude: the differential pointing seems to be independent between detector tiles.\(^7\)

In short, we see marginal evidence for spatial coherence of the, already small, differential pointing. As an example of the associated systematics, the \(I \rightarrow P\) leakage due to the differential pointing is plotted in Fig. 5.5. The amplitude of the signal is not significant compared to the detector noise. Still, there is no clear motivation for the use of a common pointing offset per detector pair with the SPIDER map-maker. Each detector is treated independently: the map-maker does not use the fact that some detectors are pairs on the focal plane. For this reason, it was decided to not force a common pointing offset per pair. Without a clear physical motivation for the per-tile grid model, it was also decided that the cosmology analysis will use the per-detector pointing offsets and not the model.

**Cross-spectra-based analysis**

This section summarises a search for the detector pointing offsets that completely works in the power spectrum domain. More specifically, the method works with angular cross-correlations between maps. Schematically, the angular cross-correlation between two intensity-only maps is calculated as follows:

\[
\hat{C}_{\ell}^{1,2} = \frac{1}{2\ell + 1} \sum_{m=-\ell}^{\ell} a_{1,\ell m}^1 (a_{2,\ell m}^2)^* ,
\]

where the \(a_{1,\ell m}^1\) are spherical harmonic coefficients of the two maps. Instead of the above equation, \(\hat{C}_{\ell}^{n,j}\) is estimated using the \texttt{PolSPICE} code [161]. \texttt{PolSPICE} partially corrects for aliasing effects due to the incomplete sky coverage of the data. \(\hat{C}_{\ell}^{n,j}\) is a lossy summary of the map that averages over all phase information; the method should therefore be less optimal than the map-domain analysis presented in the previous section. Still, we obtain almost identical results in the multipole domain. Errors in the pointing offset have a clear scale dependence: they show up at angular scales comparable to the beam scale. This means that the spectra still contain useful information about the pointing offsets. The main problem with an analysis in the multipole domain is the rather strong degeneracy between the effects.

\(^7\)Similar overall conclusions are reached with the grid models with six or ten parameters.
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Figure 5.5: Systematic $Q$ signal from assuming a common pointing offset per detector pair instead of a pointing offset per detector. The top row shows the predicted signal, created by reprocessing the Planck HFI 100 GHz data, the bottom row shows the difference with SPIDER data. To aid the visual comparison, small-scale noise in the SPIDER maps has been suppressed by applying a Gaussian smoothing ($1^\circ$ FWHM). The amplitude of the systematic signal is not significant given the noise in the SPIDER maps. Shown are full-flight data from all good detectors on the X2 telescope. The other five telescopes yield comparable results, but the morphology of the residuals varies. As a result, the systematic signal does not coherently add when data from several telescopes are joined.
from the pointing offsets and the calibration and beam window function. For this reason, the method was not pursued to the same extent that the map-domain and time-domain analyses were.

The analysis is performed completely analogously to the previous section. The only difference is that instead of evaluating the likelihood in the map domain, i.e. Eq. (5.5), we evaluate the following statistic for different values of the detector pointing offsets \( \Theta = \{ \delta_{az}, \delta_{el} \} \):

\[
R(\Theta) = \sum_{\ell=\ell_{\text{min}}}^{\ell_{\text{max}}} \left| \frac{\hat{C}^{S,P}_\ell(\Theta)}{\hat{C}^{HM1,HM2}_\ell} - 1 \right|. \tag{5.7}
\]

In this schematic representation, \( \hat{C}^{S,P}_\ell(\Theta) \) represents the angular cross spectrum between the Planck HFI map and the SPIDER map. Both are again processed identically, with the exception that the SPIDER data are binned using varying pointing offsets. \( \hat{C}^{HM1,HM2}_\ell \) represents the cross spectrum of the two half-mission splits of the HFI data used in the numerator. The cross spectrum between half-mission maps is used to avoid a noise bias: the noise in the two halves is assumed to be uncorrelated. The cross spectra are computed using Po1SPIE.\(^8\) All maps are hit-weighted and apodized using the same Gaussian apodization function (7° FWHM) as used in the map-domain analysis.

Early results and simulations indicate that the pointing offset uncertainty is comparable to the map-based analysis, but only when the calibration and beam window are left fixed. When they are simultaneously varied with the pointing offsets, a rather problematic degeneracy between the three effects becomes apparent. Such a degeneracy is not observed at this level in the map-domain analysis. This is understood as a consequence of the anisotropy of the pointing offset signal. The anisotropic signature is still largely present in the map and is distinct from the isotropic effects due to mismatches in calibration and beam window functions. By varying the lower and upper limits of the sum in Eq. (5.7), the degeneracy in the multipole domain can be increased or decreased, but not quite removed.

\(^8\)Identical results were reached with the anafast routine in HEALPix that calculates Eq. (5.6) without correcting for the sky mask. The effects of sky-mask (de)convolution essentially cancel out between the numerator and denominator in Eq. (5.7).
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**Time-domain analysis**

For optimal inference on the detector pointing offsets, an analysis in the time domain is required. Instead of using a time-domain version of the brute-force posterior exploration that we presented for the map-based approach, a slightly different approach, inspired by the BICEP2 'deprojection' method [132], was taken for **SPIDER**. The inferred pointing offsets are in complete agreement with those from the map-based analysis, which provides a great deal of credibility to both analyses. The two methods were developed independently from each other, although it should be noted that both still rely on the HFI sky maps as calibration data.

Instead of repeating the derivation of the method presented in Ref. [132], we show how the deprojection method can be derived from the general data model presented in Sec. 4.3. Furthermore, the derivation in Ref. [132] is in the context of an analysis that relies on a pair-differencing map-maker, we show that an equivalent method can be formulated for the **SPIDER** map-maker.

In short, deprojection constructs a linearised version of the pointing offset effect. This results in templates that describe the shape of the spurious signal in the time-domain, which are fitted to the data to infer the pointing offsets. The derivation of these templates in Ref. [132] starts from Taylor expanding an azimuthally symmetric Gaussian beam about a small shift in the local azimuth or elevation direction. To first order in the deviation, the perturbations to the pair-differenced beam is then expressed as derivatives (with respect to az and el) of a regular symmetric Gaussian beam. It is then shown how, after a coordinate transformation to the (θ, φ) coordinate system fixed on the sky, the time-ordered templates corresponding to this perturbed beam can be constructed using linear combination of the first derivatives (with respect to θ and φ) of regular beam-convolved maps.

When we use the data mode in Eq. (4.42) as a starting point, we see that the pointing offset templates constructed for deprojection are equivalent to the \( s = \pm 1 \) case of the full model. Let us expand on this claim a little by starting from the notion that the spurious signal due to a small pointing offset error must be proportional to the difference between the centre of the real beam and the assumed beam centre. For small offsets \( \delta_{az} \) and \( \delta_{el} \), the

---

9I did not perform the time-domain deprojection analysis. However, the deprojection method relates to the discussion in Chapter 4 and is therefore included.

