The precise characterization of the Cosmic Microwave Background (CMB) polarization will provide a wealth of information in addition to the Planck satellite CMB temperature measurement [1]. It will help to further constrain the ΛCDM cosmological model and its extensions. CMB polarization is generally described in terms of the two linear components Stokes parameters $Q$ and $U$, which can be mathematically combined to define the curl-free ‘$E$’ and divergence-free ‘$B$’ polarization patterns. CMB anisotropies are conveniently projected in harmonic space, with their statistics encoded in the angular power spectra $C^{XY}_\ell$, where $\ell$ is the multipole, and $X, Y \in \{E, B\}$. Since the anisotropies in the CMB are expected to be Gaussian distributed, all the cosmological information is contained in $C_{\ell}$.

The dominant source of $E$-modes anisotropies are scalar fluctuations at the epoch of recombination. Tensor (primordial gravitational waves) perturbations generated during inflation can act as a subdominant source of $E$-modes. Primordial $B$-modes, however, are only sourced by tensor fluctuations, and thus represent a unique observable to test inflationary physics. Their amplitude, parametrized by the tensor-to-scalar ratio $r$, can be arbitrarily low, depending on the inflation energy scale, and is expected to be maximal at large and intermediate angular scales ($\ell \lesssim 10^2$). In addition, CMB photons undergo a lensing effect induced by their passage through the gravitational field of matter between the CMB last scattering surface and us, which leads to the mixing of $E$ and $B$ modes. The lensing $B$-modes thus contaminates the primordial $B$-modes signal. Figure 1 represents the $E$-modes and the predicted lensing + tensor $B$-modes derived from the Planck best fit model [11] with an optical depth parameter $\tau = 0.06$ [2]. In addition, $E$ and $B$ tensor modes are shown for $r = 10^{-3}$, as well as instrumental noise levels between 0.1 and 50 μK.arcmin.

Due to experimental limitations and/or foreground contaminations, the effective CMB surveys sky coverage can be partial. This introduces an ambiguity in the relationship between the Stokes parameters and the $E$ and $B$ modes. In this context, the $E$ and $B$ modes are inevitably mixed and mislabelled [3,4]. Although this polarization leakage can be corrected on average [5, 6], the $E/B$ mixing signals contribute to each other spectrum variance. Since the $B$-mode signal is expected to be much lower than the $E$-mode signal, the impact of this ‘variance leakage’ is extremely problematic for $B$-modes detection and their precise measurement.

The pure pseudo-spectrum (PpCl) method presented in [3, 7, 8] is an extension of the standard pseudo-spectrum method (pCl) and currently represents the most popular solution that reduces the amount of polarization variance leakage. It has been widely investigated in e.g. [9, 10], and has been demonstrated to produce near-optimal variance power spectrum estimates for intermediate and small angular scales. The extension of the PpCl method to cross-spectra formalism offers the advantage of cross-correlate CMB maps, allowing to remove correlated noise and mitigate the impact of systematic effects, providing they are uncorrelated. However, the

\begin{figure}[h]
\centering
\includegraphics[width=\linewidth]{figure1.png}
\caption{Tensor (dashed) and total (solid) components of the E-modes (green), and B-modes (blue) spectra $\ell(\ell + 1)/(2\pi) \cdot C_{\ell}$ as a function of the multipole $\ell$, based on Planck 2015 best fit model with an optical depth $\tau = 0.06$. The primordial (tensor) polarization spectra are indicated for a tensor-to-scalar ratio $r = 10^{-3}$. Various experimental noise levels $\sigma_n [\mu K.arcmin]$ are indicated.}
\end{figure}
PpCl method requires particular sky mask apodizations which depends on the scanning strategy and on the depth of the observed CMB field. Moreover, the method has been proved to be sub-optimal for large and intermediate angular scales (ℓ ≲ 100) analysis [11–13].

Other methods consist in estimating the spectra using a pixel based approach, which is particularly relevant for large angular scale analysis, but have the drawback of being computationally more expensive. The Maximum Likelihood Estimator (MLE) and the Quadratic Maximum Likelihood (QML) have the advantage of minimizing spectra uncertainties. The latter, developed in [14] and extended to polarization in [15], gives the same error bars as the MLE and requires \( O(N_d^3) \) operations for a dataset of size \( N_d \), relative to the pCl which only demands \( O(N_d^{3/2}) \) operations [12].

In this paper, in analogy with the pseudo cross-spectra formalism, we describe a method based on the QML approach that allows to cross-correlate CMB maps that have common sky coverage. The formalism was first introduced in [16] for the 2016 Planck results. Although this spectrum estimator is not derived from a maximum likelihood, we will refer to it as the cross-QML (xQML) for simplicity. The analysis presented hereafter focuses on the case of polarization spectra and the xQML ability to reduce the impact of \( E/B \) variances leakage.

In Sec. II, we develop the formalism of the xQML estimator. We review the QML and extend it to cross-spectra. We then discuss its bias and uncertainty. In Sec. III, we forecast the uncertainty on \( r \) and the xQML ability to reduce the impact of \( E/B \) variances leakage.

In this section we review the most important steps that lead to the definition of the QML estimator, following what has been done in [14–15]. We then derive a cross-spectrum QML estimator (xQML) and compare its properties with the QML. Finally, we discuss in depth the implementation of the algorithm.

Lower case characters correspond to vectors, and upper case to matrices. Bold font, Latin indices, the trace and transpose operators are used for elements in the pixel domain, while normal font and \( \ell \) indices are used in the multipole domain.