10The term ‘deprojection’ comes from the fact that the BICEP2 analysis directly subtracts, or ‘deprojects’, the best-fitting model of the spurious data from the TOD.
difference of these beams is described by an $m = 1$ field when placed on the pole, i.e. a field that has only has parts proportional to $\delta_{\text{az}} \cos \phi$ and $\delta_{\text{el}} \sin \phi$. In terms of the spherical harmonic modes of this `difference' beam $b_{\ell 1}^I$, the part proportional to $\cos \phi$ is given by $\text{Re}\{b_{\ell 1}^I\}$, while the part proportional to $\sin \phi$ corresponds to $\text{Im}\{b_{\ell 1}^I\}$. If we rewrite the data mode in Eq. (4.42) in terms of these two beams (and neglect the polarized sky), we see that we obtain two time-ordered templates. One for a pointing offset in the local azimuth direction:

$$d_{\ell}^{\text{az}} = 2 \text{Re} \left\{ \sum_{\ell, m} \text{Re}(B_{\ell 1}^I) a_{\ell m} e^{-i \psi_t} Y_{\ell m} (\hat{n}_t) \right\} ,$$

and one for a pointing offset in the local elevation direction:

$$d_{\ell}^{\text{el}} = 2 \text{Re} \left\{ \sum_{\ell, m} i \text{Im}(B_{\ell 1}^I) a_{\ell m} e^{-i \psi_t} Y_{\ell m} (\hat{n}_t) \right\} .$$

Note that we have defined the shorthand:

$$B_{\ell 1}^I = \sqrt{\frac{4\pi}{2\ell + 1}} b_{\ell 1}^I .$$

Now, in order to fit these templates to the data and learn about the actual value of the detector offset, we use the linearity of the model, i.e. $\text{Re}\{B_{\ell 1}^I\} \propto \delta_{\text{az}}$ and $\text{Im}\{B_{\ell 1}^I\} \propto \delta_{\text{el}}$. This means that, assuming we know the functional form of $B_{\ell 1}^I$, we can use the above templates to find $\delta_{\text{az}}$ and $\delta_{\text{el}}$.

We can go one step further and connect the above description to the expression in terms of derivative maps, as used in the BICEP2 and SPIDER deprojection analysis. We do so by using Eq. (2.41): the expression for $Y_{\ell m}$ in terms of derivatives of the regular spherical harmonics. Eq. (5.8) then becomes:

$$d_{\ell}^{\text{az}} = 4 \text{Re} \left\{ e^{-i \psi_t} m (\hat{n}_t) \bar{\partial}_t \sum_{\ell, m} \frac{(\ell - 1)!}{(\ell + 1)!} \text{Re}\{B_{\ell 1}^I\} a_{\ell m} Y_{\ell m} (\hat{n}_t) \right\} .$$

Using the definition of the vector $m$ in Eq. (2.30) and the angular gradient,
this expression becomes:

\[
d_{\alpha z}^t = 2\sqrt{2} \left( \cos \psi_t \partial_\theta + \frac{\sin \psi_t}{\sin \theta_t} \partial_\phi \right)
\times \sum_{\ell,m} \sqrt{\frac{(\ell - 1)!}{(\ell + 1)!}} \Re\{B_{\ell 1}^I\} a_{\ell m} Y_{\ell m}(\hat{n}_t).
\]

(5.12)

To exactly match the expressions used in the deprojection analysis, we express the \(m = 1\) beam harmonic modes in terms of the symmetric beam window function in the following way:

\[
\Re\{B_{\ell 1}^I\} = -\frac{\delta_{\alpha z} \sigma^2}{2\sqrt{2}} \sqrt{\frac{(\ell + 1)!}{(\ell - 1)!}} B_{\ell}^I,
\]

(5.13)

and:

\[
\Im\{B_{\ell 1}^I\} = -\frac{\delta_{el} \sigma^2}{2\sqrt{2}} \sqrt{\frac{(\ell + 1)!}{(\ell - 1)!}} B_{\ell}^I,
\]

(5.14)

where \(\sigma^2\) is the Gaussian beam width.\(^{11}\) With this reparametrization, we obtain the templates in terms of derivative maps \(\partial_\theta I_{\text{eff}}\) and \(\partial_\phi I_{\text{eff}}\):

\[
d_{\alpha z}^t = -\delta_{\alpha z} \sigma^2 \left( \cos \psi_t \partial_\theta + \frac{\sin \psi_t}{\sin \theta_t} \partial_\phi \right) I_{\text{eff}}(\hat{n}_t),
\]

(5.15)

\[
d_{el}^t = -\delta_{el} \sigma^2 \left( \sin \psi t \partial_\theta - \frac{\cos \psi_t}{\sin \theta_t} \partial_\phi \right) I_{\text{eff}}(\hat{n}_t).
\]

(5.16)

\(I_{\text{eff}}\) represents the sky intensity convolved with a symmetric beam, it was already defined in Eq. (4.7).

Why is it advantageous to use the deprojection method? The smart thing is not so much the use of derivative maps; we could have equally well used the expressions in terms of SWSH transformations in Eq. (5.8) and Eq. (5.9).\(^{12}\) The SPIDER simulation pipeline is also capable of calculating

\(^{11}\)The \(\sigma^2 \sqrt{(\ell + 1)!/(\ell - 1)!/(2\sqrt{2})}\) prefactor might seem ad hoc, but this is (unsurprisingly) the approximate prefactor for the \(m = 1\) harmonic modes of a slightly displaced azimuthally symmetric Gaussian beam.

\(^{12}\)The derivative maps are computed using the \texttt{alm2map\_der1} function in HEALPix. Ultimately, these functions share the underlying routines with the \texttt{alm2map\_spin} function that is used to calculate the inverse spin-weighed spherical harmonic transforms. So there is really no meaningful numerical difference between the two approaches.
time-ordered pointing offset templates in a nonperturbative manner. The smart aspect is the linear nature of the model. Once the template has been computed, the inference step reduces to simply fitting a linear model to the data. There is no need to rescan maps for each value of the offset parameters. This enormous advantage in efficiency makes it relatively easy to jointly infer the pointing offsets together with the overall calibration and beam parameters. Although these effects are not very degenerate in the time domain, there is no obvious disadvantage to a joint inference approach.\footnote{Besides time-ordered templates for the pointing offsets, a joint analysis requires templates for calibration and beam width. These, as well as two beam ellipticity templates, can be found in Ref. [132]. The same templates have been used in the Spider analysis.}

The results of the deprojection approach are fully consistent with those from the map-based approach. The inferred pointing offsets agree to the sub-arcmin level. As expected, the deprojection method has significantly more statistical constraining power: meaningful constraints can already be made on 10-minute long data chunks. The nominal pointing offsets used by the Spider analysis are determined from a weighted average of all 10-minute data chunks that make up the entire mission length. The templates are filtered and flagged identically to the data. The 1σ statistical uncertainty obtained from the entire mission length is estimated to be $O(0.1)$ arcmin. Calibration, beam width and beam ellipticity are jointly estimated, but currently not directly used in the cosmology analysis. Null tests seem insensitive to changes in calibration and beam, so this effort has not been made. This is also the reason that, unlike the BICEP2 approach that directly removes the best-fitting templates from the TOD, we currently only use the method to infer the detector pointing offsets. Inferred values for the detector calibration and beam width seem consistent with a dedicated analysis (see next section), but these claims are still somewhat preliminary.

5.1.2 Calibration and beam window function

The detector calibration and beam window function are determined by maximising the cross correlation between Spider and Planck HFI data. The cross correlation is determined by calculating angular cross spectra of the datasets. The calibration is somewhat degenerate with the beam window function, so the two quantities are jointly inferred. The detector calibration refers to the scalar conversion factor between the sky signal measured in $\mu K_{CMB}$ and the time-ordered data expressed in analog-to-digital units.
The beam parameterisation is a Gaussian beam window function, i.e. the azimuthally symmetric Gaussian beam defined in Eq. (4.6).

Per detector, the calibration factor $c$ and the FWHM of the Gaussian window function are inferred by a brute-force evaluation of the following statistic:

$$ R(c, \text{FWHM}) = \sum_{\ell = \ell_{\text{min}}}^{\ell_{\text{max}}} c \left( \frac{\hat{C}^{S, \text{HM}1}_\ell(\text{FWHM})}{\hat{C}^{\text{HM}1, \text{HM}2}_\ell(\text{FWHM})} - 1 \right). $$

(5.17)

Note the similarity to the expression in Eq. (5.7), used for the detector pointing offset inference. $\hat{C}^{S, \text{HM}1}_\ell$ denotes the cross spectrum between SPIDER data and a rescanned half-mission HFI sky map of the appropriate frequency. $\hat{C}^{\text{HM}1, \text{HM}2}_\ell$ denotes the cross spectrum between the two HFI half-mission maps of the same frequency. The noise in the half-mission maps is approximately uncorrelated; this construction thus avoids biasing the estimate from having not modelled the HFI noise. Before processing, the HFI data are convolved with a Gaussian beam function that is specified by the FWHM parameter. Cross spectra are calculated using POLSpice with parameters that are tuned for the sky mask. All maps are weighted by the number of samples per pixel, apodized by a (7° FWHM) Gaussian function. The sum runs from $\ell_{\text{min}} = 100$ to $\ell_{\text{max}} = 275$ for the 94 GHz detectors and to 375 for the 150 GHz detectors. Only data inside the SPIDER CMB region are used. The RCW 38 data are excluded; the strong Galactic signal is avoided to keep the dependence on the SPIDER-HFI bandpass difference as small as possible.