We consider a dataset \( \mathbf{d} \), of dimension \( N_d = 3n_{\text{pix}} \) which encodes temperature and stokes parameters measurements,
\[
\mathbf{d} \equiv \begin{pmatrix} \mathbf{T} \\ \mathbf{Q} \\ \mathbf{U} \end{pmatrix}
\]

(1)

The pixels covariance matrix \( \mathbf{C} \) of the dataset is given by
\[
\mathbf{C} \equiv (\mathbf{d}, \mathbf{d}^T) = \mathbf{S} + \mathbf{N},
\]

(2)

with \( \mathbf{N} \) the pixel noise covariance matrix, and \( \mathbf{S} \) the signal covariance matrix defined as
\[
\mathbf{S} \equiv \sum_{\ell} \mathbf{P}_\ell \mathbf{C}_\ell, \quad \text{with} \quad \mathbf{P}_\ell^{ij} = \frac{\partial \mathbf{C}^{ij}}{\partial \mathbf{C}_\ell}.
\]

(3)

The vector \( \mathbf{C}_\ell \) encodes all six power spectra \( TT, EE, BB, TE, TB, EB \).

### A. QML estimator

We review important steps of the QML estimator developed in [14–15]. We can write the power spectrum estimator as a quadratic function of the pixels
\[
\hat{y}_\ell \equiv \mathbf{d}^T \mathbf{E}_\ell \mathbf{d} - b_\ell.
\]

(4)

\( \mathbf{E}_\ell \) \( (\ell = 2, \ldots) \) are arbitrary \( N_q \times N_d \) matrices, and \( b_\ell \) are arbitrary constants. From Eqs. 2 and 3, the estimator ensemble average reads
\[
\langle \hat{y}_\ell \rangle = \text{Tr} \left[ \mathbf{E}_\ell (\mathbf{d}, \mathbf{d}^T) \right] - b_\ell, \quad \text{with} \quad W_{\ell\ell'} \equiv \text{Tr} \left[ \mathbf{E}_\ell \mathbf{P}_{\ell'} \right]
\]

(5)

\[
\text{with} \quad W_{\ell\ell'} \equiv \text{Tr} \left[ \mathbf{E}_\ell \mathbf{P}_{\ell'} \right]
\]

(7)

the 'mode-mixing' matrix. Choosing \( b_\ell = \text{Tr}[\mathbf{E}_\ell \mathbf{N}] \), the unbiased estimator of the true power spectrum \( \mathbf{C}_\ell \) thus reads
\[
\hat{C}_\ell \equiv \sum_{\ell'} [W^{-1}]_{\ell\ell'} \hat{y}_{\ell'},
\]

(8)

and has the following covariance
\[
\langle \Delta \hat{C}_\ell, \Delta \hat{C}_{\ell'} \rangle = [W^{-1}]_{\ell\ell'} \langle \Delta \hat{y}_{\ell_1}, \Delta \hat{y}_{\ell_2} \rangle [W^{-1}]_{\ell_1\ell_2},
\]

(9)

where \( \Delta \hat{C}_\ell = \hat{C}_\ell - \langle \hat{C}_\ell \rangle \). The summation over repeated indices is implied. The resulting power spectrum is unbiased regardless of the choice of the \( \mathbf{E}_\ell \) matrices. However, they are usually constructed in order to minimize the estimator variance
\[
\langle \Delta \hat{y}_{\ell_1}, \Delta \hat{y}_{\ell_2} \rangle = 2\text{Tr} \left[ \mathbf{E}_{\ell_1} \mathbf{C} \mathbf{E}_{\ell_2} \right],
\]

(10)

which gives the trivial solution \( \mathbf{E}_\ell = \mathbf{0} \). We thus impose the mode-mixing matrix diagonal to be non-zero. For each \( \ell \), introducing the Lagrange multipliers \( \lambda \) and the condition \( W_{\ell\ell} = \beta \), we require the derivative of
\[
\langle \Delta \hat{y}_{\ell_1}, \Delta \hat{y}_{\ell_2} \rangle - 2\lambda \text{Tr}[\mathbf{E}_\ell \mathbf{P}_\ell - \beta],
\]

(11)

This gives minimum error bars. The polarization leakage requires that \( (N_d^2) \) operations be performed.
with respect to $E_t$ to vanish, and obtain the solution
\[ E_t = \frac{\lambda}{2} C^{-1} \mathbf{P}_t C^{-1}. \]  
(12)

Finally, imposing $W_{\ell\ell} = \text{Tr} [E_t \mathbf{P}_t] = \beta$ gives
\[ \lambda \text{Tr} \left[ C^{-1} \mathbf{P}_t C^{-1} \mathbf{P}_t \right] = \beta. \]  
(13)

We choose $\beta$ such that $\lambda = 1$ and $E_t$ is well defined. With this choice, the mode-mixing matrix $W_{\ell\ell}$ is the Fisher information matrix
\[ F_{\ell\ell} = \frac{1}{2} \text{Tr} \left[ C^{-1} \mathbf{P}_t C^{-1} \mathbf{P}_t \right], \]  
(14)

with $\langle \Delta y_{\ell t}, \Delta y_{\ell t}' \rangle = F_{\ell\ell}$ and $\langle \Delta \hat{C}_t, \Delta \hat{C}_t' \rangle = [F^{-1}]_{\ell\ell'}$.

The $E_t$ matrices are thus constructed such that the spectrum estimator has minimal variance. However, the QML estimator requires a precise knowledge of instrument properties. In the next section, we develop a method which allows to compute a cross-spectrum estimator that is unbiased independently of the choice of $N_d$.

**B. xQML estimator**

Following the same formalism as for the 'auto'-spectrum QML estimator detailed in the previous section, we now consider two datasets $d^A$ and $d^B$ from which the pixel covariance matrix reads
\[ C^{AB} \equiv \langle d^A, d^B \rangle = \mathbf{S} + N^{AB}. \]  
(15)

We assume uncorrelated noise between the two datasets, such that the cross pixel noise covariance matrix vanishes $N^{AB} = 0$. The cross-estimator now reads
\[ \hat{y}_{\ell t}^{AB} \equiv d^A T E_t d^B - b_{\ell t}^{AB}, \]  
(16)

with $b_{\ell t}^{AB} = \text{Tr} \left[ E_t N^{AB} \right] = 0$.

The covariance of the estimator is computed using Wick’s theorem,
\[ \langle \Delta \hat{y}_{\ell t}^{AB}, \Delta \hat{y}_{\ell t}'^{AB} \rangle = \left\langle \left[ \langle d_i^A, d_j^A \rangle \langle d_k^B, d_n^B \rangle + \langle d_i^A, d_n^B \rangle \langle d_j^A, d_k^B \rangle \right] E_t^{ij} E_t'^{kn} \right\rangle = \text{Tr} \left[ C^{AA} E_t C^{BB} E_t'^T + C^{AB} E_t C^{AB} E_t'^T \right], \]  
(17)

where summation on the pixels indices $i, j, k, n$ is implied. Matrices $C^{AA} = \mathbf{S} + N^{AA}$ and $C^{BB} = \mathbf{S} + N^{BB}$ are respectively the pixel covariance matrix of the datasets $A$ and $B$. As in Eqs. (8) and (9) for the QML method, the unbiased estimator reads
\[ \hat{C}_t \equiv \sum_{\ell'} [W^{-1}]_{\ell \ell'} \Delta \hat{y}_{\ell t}^{AB}, \]  
(18)

and its covariance
\[ \langle \Delta \hat{C}_t, \Delta \hat{C}_t' \rangle = [W^{-1}]_{\ell \ell'} [\Delta \hat{y}_{\ell t}^{AB}, \Delta \hat{y}_{\ell t}'^{AB}] [W^{-1}]_{\ell t'}. \]  
(19)

As in Eq. (11) for the QML, we seek for the $E_t$ matrices that minimize the estimator variance of Eq. (17). We get the equation
\[ C^{AA} E_t C^{BB} + C^{AB} E_t'^T C^{AB} = \lambda \mathbf{P}_t, \]  
(20)

which is a generalized form of the Sylvester equation [17]. Although the exact solution exists, as discussed in Sec. [17] it requires to solve a system of $N^2$ equations, which quickly becomes computationally prohibitive for large datasets. For this reason, we derive an approximate solution by considering two extreme signal-to-noise ratio (SNR) cases:

**HS :** High SNR, such that $S \gg N$, and $C^{AA} \sim C^{BB} \sim S$.

**LS :** Low SNR, such that $S \ll N$, and $C^{AA} \sim N^{AA}$, $C^{BB} \sim N^{BB}$.

For both limits, Eq. (20) admits a solution of the form
\[ E_t \simeq \frac{\lambda}{\alpha} (C^{AA})^{-1} \mathbf{P}_t (C^{BB})^{-1}, \]  
(21)

where $\alpha$ is a normalization coefficient that depends on the SNR, with $\alpha = 2$ for the HS regime, and $\alpha = 1$ for the LS regime. The impact of the approximation made in Eq. (21) on the spectrum variance is discussed in Sec. [17]. Finally, imposing $W_{\ell\ell} = \text{Tr} [E_t \mathbf{P}_t] = \beta$ gives
\[ \lambda \frac{\alpha}{\beta} \text{Tr} \left[ (C^{AA})^{-1} \mathbf{P}_t (C^{BB})^{-1} \mathbf{P}_t \right] = \beta. \]  
(22)

We choose $\beta$ such that $\lambda/\alpha = 1/2$, and we recover the QML solution for $A = B$. Inserting $E_t$ of Eq. (21) in the mode-mixing matrix defined in Eq. (7), one obtains
\[ W_{\ell\ell} = \frac{1}{2} \text{Tr} \left[ (C^{AA})^{-1} \mathbf{P}_t (C^{BB})^{-1} \mathbf{P}_t \right]. \]  
(23)

Using Eqs. (17), (19), (21) and (22), the cross-spectrum estimator covariance reads
\[ \langle \Delta \hat{C}_t, \Delta \hat{C}_t' \rangle = \frac{1}{2} \left[ W^{-1} \right]_{\ell \ell'} \left[ W^{-1} \right]_{t t'} G_{t t'} \left[ W^{-1} \right]_{\ell t'} \]  
(24)

where we define
\[ G_{\ell t'} \equiv \frac{1}{2} \text{Tr} \left[ (C^{AA})^{-1} \mathbf{P}_t (C^{BB})^{-1} C^{AB} \times (C^{AA})^{-1} \mathbf{P}_t (C^{BB})^{-1} C^{AB} \right]. \]  
(25)

---

1. Using matrix identities $\partial_{\mathbf{E}} \text{Tr} [\mathbf{C} \mathbf{E}^\dagger \mathbf{C}^\dagger] = 2 \mathbf{C}^\dagger \mathbf{E}^\dagger \mathbf{C}^\dagger$.