In an attempt to improve numerical efficiency, it was found that the following expression provides identical results to Eq. (5.17):

$$ R(c, \text{FWHM}) = \sum_{\ell = \ell_{\text{min}}}^{\ell_{\text{max}}} c \left( \frac{1}{B^T_\ell(\text{FWHM})} \frac{\hat{C}^{S, \text{HM}1}_\ell}{\hat{C}^{\text{HM}1, \text{HM}2}_\ell} - 1 \right). $$

(5.18)

$B^T_\ell$ is defined in Eq. (4.6). This expression is more efficient because the ratio of cross spectra is not recomputed for each new value of the FWHM parameter. The HFI maps are not beam convolved before rescanning.\(^{14}\) The expressions is not formally equivalent to Eq. (5.17), as beam convolution does not commute with the transformations due to the sky cut and the

\(^{14}\)Except for a 12 arcmin Gaussian beam window function that is there to reduce pixel aliasing effects.
filtering applied by the data processing. However, these effects are negligible for the multipole range used. For this reason, the more efficient expression is used in the actual analysis.

The 100 and 143 GHz Planck HFI data are calibrated using the orbital dipole [36]. By calibrating on HFI data, SPIDER does as well. In terms of statistical power per detector, a relative error (at $1\sigma$ uncertainty) of approximately 1% is obtained on the calibration factor. Given that uncertainty in the detector calibration does not induce $I \rightarrow P$ leakage with the map-making scheme used for SPIDER, a 1% uncertainty is sufficient. It is also checked whether calibrating on HFI data that are corrected for the SPIDER frequency bandpasses changes the outcome. Results indicate that the calibration is insensitive to the band-pass differences in the CMB region. The relative error on the FWHM parameter of the beam window function is approximately 2% at $1\sigma$. Similar to the calibration case, this uncertainty does not contribute significantly to the overall error budget of the experiment as it does not directly cause $I \rightarrow P$ leakage.

Several attempts have been made to move away from the assumption of a Gaussian window function. There is relatively strong prior belief in the existence of beam sidelobes due to the baffling of the telescopes (see the next section). To leading order, such sidelobes cause a non-Gaussian excess in power in the window function at low ($\ell < 50$) multipoles. Attempts to estimate this excess using parameterisations of the window function that allow for a rise at low multipole have not been successful. Two issues are identified: the sensitivity of the processed SPIDER data drops off sharply at low multipole order due to the aggressive time-domain filtering and the limited sky region. As a result, the inferred window functions, either at the detector or focal plane level, gain a large uncertainty at $\ell < 50$, the range of interest. The second issue is that, although the resulting non-Gaussian window functions significantly improve the (SPIDER − HFI) large-scale residual (largely by construction), the corresponding sidelobe amplitudes are too large to be physical. A likely explanation is spurious signal in the SPIDER data that is interpreted as sidelobe signal. The bandpass difference between SPIDER and HFI has been excluded as an explanation for this spurious signal: the same results are reached with bandpass-corrected HFI maps as input.

While the aggressive time-domain filtering makes it difficult to characterise the expected beam sidelobes, it also means that the systematic effects due to sidelobes are strongly suppressed. Preliminary results indicate that null tests are essentially insensitive to the addition of sidelobes to the data model.
For this reason, the nominal analysis keeps the Gaussian beam window function. Still, a contribution from beam sidelobes is expected to present. In Sec. 5.2 the amplitude of the systematic sidelobe signal is estimated using optical simulations and the \texttt{beamconv} code.

## 5.2 Simulating optical systematics

As explained in Sec. 5.1.2, the nominal \textsc{Spider} analysis currently approximates the beam of the instrument with a Gaussian beam window function. All detectors on a given telescope are thus assumed to have the same Gaussian beam and six FWHM parameters completely specify the optical response of the instrument. We investigate how problematic this approximation is by calculating the expected residual signal due to neglected optical effects with the use of optical simulations and the \texttt{beamconv} code.

Several preflight studies into systematic contamination were performed for the \textsc{Spider} mission. Table 2 from Ref. [92] lists 12 systematic effects that could potentially limit the science goals along with target limits. Many of those targets are informed by simulations described in Ref. [162] or Ref. [163]. The simulations described in both of those papers were performed using a limited number of detectors while assuming a 4-day flight from Alice Springs, Australia with a different scanning strategy than the one used in the 2015 Antarctic flight [92]. The study presented here updates a number of the previously quantified systematic effects, but also adds a number of new systematics. The results presented in this section will be included in a future publication of the \textsc{Spider} collaboration and should be considered as preliminary.

### 5.2.1 Description of the method

Our approach is as follows: we forward-propagate different systematic effects through the analysis pipeline and assess their effects on the inferred $B$-mode power spectrum. The systematic signal are thus treated the same as the real data. After all processing has taken place and the simulated data are binned using the map-maker, the resulting $B$-mode power spectrum is estimated and compared to the amplitude of the primordial spectrum. As the input signal contains $I$ and $E$-mode signal but no $B$-mode signal, all resulting signal is necessary from $I \rightarrow P$ and $E \rightarrow B$ leakage. The systematics are treated independently from each other, we neglect the possibility that two
types conspire to have a larger combined effect. The approach thus yields an estimate of the relative importance of known types of systematics.

To simulate the CMB random generated $I$, $Q$ and $U$ maps with best-fitting ΛCDM spatial (cross-)correlations are generated using synfast and synalm functions in healpy. As an estimate for the polarized dust and polarized synchrotron signal Commander estimates [102] tailored to the SPIDER frequency bandpasses are used. No masking is applied to the maps before beam convolution. To reduce aliasing effects the SWSH coefficients of the maps are computed up to $\ell_{\text{max}} = 4000$. The resulting coefficients are truncated to a multipole of 1000, which is still beyond the band limit of SPIDER, in order to speed up to inverse SWSH transforms in beamconv.

Time-ordered data are produced by the beamconv code with the above input for all detectors that are included in the current analysis on one of the 94 GHz telescopes and one of the 150 GHz telescopes. The same pointing data used for the main analysis are provided to beamconv. The data corresponds to roughly 12 consecutive days (before data cuts) or 24 HWP steps sampled at 119 Hz per detector. The resulting time-ordered data is given as input to the SPIDER simulation pipeline in order to apply the same linear filtering and data cuts that are applied to the real data. There is no noise added to the simulation. The filtering amounts to a fifth order Legendre polynomial that is fitted to the data in the azimuth domain and subtracted. The fit is done independently for each detector over each azimuthal scan and is meant to remove large-scale, azimuthally-fixed spurious signal due to any optical or otherwise scan-synchronous pickup. Since the filter operation is linear, we may study its effect on the simulated beam-induced signal by simply applying it. It does not require knowledge of the real data.

The processed data are binned into a sky map by using the same map-making algorithm used in the nominal SPIDER analysis. The algorithm is a pencil-beam binning algorithm similar to the one described in 4.1.2. No attempt to correct for the bias due to the polynomial filter is made during the mapmaking stage. Besides an overall per-detector scalar weight, inferred from the effective white-noise level per detector, no inverse noise-covariance weighting is applied.