2. Using matrix identities $\partial_{\mathbf{E}} \text{Tr} [\mathbf{A} \mathbf{B}^\dagger \mathbf{E}] = \mathbf{A}^\dagger \mathbf{B}^\dagger \mathbf{E} + \mathbf{B}^\dagger \mathbf{E}^\dagger \mathbf{A}^\dagger$ and $\partial_{\mathbf{E}} \text{Tr} [\mathbf{A} \mathbf{B}^\dagger \mathbf{E}] = \mathbf{A}^\dagger \mathbf{B}^\dagger + \mathbf{A} \mathbf{B}^\dagger$.

3. We remark that when $C^{AA} \sim C^{BB}$, and more specifically for high signal-to-noise ratio : $E_t \simeq E_t^T$. 

4. Wick's theorem, $\text{Tr} \left[ C^{-1} \mathbf{P}_t C^{-1} \mathbf{P}_t \right] = \lambda$. 

5. Extreme signal-to-noise ratio cases : High SNR, such that $S \gg N$, and $C^{AA} \sim C^{BB} \sim S$.

6. Low SNR, such that $S \ll N$, and $C^{AA} \sim N^{AA}$, $C^{BB} \sim N^{BB}$.
In the $E$ regime, $G_{\ell \ell'} \sim W_{\ell \ell'}$, such that $V_{\ell \ell'} = [W^{-1}]_{\ell \ell'}$. In the $L$ regime, the second term $[W^{-1}]_{\ell_1 \ell_1'} G_{\ell_1 \ell_1'} [W^{-1}]_{\ell_1' \ell_1}$ in Eq. (24) contributes at second order to the cross-spectrum variance. As a representative example, the diagonal elements of those two terms are compared on Fig. 2 for the $EE$ and $BB$ spectra, with a $10 \mu K\cdot \text{arcmin}$ noise level. With this choice, the $E$-mode is signal dominated, and corresponds to the $H$ regime, while the $B$-mode SNR is low for most of the multipoles $(\ell \gtrsim 10)$, and corresponds to the $L$ case.

![FIG. 2: Diagonals of the covariance matrix terms $W_{\ell \ell}^{-1} G_{\ell \ell} W_{\ell \ell}^{-1}$ (dashed) and $W_{\ell \ell}^{-1}$ (plain) of Eq. (24). EE and BB components are plotted in green and blue respectively. The noise level is $10 \mu K\cdot \text{arcmin}$.](image)

We successfully defined a quadratic estimator based on datasets cross-correlation which does not require the subtraction of noise bias. Moreover, we derived an approximation of the $E_\ell$ matrices that minimizes its variance. We also recover the QML estimator when $A = B$, with a non vanishing noise bias term $b_\ell$.

C. Implementation

In this section we detail some important steps of the xQML implementation. We first discuss the pixel covariance matrix construction. We then derive an exact solution for the Sylvester Eq. (20). Finally, we describe a method for binning the xQML spectrum estimator.

1. Pixel covariance matrix

The datasets beams and pixel window functions are directly included in the $P_\ell$ matrices of Eq. (3). We do not discuss their construction, for which further details can be found in [15].

The covariance matrix $\mathbf{C}$ introduced in equation (2) includes correlations between pixels for each Stokes parameters,

$$\mathbf{C} = \begin{pmatrix} C^{TT} & C^{TQ} & C^{TU} \\ C^{QT} & C^{QQ} & C^{QU} \\ C^{UT} & C^{QU} & C^{UU} \end{pmatrix}. \quad (26)$$

We can separate the temperature and polarization measurements by using an approximated pixel covariance matrix

$$\tilde{\mathbf{C}} = \begin{pmatrix} C^{TT} & 0 & 0 \\ 0 & C^{QQ} & C^{QU} \\ 0 & C^{QU} & C^{UU} \end{pmatrix}. \quad (27)$$

This matrix does not mix temperature with polarization estimates. As a result, the $\tilde{C}_\ell$ estimator is not optimal any more, while still an unbiased estimator of the true $C_\ell$. As shown in [13], the price to pay is a slight error bar increase of the order of one percent. Using this choice, temperature and polarization analysis can be done completely separately. For the rest of this paper, we focus our analysis on polarization measurement only. The method can be implemented for the temperature spectrum estimation following the same approach.

In Eq. (3), the summation over $\ell$ is theoretically infinite. It can however be truncated at a given $\ell_{\text{max}}$ as long as the remaining contributions from $C_{\ell > \ell_{\text{max}}}$ are negligible. This can be accomplished manually by smoothing the dataset $d$ (e.g. by convolving the spectrum with a decreasing function). In the framework of our analysis, we simply generated CMB simulations while filtering all $C_{\ell > \ell_{\text{max}}}$.

The xQML variance has been shown to be minimal if the fiducial $\mathbf{C}$ matrix is built from the true $C$. In practice, it is not always possible to estimate precisely the latter. We can compute the estimator variance in Eq. (19) for any fiducial $\mathbf{C}$

$$\langle \Delta \hat{C}_\ell, \Delta \hat{C}_\ell' \rangle = \left[ \tilde{W}^{-1} \right]_{\ell \ell'} \left[ \mathbf{C}^{TT} \mathbf{E}_\ell \mathbf{C}^{BB} \mathbf{E}_{\ell'}^T \right] \left[ \tilde{W}^{-1} \right]_{\ell' \ell'} + \left[ \tilde{W}^{-1} \right]_{\ell \ell'} \left[ \mathbf{C}^{AB} \mathbf{E}_\ell \mathbf{C}^{AB} \mathbf{E}_{\ell'}^T \right] \left[ \tilde{W}^{-1} \right]_{\ell' \ell'}, \quad (28)$$

where $\mathbf{E}_\ell$ and $\tilde{W}_{\ell \ell'}$ are computed using $\tilde{C}$ in Eqs. (21) and (23).

To estimate the impact on the spectra estimations variance of small deviations of the fiducial $\mathbf{C}$ from the true $\mathbf{C}$, we consider a simplified toy-model with $\mathbf{C}^{AA} = \mathbf{C}^{BB} = \mathbf{C}$. We also restrict our calculation to the first term of Eq. (25), since we showed that, depending on the noise level, the second term is either negligible, either equal to the first one. Any small perturbation to the fiducial $\mathbf{C}$ around the true $\mathbf{C}$ can be written as

$$\tilde{\mathbf{C}} = \mathbf{C} + \epsilon, \quad \text{with} \quad \epsilon \ll \mathbf{C}, \quad (29)$$

and thus

$$\tilde{\mathbf{C}}^{-1} = \mathbf{C}^{-1} - \mathbf{D}, \quad \text{with} \quad \mathbf{D} \equiv \mathbf{C}^{-1} \epsilon \mathbf{C}^{-1} \ll \mathbf{C}^{-1} \quad (30)$$

At first order in $\mathbf{D}$,

$$\text{Tr} \left[ \mathbf{C} \mathbf{E}_\ell \mathbf{C} \mathbf{E}_{\ell'}^T \right] \simeq \text{Tr} \left[ \mathbf{C}^{-1} \mathbf{P}_\ell \mathbf{C}^{-1} \mathbf{P}_{\ell'} - 4 \mathbf{C}^{-1} \mathbf{P}_\ell \mathbf{D} \mathbf{P}_{\ell'} \right] \quad (31)$$

and

$$\tilde{W}_{\ell \ell'} \simeq \text{Tr} \left[ \mathbf{C}^{-1} \mathbf{P}_\ell \mathbf{C}^{-1} \mathbf{P}_{\ell'} - 2 \mathbf{C}^{-1} \mathbf{P}_\ell \mathbf{D} \mathbf{P}_{\ell'} \right]. \quad (32)$$
Inserting both expressions in Eq. (28),
\[
\langle \Delta \hat{C}_\ell, \Delta \hat{C}_\ell' \rangle = \frac{\operatorname{Tr}[C^{-1}P_\ell C^{-1}P_\ell'] - 4\operatorname{Tr}[C^{-1}P_\ell DP_\ell]}{\operatorname{Tr}[C^{-1}P_\ell C^{-1}P_\ell] - 2\operatorname{Tr}[C^{-1}P_\ell DP_\ell] - 2} \approx \frac{\operatorname{Tr}[C^{-1}P_\ell C^{-1}P_\ell]^{-1}}{2} = V_{\hat{C}_\ell}.
\]

We see that if a fiducial $\hat{C}$ sufficiently close to the true $C$ induces only second order deviations of the spectrum estimation variance from the optimal variance $V_{\hat{C}_\ell}$. For low SNR, the choice of the fiducial $\hat{C}_\ell$ have little impact on $C$. Conversely, for signal dominated datasets, deviations of $\hat{C}_\ell$ can have non-negligible impact on the spectrum error. A solution is to run the xQML method iteratively as recommended in [15], with previous spectrum estimation as the new fiducial model. This especially applies for the tensor-to-scalar ratio and reionization fiducial parameters. We have found that the choice of their fiducial values, if far from their true values, can greatly increase the order of 2% in the worse case, when the signal and the noise level are of the same order. We can thus safely use the approximated solution of Eq. (21) for the implementation of the xQML method.

3. Binning

CMB observations are only available on a limited sky fraction, as a result, individual multipole can be strongly correlated when reconstructing the CMB spectra. It is thus convenient to bin the power spectra in multipoles bandpowers, labelled $b$ hereafter. We define the binning operators,
\[
R_{b\ell} = \begin{cases} 
\Delta_b^{-1} & \text{if } \ell \in b \\
0 & \text{otherwise}
\end{cases}, \quad Q_{b\ell} = \begin{cases} 
1 & \text{if } \ell \in b \\
0 & \text{otherwise}
\end{cases},
\]
with $\Delta_b$ the width of the $b$th bin, which can be varied from one bin to another. The binned estimator is written
\[
\hat{y}_b \equiv \sum_{\ell} R_{b\ell} \hat{y}_\ell,
\]
for which the covariance reads
\[
\langle \Delta \hat{y}_b, \Delta \hat{y}_b' \rangle = \operatorname{Tr}[C^{AB}E_b C^{BB}E_b' + G^{AB}E_b G^{BB}E_b'] = \frac{1}{2\Delta_b} (W_{bb'} + G_{bb'})
\]
with $W_{bb'} = R_{b\ell} W_{\ell\ell'} Q_{b\ell'}$, and $G_{bb'} = R_{b\ell} G_{\ell\ell'} Q_{b\ell'}$. The true binned spectrum is thus
\[
C_b \equiv \sum_{\ell,\ell'} [W^{-1}]_{bb'} R_{b\ell} W_{\ell\ell'} C_{\ell'},
\]
and its unbiased binned estimation becomes
\[
\hat{C}_b \equiv \sum_{\ell} [W^{-1}]_{bb'} \hat{y}_\ell,
\]
with covariance
\[
V_{bb'} = \frac{1}{2\Delta_b} \left( [W^{-1}]_{bb'} + [W^{-1}]_{bb_1} G_{b_1 b_2} [W^{-1}]_{b_2 b'} \right).
\]