The $B$-mode power spectrum is estimated from the resulting $Q$ and $U$ maps using the PolSPICE code [161]. The input maps are masked with the same sky mask as used in the cosmological analysis, the PolSPICE parameters are tuned for the mask. The resulting spectra are divided by the nominal SPIDER Gaussian window function $(B_{\ell}^2)_{\text{adj}}$ before plotting. This pro-
5.2. SIMULATING OPTICAL SYSTEMATICS

5.2.2 Description of included optical systematics

**Realistic main beams** Physical optics (PO) simulations of the main beam of each of the SPIDER detectors produced with the GRASP software package\(^{15}\) are used to study the effects of realistic beams. Compared to the single-Gaussian beam parametrisation used in the nominal analysis, the PO beams capture the differences in effective beam width across the focal plane, the beam asymmetry, the non-Gaussian aspects due to diffraction and the small cross-polar beam component. A detailed description of the GRASP simulations is beyond the scope of this thesis. Roughly speaking, an initial electric field originating from the detector (the phased antenna array) is modelled as the beam corresponding to a square aperture set by the geometry of the antenna arrays). This initial beam, or pixel beam, is then propagated though the optical system that, for this simulation, includes the two anti-reflection-coated lenses and the reflecting baffles seen in Fig. 3.4. The resulting (monochromatic) beams are comparable to the beams depicted in Fig. 4.5 (albeit without the ghosting beam). As the PO predictions for the off-axis response are poorly understood, the beams are truncated at \(4^\circ\) from the beam centre and apodized before the SWSH coefficients are computed. The beam asymmetry is relatively modest, which allows the beam azimuthal modes to be truncated at \(s_{\text{max}} = 4\). The two detectors in each detector pair share the PO beam up to a complex phase set by the polarization angle.

**Elliptical Gaussian beams** To investigate the effect of an elliptical Gaussian approximation, an elliptical Gaussian is fitted to each of the PO beams. This beam model still captures the varying beam width and beam asymmetry over the focal plane but neglects cross-polar or non-Gaussian beam components.

**Sidelobes** Method-of-Moments (MoM) computations produced with the GRASP software package are used to estimate the beam sidelobes due to the baffling of the telescopes. Compared to the PO technique used for the main beams, the MoM technique jointly solves for the electric

\(^{15}\)http://www.ticra.com/software/grasp/
field on all surfaces rather than relying on a sequential approach which results in more reliable off-axis predictions. Both methods agree at the percent level for the optical response within $1^\circ$ of the beam centre. The MoM computations are however significantly more numerically intensive. As a result, only a single sidelobe estimate, computed for a detector centred on the focal plane, is used per focal plane. A hybrid representation of the PO main beams and sidelobe contribution is thus created. The two types are merged at the $4^\circ$ edge of the PO beam; the MoM estimate is truncated outside a polar cap of $45^\circ$ around the beam centre. Uncertainty in optical modelling results in several estimates for the sidelobe beam; only the most pessimistic (largest amplitude) sidelobe is used here. The estimate is comparable in amplitude, cross-polar response and morphology to the annulus-shaped sidelobe in Fig. 4.4 (again, without the ghost beam).

**Optical ghosting** A sidelobe due to optical ghosting is caused by internal reflections in the optics of the telescope. The effect is common in refractive telescopes and results in a secondary beam on the sky that is mirrored across the boresight of the telescope [162]. The effect is incorporated in `beamconv` by combining the TOD from the main beam with that of a scaled-down version of the main beam with a reflected detector pointing offset (i.e. the ghost). A single ghost is added to each detector. A 1% amplitude is used for the ghost beams, which is slightly more pessimistic than the goal stated in Ref. [92].

**Polarization angle miscalibration** Miscalibrated polarization angles are simulated by introducing an offset between the angles used in `beamconv` to produce the TOD and the angles used during map-making. Two cases are simulated: a $1^\circ$ systematic polarization angle offset that is shared among detectors and a random Gaussian ($\mu = 1^\circ, \sigma = 1^\circ$) offset added per detector. A $1^\circ$ offset is pessimistic given the accuracy of the pre-flight polarization angle measurements [105].

**Row cross-talk** The detector readout system correlates signals from detectors that are adjacent in the read-out chain. For the SPIDER focal planes, the effect is that each detector gains a secondary beam roughly $2^\circ$ away from the main beam. To simulate this type of detector cross-talk, an approach similar to the optical ghosting approach is taken. The amplitude of the secondary beams is taken to be 0.3% in accordance with Ref. [132].
5.2. SIMULATING OPTICAL SYSTEMATICS

A/B cross-talk

Cross-talk between the two detectors in a pair is expected to be present at the 0.5% level [108]. The effect is simulated by adding 1% of the signal received by each detector to its partner.

Figure 5.6: Expected systematic B-mode residual for the 150 GHz X1 SPIDER telescope from various types of optical non-idealities. Residuals are compared to theoretical B-mode power spectra (solid black curves) for four different choices for the tensor-to-scalar ratio $r$. For each choice of $r$, the total B-mode power spectrum is constructed out of the primordial spectrum and the spectrum due to weak gravitational lensing of E-mode polarization. The meaning of each label is described in Table 5.1.

5.2.3 Results and conclusions

The expected residual signal for the 150 GHz telescope is plotted and compared to the theoretical B-mode power spectrum in Fig. 5.6. Qualitatively equal results are obtained for the 94 GHz telescope. In Table 5.1 additional information for each curve is provided. All considered effects seem to be an
order of magnitude below the $r = 0.03$ amplitude. The $E \rightarrow B$ leakage due to miscalibrated polarization angles dominates the residual at intermediate and small angular scales. On large angular scales sidelobe coupling to the Galaxy dominates.

Overall, the results agree well with those from the satellite test-case presented in Paper I and discussed in Sec. 4.5. The $I \rightarrow P$ leakage due to the asymmetry of the PO beams is suppressed effectively by the HWP modulation. The elliptical Gaussian approximation yields an even smaller residual. It should be noted that, similar to the satellite test-case, there is virtually no ‘differential asymmetry’, i.e. the two detectors in each pair share their $\tilde{I}$ beam (but are not exactly co-aligned). Even without HWP modulation the $I \rightarrow P$ signal induced by an asymmetric beam will approximately cancel out with the signal from the partner detector. The surviving spurious signal comes from the detectors that do not have a functioning partner; see Fig. 12 in Paper I. The fact that the curves of the two types of miscalibrated polarization angles overlap implies that the residual due the random offsets is completely negligible compared to that of a systematic polarization angle offset. The effects from the ghost beams and the secondary beams due to row cross-talk are similar to that of beam asymmetry and are thus suppressed by the HWP modulation. The A/B cross-talk is not suppressed by the HWP but is too small to be an issue.

It should be noted that the actual cosmological analysis would effectively divide out a ‘transfer function’ from the curves in Fig. 5.6 to undo the suppression of large-scale signal due to the time-domain filtering. Dividing out the SPIDER transfer function $F_\ell$ would result in factor three increase in residual at $\ell \approx 25$ and a $60\%$ increase at $\ell \approx 80$. Due to the logarithmic scaling of the y-axis, this is a small effect by eye. Note that sky signal below $\ell \approx 25$ is currently not effectively probed by SPIDER.

<table>
<thead>
<tr>
<th>Label</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PO (synf.)</td>
<td>Physical optics main beams scanning a random Gaussian $I$ and $E$-mode CMB.</td>
</tr>
</tbody>
</table>

Continued on the next page
Description for each label in Fig. 5.6 (cont.).

<table>
<thead>
<tr>
<th>Label</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PO + ghosts (synf.)</td>
<td>Same as PO (synf.) but with the addition of a ghost beam: a copy of the main beam with a pointing offset that is diametrically opposite from that of the main beam and scaled down to 1% of the main beam peak amplitude.</td>
</tr>
<tr>
<td>EG (synf.)</td>
<td>Same sky input as PO (synf.) but scanning is done with the best-fitting elliptical Gaussian approximation to the physical optical beam.</td>
</tr>
<tr>
<td>1-deg syst.polerr. (synf.)</td>
<td>Nominal Gaussian beam with a systematic 1° polarization angle offset for all detectors, scanning a random Gaussian $I$ and $E$-mode CMB.</td>
</tr>
<tr>
<td>1-deg rand.polerr. (synf.)</td>
<td>Nominal Gaussian beam with a Gaussian random ($\mu = 1°, \sigma = 1°$) polarization angle offset for each detector, scanning a random Gaussian $I$ and $E$-mode CMB.</td>
</tr>
<tr>
<td>0.3% row xtalk (synf.)</td>
<td>Nominal Gaussian beam with 0.3% cross-talk between adjacent detectors in the read-out chain, scanning a random Gaussian $I$ and $E$-mode CMB.</td>
</tr>
<tr>
<td>1% A/B xtalk (synf.)</td>
<td>Nominal Gaussian beam with 1% cross-talk between the two detectors (A and B) in each detector pair, scanning a random Gaussian $I$ and $E$-mode CMB.</td>
</tr>
<tr>
<td>PO + sidelobes (synf.+dust+synch)</td>
<td>Physical optics main beams and the sidelobe beam scanning over a sky consisting of the $I$ and $E$-mode CMB signal and polarized dust and synchrotron emission.</td>
</tr>
</tbody>
</table>
Chapter 6

Primordial Tensor Non-Gaussianity

The advent of sensitive $B$-mode CMB data from experiments like SPIDER and its successors will allow us to extend the search for the non-Gaussianity of the initial conditions of the large-scale structure of the Universe. This ‘primordial’ non-Gaussianity is a particular sensitive probe of the early Universe. Models of inflation other than the currently favoured single-field slow-roll (SFSR) models of cosmic inflation may often only distinguish themselves clearly through a non-Gaussian signature. At the moment there is no observational evidence for primordial non-Gaussianity. The most recent constraints from the Planck CMB data give the strongest upper-limits [66, 164]. Despite this null result, there is merit in further constraining primordial non-Gaussianity. Here we will describe one possible way to do so.

6.1 Introduction

As we have seen in Sec. 2.3.2, $B$-mode data allow much more efficient inference on the primordial tensor perturbation compared to temperature (or $E$-mode) CMB data. This advantageous property holds when the tensor field is Gaussian distributed, i.e. in case of the search for the tensor-to-scalar ratio $r$, but also in the case of a non-Gaussian primordial tensor field. This last insight has only been formulated relatively recently [23] and is what we will exploit in this chapter. More specifically, we will explore how
B-mode data offer a relatively unique observational window on the scalar-scalar-tensor (SST) 3-point correlation function: a non-Gaussian correlation between the primordial tensor perturbation $h$ and the scalar perturbation $\zeta$, both of which were introduced in Sec. 2.2. The SST 3-point correlation function is an essentially unconstrained probe of the very early Universe. Moreover, the correlation function is part of a consistency relation that applies to a large class of inflationary models [26, 165, 166]. We will thus see how B-mode data enables testing of a rather robust prediction of the inflationary paradigm. By detecting a SST correlation that violates this consistency relation we would rule out the majority of formulated inflation models.

This chapter mainly serves as an introduction to paper II. The paper describes the preparations for an analysis that would constrain the primordial SST function with upcoming CMB data. The best constraints on primordial non-Gaussianity, made using the Planck data [66, 164], mainly apply to the scalar-only case: the scalar-scalar-scalar (SSS) 3-point and SSSS 4-point function; the SST 3-point function requires a dedicated analysis. An important part of the preparation is the development of a dedicated method; the bulk of paper II therefore deals with the derivation of such a method. The resulting estimation method makes use of the 3-point functions constructed out of the CMB temperature and $E$- and $B$-mode anisotropies: the $TTB$, $TEB$, and $EEB$ functions, to constrain the primordial SST correlation. As the use of these 3-point functions is numerically demanding, a large emphasis is placed on the numerical efficiency of the method. From an observational point of view, the analysis will strongly benefit from upcoming small-aperture ground-, balloon- or satellite-based instruments that search for the $B$-mode power spectrum: the analysis will make use of the same data.

6.1.1 The bispectrum

We start by introducing the observable of interest: the harmonic representation of the CMB 3-point function, or the ‘bispectrum’. Let us denote this 3-point function as follows:

$$B_{m_1 \ell_1 m_2 \ell_2 m_3 \ell_3}^\ell \equiv \langle a_T, \ell_1 m_1 a_T, \ell_2 m_2 a_T, \ell_3 m_3 \rangle,$$  \hspace{1cm} (6.1)

with angled brackets that denote an ensemble average. Similar to how isotropy constraints the 2-point correlation function to be described by $C_\ell$,
see Eq. (2.63), isotropy constraints the 3-point correlation function to be described by the angle-averaged bispectrum $B_{\ell_1 \ell_2 \ell_3}$ [167, 168]:

$$B_{m_1 m_2 m_3}^{\ell_1 \ell_2 \ell_3} \equiv \left( \begin{array}{ccc} \ell_1 & \ell_2 & \ell_3 \\ m_1 & m_2 & m_3 \end{array} \right) B_{\ell_1 \ell_2 \ell_3}.$$  \hspace{1cm} (6.2)

We refer to the left-hand side of the above equation as the bispectrum, i.e. an isotropic harmonic 3-point function. The bispectrum can always be written as the above equation: a purely geometric part, the Wigner 3-$j$ symbol, and the angle-averaged bispectrum. The Wigner 3-$j$ symbol in Eq. (6.2) enforces that $m_1 + m_2 + m_3 = 0$ and $|\ell_1 - \ell_2| \leq \ell_3 \leq \ell_1 + \ell_2$. So we only define the angle-averaged bispectrum over the $(\ell_1, \ell_2, \ell_3)$ triplets that obey this triangle inequality.

Fig. 6.1 shows a slice through an example of an angle-averaged bispectrum. The observed checkerboard pattern, i.e. the fact that $B_{\ell_1 \ell_2 \ell_3}$ is only nonzero for $\ell_1 + \ell_2 + \ell_3 = \text{even}$, means that this particular bispectrum is invariant under the parity transformation. As the $a_{\ell,\ell m}$ harmonic modes transform like Eq. (2.53) under parity, their (angle-averaged) bispectra must pick up a factor $(-1)^{\ell_1 + \ell_2 + \ell_3}$ under parity.

**Bispectrum including polarization**

We are interested in the $TTB$, $TEB$ and $EEB$ CMB 3-point functions. Generalising the 3-point correlation function to include the $E$- and $B$-mode fields is straightforward:

$$B_{m_1 m_2 m_3, X_1 X_2 X_3}^{\ell_1 \ell_2 \ell_3} \equiv \left\langle a_{X_1, \ell_1 m_1} a_{X_2, \ell_2 m_2} a_{X_3, \ell_3 m_3} \right\rangle,$$  \hspace{1cm} (6.3)

with $X_1, X_2, X_3 \in \{T, E, B\}$. The generalisation of the angle-averaged bispectrum obeys the exact analogue of Eq. (6.2). Interestingly, while isotropy does not allows an angular power spectrum that is odd under parity, i.e. $C_T^{EB}$ and $C_E^{EB}$ must vanish, it allows certain parity-odd non-Gaussian correlations. For the bispectrum this means that, even in a parity-conserving theory, bispectra of all combinations of $T$, $E$ and $B$ are allowed to be nonzero.\footnote{The only caveat is that bispectra with a single or three $B$-mode components are only nonzero for configurations with $\ell_1 + \ell_2 + \ell_3 = \text{odd}$ if one requires invariance under parity. For bispectra with zero or two $B$-mode components the opposite behaviour holds: only $\ell_1 + \ell_2 + \ell_3 = \text{even}$ configurations are nonzero. A particularity of the harmonic representation is that the (angle-averaged) bispectrum is purely imaginary for configurations with $\ell_1 + \ell_2 + \ell_3 = \text{odd}$; it is real otherwise [169].}
Figure 6.1: A small part of a two-dimensional slice of a typical angle-averaged bispectrum $B_{\ell_1,\ell_2,\ell_3}$. The slice is restricted to $\ell_1 \leq \ell_2 \leq \ell_3$. With the $\ell_1$ multipole set to 40, this triangle inequality is responsible for the (isosceles) trapezoidal shape of the slice. The checkerboard pattern is a consequence of the assumed parity invariance of the bispectrum.