We remark that the binning can also be achieved by computing $P_b \equiv \sum_{\ell} P_{\ell}$ directly (without the normalization term $\Delta_b$), or equivalently $P_b \equiv \sum_{\ell} P_{\ell} Q_{b\ell}$. With this definition of $P_b$, the xQML components can be computed as usually defined in Eqs. (16), (18), (21) and (23) for the spectrum estimate $\hat{C}_\ell$, and Eqs. (24), (25) and (23) for its analytical covariance (replacing all subscripts $\ell$ by $b$). This method is computationally more efficient compared to the method presented above.

III. MONTE CARLO SIMULATIONS

In this section we describe two simulated surveys on which we test the xQML estimator. We first consider a nearly full sky experiment aiming at the measurement of the reionization signal ($\ell \lesssim 10$). The second
FIG. 3: \( EE \) (green) and \( BB \) (blue) mean power spectra xQML estimates \( \ell (\ell + 1) / 2\pi \cdot \langle \hat{C}_\ell \rangle \), and residues \( R_t[\hat{C}_\ell] \) from Eq. (43), computed from \( n_{\text{MC}} = 10^5 \) Monte-Carlo (MC) simulations. Spectra model are plotted in black solid line. Left panel corresponds to the reionization survey simulations \( (\ell_{\text{side}} = 16, f_{\text{sky}} \approx 0.7\%) \), right panel corresponds to the recombination survey simulations \( (\ell_{\text{side}} = 128, f_{\text{sky}} \approx 1\%) \). Noise level \( \sigma_n = 1 \mu \text{K.arcmin} \) for both surveys.

The 'reionization survey' sky patch is based on the Planck 2015 best fit spectrum model \( \Pi \) shown on Fig. 1 with a tensor-to-scalar ratio \( r = 10^{-3} \), and a reionization optical depth \( \tau = 0.06 \). Noise levels are between \( 0.1 \leq \sigma_n \leq 50 \mu \text{K.arcmin} \) for each of the cross dataset, and are indicated on Fig. 1. This choice roughly covers the characteristics of future ground experiments from CMB Stage-4 (S4) \( [19] \) (\(~ 1 \mu \text{K.arcmin}\)), or satellite such as LiteBIRD, CORE, and PICO (between 1 and 5 \( \mu \text{K.arcmin}\) \( [20–22] \), up to Planck noise level (around 50 \( \mu \text{K.arcmin}\) \( [23] \).

A. Reionization survey

For the large angular scales analysis, referred as the 'reionization survey', we consider an observed sky fraction \( f_{\text{sky}} \approx 70\% \). A binary mask is built from the 353 GHz Planck polarization maps, for which pixels with the highest polarization amplitude \( (Q^2 + U^2)^{1/2} \) accurately traces the galactic polarized dust. We choose to follow the instrumental specifications of the satellite mission LiteBIRD \( [20] \) considering a beam-width of 0.5 deg, and a white homogeneous noise. The analysis is done at the map resolution \( \ell_{\text{side}} = 16 \), over the multipoles range \( \ell \in [2, 47] \), and a beam-width of 0.5 deg. Due to the limited sky fraction, individual multipoles are strongly correlated. We thus reconstruct the spectrum using the binning scheme described in Sec. II C. We show the results starting from \( \ell = 48 \) to account for the insensitivity of the survey to large angular scales, and define 24 bins up to \( \ell = 383 \) with \( \Delta \ell = 14 \).

B. Recombination survey

The 'recombination survey' sky patch is based on the public BICEP2 \( [24] \) apodized mask \( M \in [0,1] \). We build a binary mask using all pixels \( i \) for which \( M_i \geq 0.1 \). Rather than considering a homogeneous noise as for the reionization survey, we apply an inverse weighting noise distribution based on the mask \( M \). The effective sky fraction is therefore \( f_{\text{sky}} = (\sum M_i^2) / \sum M_i \approx 1\% \), as defined in \( [23] \). Our analysis is done with maps resolution \( \ell_{\text{side}} = 128 \), and a beam-width of 0.5 deg. Due to the limited sky fraction, individual multipoles are strongly correlated. We thus reconstruct the spectrum using the binning scheme described in Sec. II C. We show the results starting from \( \ell = 48 \) to account for the insensitivity of the survey to large angular scales, and define 24 bins up to \( \ell = 383 \) with \( \Delta \ell = 14 \).