Contributions to the CMB bispectrum

Roughly speaking, we may identify three causes for non-Gaussianity in the CMB. In terms of the bispectrum, the types are the linearly-propagated bispectrum, the intrinsic bispectrum and the secondary bispectrum. We will define the three types below below. Analogous to the case of the CMB power spectrum, the dependence on $\ell_1$, $\ell_2$, and $\ell_3$, as well as the electromagnetic signature of different bispectra allows us to distinguish their contributions to the observed CMB. As the sensitivity of our measurements improves, an increasingly important part of research into CMB non-Gaussianity will revolve around our ability to distinguish different sources of non-Gaussian signal.

The linearly propagated bispectrum is our main focus. It represents the bispectrum sourced by non-Gaussian initial perturbations. The name refers to the fact that the cosmological evolution of the non-Gaussian perturbations is described with linear perturbation theory, see e.g. Eq. (2.22). All resulting non-Gaussian structure in the CMB is thus linearly related to the
primordial non-Gaussianity [170]. The required smallness of the primordial non-Gaussian contribution means that a linear description suffices. Even the most prominent non-linear effect, gravitational lensing, has a small effect on bispectra sourced by primordial non-Gaussianity [171]. As mentioned before, no observational evidence for primordial non-Gaussianity exists; the linearly propagated bispectrum is therefore not observed.

The intrinsic bispectrum represents the opposite case, it is the CMB bispectrum sourced by non-linear evolution of the initial Gaussian perturbations [172, 173]. More specifically, we define the intrinsic bispectrum to be the bispectrum produced by second-order cosmological perturbation theory. The resulting bispectrum can be computed by a second-order Einstein-Boltzmann solver [174]. The amplitude of the intrinsic bispectrum is too small to be detected by current, i.e. Planck, data. The required statistical power for a 1σ detection will likely be reached with the addition of upcoming data from ground-based experiments [173]. The intrinsic bispectrum is unlikely to bias the inference on the primordial SST correlation so we will ignore it.

Finally, there is the class of secondary bispectra. Strictly speaking, these are also ‘intrinsic’: they are present even with Gaussian initial conditions. However, it is useful to distinguish them from the intrinsic bispectrum. Secondary bispectra are sourced by non-linear cosmological effects that are not well-described as second-order perturbations of the initial conditions. These effects are due to late-time cosmological effects such as gravitational lensing, the Sunyaev Zel’dovich effect and the signal from the Cosmic Infrared Background. Secondary bispectra are interesting observational targets on their own: they contain information on the late-time cosmological evolution of the large-scale structure that is not contained in the power spectrum. In Ref. [175] several unpolarized secondary bispectra are detected using a combination of Planck HFI and ACTPol data. In terms of providing a bias for inference on primordial non-Gaussianity, the effects of secondary bispectra have been relatively modest. The bispectrum sourced by the correlation between the gravitational lensing and the integrated Sachs-Wolfe (ISW) effect, the lensing-ISW bispectrum [176], provides the only relevant bias for the Planck non-Gaussianity analysis (and then only really for the ‘local’ model) [66, 164]. For sensitivities beyond Planck, biases by a range of secondary bispectra quickly become relevant; an overview of the relative importance of different secondary (unpolarized) bispectra is given in Ref. [177]. It should be noted that the expected importance of secondary
sources is only true for inference on unpolarized bispectra. There are relatively few secondary contributions to the bispectrum of CMB polarization. The main contributions are unclustered extragalactic point sources \[178\], as well as a secondary bispectrum sourced by the correlation between the polarized reionization signal and the gravitational lensing signal \[169\]. The former has not been detected in the foreground-cleaned data that the Planck analysis uses; the latter has been detected, but does not provide a significant bias \[66, 164\].

The lack of secondary signal implies that polarized bispectra are a cleaner probe of the primordial signal compared to the unpolarized bispectrum. This seems especially true for inference using bispectra with a large-angular-scale $B$-mode contribution (the bispectra of interest for the primordial SST correlation); little relevant secondary signal is expected. We expand the discussion on expected secondary signal in paper II.

### 6.1.2 The scalar-scalar-tensor 3-point correlation function

It is important to understand how primordial non-Gaussianity is exactly defined. Similar to how the primordial power spectrum, introduced in Sec. 2.2.2, describes the 2-point correlation of the constant super-horizon amplitudes of the curvature (or tensor) perturbation, primordial non-Gaussianity refers to any non-Gaussian correlations of these amplitudes. Recall that although both $\zeta$ and $h$ are functions of $x$ and $t$, they are assumed to be constant with time before they enter the horizon; For that reason a description in terms of a three-dimensional fields suffices, as long as we describe the correlation early in the radiation-dominated epoch, i.e. before any of the modes we observe today entered the horizon.

The specific type of primordial non-Gaussianity we are interested in, the SST correlation function, thus refers to the 3-point function of the three-dimensional super-horizon amplitudes: $\zeta_k$ and $\pm 2h_k$. It is convenient to work with the Fourier coefficients of the amplitudes due to the assumed homogeneity of the correlation. The SST 3-point correlation function is parametrised as follows:

$$
\langle \zeta_{k_1} \zeta_{k_2} (\pm 2)h_{k_3} \rangle = (2\pi)^3 \delta^{(3)}(k_1 + k_2 + k_3) f^{(\zeta\zeta h)}(k_1, k_2, k_3) \times (\hat{k}_1)^i (\hat{k}_2)^j e^{\pm 2}_{ij} (\hat{k}_3) .
$$

(6.4)
The delta function is a consequence of homogeneity: it forces the three wave vectors to form a triangle. The other terms in Eq. (6.4) provide a relative weight to each possible triangle. Isotropy means that the absolute orientation of the triangle should be irrelevant. Indeed both the $f(\zeta \zeta h)$ term and the $(\hat{k}_1)^i(\hat{k}_2)^j e_{ij}^{\pm 2}(\hat{k}_3)$ term are invariant under spatial rotations.

The term in the second line of Eq. (6.4), the contracted angular term, is specific to the SST correlation. It suppresses triangles for which the wave vector associated to the tensor perturbation is (anti-)aligned with one or both of the other wave vectors. The shape function $f(\zeta \zeta h)$ specifies a weight depending on the lengths of the three sides of the triangle: $k_1$, $k_2$, and $k_3$. Various parametrizations are used in the literature [23, 26, 179]; in paper II the following is used:

$$f(\zeta \zeta h)(k_1, k_2, k_3) = 16\pi^4 A_s^2 f_{\text{NL}} f(\zeta \zeta h) f(k_1, k_2, k_3). \quad (6.5)$$

The parameter $A_s$, defined in Eq. (2.66), represents the amplitude of the curvature perturbation. $f_{\text{NL}}$ is a dimensionless parameter that specifies the overall amplitude of the 3-point function. The shape function $f(k_1, k_2, k_3)$ further differentiates different models.

If we were certain that the initial perturbations were set up during a SFSR type of inflationary phase, the SST 3-point function would not be a revealing probe. The SST 3-point correlation function predicted for SFSR inflation models is too small to be observable through the CMB. $f_{\text{tot}}^{\text{NL}}$ in Eq. (6.5) would be approximately equal to $r/16$, where $r$ is the tensor-to-scalar ratio [24]. Going beyond the SFSR paradigm opens up the possibility for a more sizeable and possibly observable SST correlation. There has been a sharp increase in research into these scenarios in the recent literature [179–184]. A rather robust observational test of the inflationary paradigm comes in the form of so-called consistency relations for the squeezed 3-point function [25]. ‘Squeezed’ refers to the fact that the correlation is most prominent for wave vectors that obey $k_3 \ll k_1 \sim k_2$, i.e. squeezed triangles. The consistency relation for the SST 3-point function dictates that the correlation must be unobservable in the squeezed limit where the wavelength of the tensor perturbation is much longer than those of the scalar perturbations. Roughly speaking, this consistency relation will hold for all models of inflation in which the tensor perturbation does not become constant with time as it leaves the horizon during the accelerated expansion. This ‘adiabaticity’ of the tensor perturbation is a property common to the majority of formulated models of inflation [26]. This seemingly universal property may be
used as a motivation for a targeted search for the squeezed SST correlation. If a nonzero squeezed SST correlation is detected, the consistency relation would be violated and a large number of inflation models would be ruled out.

### 6.1.3 The scalar-scalar-tensor bispectrum

We aim to constrain the primordial SST correlation by constraining its associated CMB bispectrum $B^{(\zeta \zeta h)}$. It is straightforward to write down a closed-form expression for the linearly propagated bispectrum using the expressions for $a_{\ell m}$ sourced by $\zeta$ and $h$ in Eq. (2.61) and Eq. (2.74). We insert these relations into the expression for the bispectrum in Eq. (6.3); the result is an expression that directly relates the SST CMB bispectrum to the primordial SST correlation by means of the transfer functions $T_{\ell}(k)$ that were introduced in Chapter 2:

$$
B_{m_1 m_2 m_3, 123}^{\ell_1 \ell_2 \ell_3 (\zeta \zeta h)} = \prod_{n=1}^{3} 4\pi (-i)^{\ell_n} \int \frac{d^3 k_n}{(2\pi)^3} \mathcal{T}_{X_n, \ell_n}(k_n)
$$

$$
\times Y_{\ell_1 m_1}(\mathbf{k}_1) Y_{\ell_2 m_2}(\mathbf{k}_2) \sum_{\lambda \in \pm 2} \text{sgn}(\lambda) \lambda^{+x_3 - \lambda} Y_{\ell_3 m_3}(\mathbf{k}_3)
$$

$$
\times \langle \zeta_{k_1} \zeta_{k_2} (-\lambda) h_{k_3} \rangle.
$$

(6.6)

Note that $X_3 \in \{I,E,B\}$ while $X_1, X_2 \in \{T,E\}$. The lowercase $x_3$ denotes whether the $X_3$ is $B$ ($x_3 = 1$) or $T$ or $E$ ($x_3 = 0$). We only consider the $x_3 = 1$ case, but the equation is also valid for $x_3 = 0$: the SST correlation also sources bispectra without a $B$-mode component.

### 6.2 Estimator

The main goal of paper II is the derivation of a method to estimate the amplitude of the primordial SST correlation function using the CMB bispectrum. The shear size of the bispectrum requires a different approach than the standard CMB inference that treats cosmological parameter estimation as a Bayesian inference problem. Inference on primordial non-Gaussianity is generally done using statistical ‘estimators’. This is also the approach we use. Loosely speaking, an estimator is a rule to transform observed data into a statistical point estimate, i.e. the single best-fitting parameter. In this
case, the estimator would produce the best-fitting amplitude of a primordial 3-point function with the use of the CMB bispectrum.

### 6.2.1 Standard KSW estimator

The estimator derived in Paper II is a generalisation of the standard Komatsu-Spergel-Wandelt (KSW) estimator [185]. The KSW approach reduces the computational scaling of non-Gaussianity estimation from $O(\ell_{\text{max}}^5)$ to a much more manageable $O(\ell_{\text{max}}^3)$. Here $\ell_{\text{max}}$ denotes the band-limit, i.e. resolution, of the data. The computational reduction is of crucial importance for modern high-resolution data.

The KSW estimator produces a statistically optimal, unbiased estimate $\hat{f}_{NL}^\zeta\zeta\zeta$ of the amplitude $f_{NL}^\zeta\zeta\zeta$ of the primordial SSS 3-point correlation. This 3-point function can be parametrised as follows:

$$\langle \zeta_{k_1} \zeta_{k_2} \zeta_{k_2} \rangle = (2\pi)^3 f_{NL}^\zeta\zeta\zeta \delta^{(3)}(k_1 + k_2 + k_3) f^{(\zeta\zeta\zeta)}(k_1, k_2, k_3).$$

(6.7)

To estimate the amplitude of the SSS 3-point correlation $\hat{f}_{NL}$, the following is calculated:

$$\hat{f}_{NL}^\zeta\zeta\zeta = \frac{1}{I_0} \int_{S^2} d\Omega(\hat{n}) \int_0^\infty r^2 dr \left( A^{(c)}[f] A^{(c)}[g] A^{(c)}[h] \right)(r, \hat{n}),$$

(6.8)

where we have used the notation from Paper II. The normalising factor $I_0$ represents the Fisher information: a single number that in practise would be estimated using simulations. The $r$ parameter is the comoving distance from the (flat) RW metric in Eq. (2.3). The $A$ symbols represent functionals that take an input function $f(k)$ and use that function to optimally filter the data. The resulting filtered data are represented as a map of the sky as function of $\hat{n}$, the filter depends on the value of $r$. The integrand roughly peaks at $r_{\text{rec}}$: the distance traveled by a photon since the epoch of recombination. The input functions $f$, $g$, and $h$ refer to the fact that it is assumed that the shape function $f(k_1, k_2, k_3)$ in Eq. (6.7) is separable in the three comoving wavenumbers:

$$f^{(\zeta\zeta h)}(k_1, k_2, k_3) = \frac{1}{6} f(k_1) g(k_2) h(k_3) + (5 \text{ perm.}).$$

(6.9)

It is important to realise that for the standard KSW estimator, the filter operation inside the $A$ functionals is always isotropic. In terms of the spherical harmonic decomposition, the filter only has a $\ell$ dependence;
similar to the case of the symmetric beam window function \( B_\ell \) discussed in Chapter 4, the filter thus treats all \( m \)-modes of the data for a given \( \ell \) on equal footing.

### 6.2.2 Generalised KSW estimator

As explained in Paper II, the KSW approach as formulated in Eq. (6.8) is not suited to estimate the amplitude \( \hat{f}_{\zeta \zeta h}^{\mathrm{NL}} \) of the SST correlation. The reason is the \((\hat{k}_1)^i(\hat{k}_2)^j e_{ij}^{\pm 2}(\hat{k}_3)\) term in the expression for the SST correlation in Eq. (6.4). As it turns out, it is possible to formulate a generalisation of the KSW estimator that does apply to the SST correlation in Eq. (6.4). The details are kept in Paper II, here we summarise the results.

The generalised KSW estimator that produces an estimate \( \hat{f}_{\zeta \zeta h}^{\mathrm{NL}} \) for the amplitude of the SST correlation in Eq. (6.4) is given by:

\[
\hat{f}_{\zeta \zeta h}^{\mathrm{NL}} = \frac{\sqrt{2}}{54 I_0} \sum_{m_a, m_b, M} \left( \begin{array}{ccc} 1 & 1 & 2 \\ m_a & m_b & M \end{array} \right) \int_{S^2} d\Omega(\hat{n}) \times \int_0^\infty r^2 dr \left( A^{(c)}_{(1,m_a)}[f] A^{(c)}_{(1,m_b)}[g] A^{(h)}_{(2,M)}[h] \right)(r, \hat{n}).
\]

(6.10)

The main difference compared to Eq. (6.8) are the indices of the \( A \) functionals. They represent the fact that the filtering applied to the data by each \( A \) is no longer isotropic. The anisotropic filtering reflects the anisotropy of the different elements in the sum over \( i \) and \( j \) in the \((\hat{k}_1)^i(\hat{k}_2)^j e_{ij}^{\pm 2}(\hat{k}_3)\) term. The sum of elements is isotropic, but the individual elements are not. The same is true for the filtering: each allowed combination of \( m_a, m_b, \) and \( M \) results in a set of filters that filter the data in an anisotropic manner. Note that the only required combinations are given by:

\[
(m_a, m_b, M) \in \{ (1, 1, -2), (1, 0, -1), (0, 1, -1), (1, -1, 0), (0, 0, 0) \}.
\]

(6.11)

Only when the combinations from these five combinations are summed (and weighed by the Wigner 3-\( j \) symbol), the result is isotropic again (which is required since the SST correlation in Eq. (6.4) is isotropic).