C. Power spectra reconstruction

We verify with simulations that the reconstructed power spectra are unbiased with respect to the input model \( C_\ell \). From the central limit theorem we expect that, as \( n_{\text{MC}} \) is large, the mean spectra residues

\[
R_t[\hat{C}_\ell] \equiv \frac{C_\ell - \langle \hat{C}_\ell \rangle}{\sqrt{\sigma^2(C_\ell^{\text{MC}})/n_{\text{MC}}}} \tag{43}
\]

are expected to be normally distributed around zero for all \( \ell \) if the spectra are unbiased, with
\( \sigma^2(\hat{C}_{\text{MC}})/n_{\text{MC}} \) the MC variance of the mean spectra. We carefully checked that this is the case for all noise levels \( 0.1 \leq \sigma_n \leq 50 \mu \text{K.arcmin} \). Power spectra and their residues are shown on Fig. 3 for \( 1 \mu \text{K.arcmin} \). Given the residues distribution for \( n_{\text{MC}} = 10^5 \) simulations, we conclude that the spectra bias level is less than one percent of the spectra errors.

The MC spectra variance and that derived analytically \( \sigma^2(\hat{C}_{\text{ana}}) = V_\ell \) in Eq. (24) are shown to be in excellent agreement, as displayed on Fig. 5. The covariance matrix, not shown here, is band diagonal over the whole multipoles range, meaning that correlations are low and only occur between neighbouring bins.

We successfully verified that the xQML spectrum reconstruction is unbiased, and that the MC covariance corresponds to that expressed analytically. The xQML thus gives near minimal spectrum error.

### IV. EB LEAKAGE

#### A. Modes mixing

The mode-mixing matrix \( W_{\ell\ell'} \) introduced in Eq. 7 quantifies the contribution of all \( \ell' \)-modes to the spectrum estimator at angular scale \( \ell \). The rescaled matrix

\[
\bar{W}_{\ell\ell'} = \frac{W_{\ell\ell'}}{\sqrt{W_{\ell\ell}W_{\ell'\ell'}}},
\]

is displayed on Fig. 6 in log-scale for \( \sigma_n = 1 \mu \text{K.arcmin} \). The off-diagonal blocks quantify the \( E/B \) modes mixing, also known as polarization leakage. This mixing appears as soon as maps are partially masked, making some modes ambiguously belonging to both \( E \) and \( B \) polarizations patterns.

We remark that the \( E/B \) mixing is on average very low. Most of the \( E \)-to-\( B \) leakage is localized at \( \ell \lesssim 10 \) for the reionization survey. The recombination survey also suffers from a polarization mixing increase at \( \ell \gtrsim 250 \). This effect is caused by the pixel resolution of the maps. It appears when the multipole angular scale is close to the typical pixel scale, and disappears as soon as we increase the datasets pixel resolution. The effect remains however very small. For the multipoles ranges of interest, it induces a negligible increase of variance as shown hereafter.
B. Variance induced leakage

Due to polarization leakage, $E$ and $B$ modes respective uncertainty contribute to each other variance. For noise-dominated datasets, this variance leakage has a small impact since both polarizations have the same noise, and their mutual contributions are equivalent. Conversely, when the noise is much below the signal level, the uncertainty is limited by the intrinsic ‘cosmic variance’, arising from the finite number of modes that can be sampled on the sky. The $E$-modes signal, thus its cosmic variance, is much higher than that of $B$-modes. As a consequence, even for small polarization mixing, the impact of the $E$-to-$B$ variance leakage can become non-negligible.

Since by construction the error of the xQML estimator is minimal, it also minimizes the amount of variance leakage. The $BB$ uncertainty is represented on Fig. 7 for which we compare the cases with and without leakage. The latter is obtained by simulating CMB polarization maps using null $EE$ and $TE$ spectra. We also show the absolute level of variance leakage $[\sigma(C^\text{leak}_\ell) - \sigma(C^\text{noleak}_\ell)]/\sigma(C^\text{noleak}_\ell)$. We observe that the recovered spectra uncertainties for $\sigma_n = 0.1$ and $\sigma_n = 1 \mu K.\text{arcmin}$ are both mostly cosmic variance limited by the lensing $B$-modes signal. We also recover that the impact of the cosmic leakage gets less important as the SNR decreases.

For the reionization survey, the variance leakage is observed to be maximal at large angular scales, up to a 80% increased uncertainty around $\ell \lesssim 10$, which quickly drops to 30% for higher $\ell$‘s. This is not surprising since, for this multipoles range, the $EE$ cosmic variance as well as the $E$-to-$B$ mixing in $W_{\ell\ell'}$ are maximal.

For the recombination survey the impact is maximal for the first bins. This is again related to the higher polarization mixing in $W_{\ell\ell'}$ at those multipoles. It then drops to 20% for $\ell \gtrsim 90$, followed by a slight increase at $\ell \gtrsim 250$. This is consistent with the previous $E/B$ mixing observations made on $W_{\ell\ell'}$ for this multipoles range. The impact at low $\ell$‘s remains however smaller since the $E$-modes cosmic variance level is much lower for those angular scales.

We conclude that, even if the mixing between polarization modes is minimized when using the xQML estimator, the induced variance increase can however be non-negligible, especially at large angular scales.

C. Comparison with pseudo-spectra

The uncertainty on the reconstructed $B$-mode power spectrum from the xQML is compared on Fig. 8 with other methods such as the standard pCl and the (pure) PpCl approach, using $10^4$ MC simulations. We follow the cross PpCl formalism described in [9], for which the mask and its first derivative are required to be equal to zero on its boundaries. This is achieved by applying the apodization function ‘C2’ defined in [9] to our binary masks, parametrized by the apodization length parameter $\theta_\ast [\text{deg}]$. This parameter needs to be adapted to the SNR, i.e., for each multipole.