An important point is that the evaluation of the estimator in Eq. (6.10) still scales as \( O(\ell_{\max}^3) \). This allows the use of high resolution data and thus makes the estimator particularly suitable for inference on the amplitude of
the squeezed SST correlation. Note that the estimator requires the assumption that the $f^{(\zeta h)}(k_1, k_2, k_3)$ shape function in the expression for the SST correlation is separable like Eq. (6.9). Although, it is also possible to use a shape function that can be written as a sum of separable terms. This is the same assumption that is required for the standard KSW estimator. It should additionally be noted that the generalised approach introduced here also applies to different types of correlation functions involving tensor modes; in Appendix A of Paper II the estimators for a number of different primordial correlations are derived.

6.3 Discussion and future work

In addition to the derivation of the estimator presented in the previous section, Paper II also describes how the expected upper-limits on the amplitude of the SST correlation can be estimated using the Fisher information. In Paper II, this approach is used to estimate how the upper-limits obtainable by upcoming experiments will depend on parameters such as noise level, data resolution and the amount of contamination by $B$-modes from weak lensing. This method is used to forecast the performance of the upcoming Simons Observatory (SO) and the CMB-S4 experiments in Paper III and Paper V. The forecasts suggest that current constraints on the SST correlation will be improved by more than an order or magnitude. On the other hand, the constraints on the SSS correlation will only improve by a factor of two from the SO and CMB-S4 data. Constraints on the SSS 3-point function will eventually be improved by large-scale structure probes [186–189], but these upcoming constraints will not directly translate over to constraints on the squeezed SST correlation; the CMB constraints will likely be the most constraining in the foreseeable future.\footnote{It should be noted that the tensor consistency relation can in principle be probed with the 4-point correlation function of the CMB temperature or $E$-mode anisotropies [26] or the 4-point function of galaxy counts [190]. Both are not as constraining as the search involving CMB $B$-mode data considered here [26].}

It is important to understand that the limits in Papers II, III and V constitute a baseline to which more realistic forecasts will have to be compared to. The Planck analysis of primordial non-Gaussianity was able to neglect almost all complications due to secondary non-Gaussian signals; Fisher estimates gave a good prediction of the obtained upper-limits. For upcoming data from e.g. SO or CMB-S4, this will likely not be the case; the contribu-
tion from secondary non-Gaussian signal (that cannot easily be included in
the Fisher estimates) will become more important.

The Fisher estimates presented in Paper III and Paper V are made using
estimates of the effective Gaussian noise power spectrum \( N_\ell \) after foreground
cleaning. This means that, in addition to the detector- and atmospheric
noise, the uncertainty due to the imperfect removal of Galactic foregrounds
is also included. However, this is only a Gaussian estimate of what is likely
a non-Gaussian residual in the map. Extra non-Gaussian signal will bias
and/or increase the estimator variance. Besides residual from Galactic fore-
grounds, there is a contribution to the estimator variance expected from the
non-Gaussian 4-point correlation function due to weak gravitational lens-
ing [191]. For the \( \ell_{\text{max}} \approx 2000 \) band-limit of the Planck analysis the term
constitutes a 20\% increase in variance and was therefore ignored. With the
extra resolution of SO or CMB-S4, the contribution to the variance becomes
a serious issue. At this point it is unclear how much delensing will help to
counter this lensing-induced estimator variance.

The estimator derived in Paper II will be the primary method to estimate
the effects of secondary non-Gaussian signal. By producing simulated sky
maps that include residual Galactic signals or non-Gaussian lensing con-
tributions, the estimator variance and possible biases can be determined
simply by applying the estimator to ensembles of simulations. This effort is
currently underway to prepare for the analysis of the upcoming SO data.
Summary and Outlook

The detection of a stochastic background of gravitational waves would provide strong evidence for an initial inflationary phase of the Universe. An indirect detection would come from the observation of the associated $B$-mode patterns in the polarization of the CMB. A large part of my thesis revolved around the practical aspects of measuring the $B$-mode signal searched for by experiments such as SPIDER, a dedicated $B$-mode experiment, which I described in Chapter 3. Due to their faint nature, great care must be taken to eliminate fake $B$-mode signals. In Chapter 4, I studied how the telescopes that are used to gather the microwave light create a spurious signal by themselves. I presented an efficient simulation method, beamconv, to predict the bias in the $B$-mode signal. In Chapter 5, I applied my findings to SPIDER and determined the expected bias due to imperfections in the instrument’s telescopes. In addition, I contributed to the calibration and characterisation of the instrument. In Chapter 6, I described how future experiments may potentially yield more exact information about the mechanism that generated the gravitational waves by combining their $B$-mode data with other cosmic microwave background probes.

The publicly available beamconv code library that is presented in Chapter 4 is capable of simulating the systematic effects caused by arbitrarily complicated instrumental beams and scan strategies. The code does not rely on ad hoc assumptions about the instrumental beam. By computing the beam-convolution operation in the harmonic domain, the algorithm is optimised for the low-resolution beams of $B$-mode experiments and is able to include the large-angular-scale sidelobes that are important for $B$-mode measurements on degree-angular-scales. Together with a series of realistic optical simulations, the code is used to predict the level of systematic bias, resulting from optical non-idealities, for a hypothetical satellite instrument.
and the SPIDER instrument. In both cases, I concluded that bias due to beam asymmetry and non-trivial cross-polarized beam components was at an acceptable level. It can be noted, however, that beam sidelobes contribute to a potentially problematic contaminant on large-angular scales that will be hard to characterise in practise. The post-flight instrument characterisation for the SPIDER experiment presented in Chapter 5 suggests that characterisation using the external Planck HFI data is appropriate for the detector calibration, beam window function and detector pointing offsets. The various explored characterisation methods seem to yield consistent instrumental parameters. The inferred detector pointing offsets suggest an insignificant amount of differential pointing. The associated systematic effect does not pose a serious problem for SPIDER. Overall, it seems hardly justified to go beyond the standard modelling of the instrumental response for SPIDER. The yet-to-be explored BTT, BTE, and BEE 3-point correlation functions, or CMB bispectra, that are the subject of Chapter 6, form well-defined observables that can be probed with future polarization data. These bispectra probe the scalar-scalar-tensor correlation of the primordial scalar and tensor perturbations. As a results, inference on these bispectra is complementary to existing searches for primordial non-Gaussianity. It is shown how a generalised KSW bispectrum estimator can be used to infer the amplitude of such bispectra. Furthermore, it is demonstrated how the expected upper-limits on the bispectrum sourced by the scalar-scalar-tensor correlation depend on various instrumental properties such as spatial resolution and noise levels. The expected upper-limits on the amplitude of this bispectrum are forecasted for the SO and CMB-S4 experiments. The forecasts confirm that the CMB constraints on this type of non-Gaussianity can still be improved substantially over the results currently to be obtained by e.g. the Planck data.

The error analysis presented for SPIDER in Chapter 5 will be part of a series of papers analysing the SPIDER data. A similar post-flight instrument characterisation effort is planned for the data produced by the second SPIDER flight. The beamconv code used to determine the error analysis is now applied to forecast the optical systematic performance of the SO experiment. It is foreseen that the code must be updated to handle the vastly increased number of detectors. Suggestions for such updates are made in Paper I. The inclusion of several new types of systematic signal, such as HWP non-idealities, is also planned for the updated code. The forecasts for the primordial scalar-scalar-tensor correlation discussed in Paper II, III,
and V will be updated to include more realism. In the context of the SO experiment, the estimator derived in Paper II will be used to assess the effects of secondary non-Gaussian signals from Galactic foregrounds and weak gravitational lensing.
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