As illustrated on Fig. 8, the pCl leads to higher uncertainties. The $E$-modes cosmic leakage contribution is particularly visible on the recombination survey $B$-modes variance, for which the two bumps $\ell \simeq 100$ and $\ell \gtrsim 300$ follow the $E$-modes power spectrum at those scales.

Compared to the xQML, we observe a significant rise of the PpCl uncertainty at large angular scales, which tends to decrease as $\ell$ increases. This behaviour is visible on both the reionization and recombination surveys, and is expected since the variance leakage is maximal for this multipoles range, as previously showed in Sec. [11]. As smaller angular scales are probed, the polarization mixing impact is less important. The effect of the mask shape for the
PpCl method is clearly visible: broader apodization lengths reduce the amount of leakage at large angular scales ($\ell \lesssim 15$ for the reionization survey, and $\ell \lesssim 90$ for the recombination survey), but also reduces the effective observed sky fraction, thus rising the sampling variance at the remaining higher multipoles. A possible solution is to select for each multipole the mask apodization for which the mode estimate has minimal variance. Each mode can thus be combined to reconstruct an unbiased spectrum estimate, which covariance matrix can be evaluated using MC simulations. This process has to be repeated depending on the noise level. The resulting spectrum uncertainty $\sigma(\hat{C}_\ell^\text{comb})$, shown on Fig. 8 is close to the joined spectra minimum variances, that is to say $\sigma(\hat{C}_\ell^\text{comb}) \simeq \min \{ \sigma(\hat{C}_\ell^\text{pCl}), \ldots, \sigma(\hat{C}_\ell^\text{xQML}) \}$. In order to fully visualize the apodization effect, we also show PpCl errors for each apodization length value. Longer apodization lengths do not improve further the large scale spectra uncertainties ($\theta_0 \geq 30^\circ$ for the reionization, and $\theta_0 \geq 10^\circ$ for the recombination survey).

We conclude that the xQML method is particularly suited for reducing the B-modes variance leakage for large angular scale analysis compared to the PpCl approach. It produces smaller error bars and does not require mask apodization optimizations. This is of special interest for primordial $B$-modes detection.

V. E-B CORRELATION SPECTRUM

Although first order primordial $E$-$B$ and $T$-$B$ correlations are predicted to be null in the frame of the $\Lambda$CDM model, non-standard cosmological mechanisms, such as cosmic birefringence, could induce non-zero correlation spectra \cite{26, 27, 28, 29, 30, 31, 32}. In addition to providing an important probe to non-standard physics, measuring $E,B,TB$ spectra could also help to diagnose instrumental systematic effects \cite{33, 34}.

We focus on the $E$-$B$ correlation, for which we compute the $EB + BE$ spectrum variance. The rescaled mode-mixing matrix introduced in Eq. (11) is extended to $EB$ multipoles as displayed on Fig. 6 for $1\mu K\cdot\text{arcmin}$. Apart from a negligible resolution effect for high $\ell$'s, we observe no mixing between $EB$ and $EE, BB$ when using the xQML method. Note however that this statement is not true if we consider particular models with non-zero $\tilde{C}_{E}^{EB}$.

As in the previous section for the $BB$ uncertainty, we compare our results with the pCl and PpCl methods. The latter is computed using the hybrid approach proposed in \cite{10}, where the $E$-modes are obtained using the classic pseudo-spectrum, and the $B$-modes using the pure method. Variances are shown on Fig. 6 for $1\mu K\cdot\text{arcmin}$. The PpCl uncertainty is about 20%-60% higher than that of the xQML for the reionization survey. Longer mask apodization lengths improve the PpCl error for $\ell \lesssim 10$. On the recombination survey, the xQML gives significant lower $EB$ uncertainty only for $\ell \lesssim 100$. The conclusion is similar as for the $BB$-spectrum analysis. The xQML method provides an efficient estimator for large angular scales analysis.

VI. CONCLUSION

In this paper, we derived a pixel-based spectrum estimator which allows to cross-correlate CMB datasets. The method is very similar to the QML, but does not require a precise knowledge of the datasets noise covariance matrices to subtract the noise bias. We also provided an approximation to the Sylvester equation that has little impact on the optimality of the estimator, which, by construction, provides near-minimal error bars. The estimator variance is shown to be sensitive to only second order perturbations of the fiducial pixels covariance matrix. Moreover, using no $TQ$ and $TU$ correlations for the construction of this matrix, temperature and polarization analysis can be done completely separately.

We showed that the xQML estimator is unbiased, and that the error bars on the recovered spectrum obtained from Monte-Carlo simulations correspond to the variance derived analytically. We presented two CMB surveys aiming at the reionization and recombination polarized signals measurement, with a fiducial
FIG. 9: $EB$ spectrum errors from xQML, PpCl (pure pCl), and classic pCl estimators, for the reionization (left) and recombination (right) surveys, at noise level $\sigma_n = 1\mu K \text{arcmin}$. The mask apodization lengths $\theta_n$ [deg] are specified for each pseudo-spectrum, the uncertainty from the combined PpCl apodizations is in dashed red.

FIG. 10: The normalized mode-mixing matrix $\tilde{W}_{\ell\ell'}$ defined in Eq. (11) in log-scale, for the reionization (up) and recombination (down) surveys, for $\sigma_n = 1\mu K \text{arcmin}$.

tensor-to-scalar ratio $r = 10^{-3}$. The source of polarization leakage can be identified in the mode-mixing matrix $W_{\ell\ell'}$. We showed in Sec. IV that it is consistent with the increase of $B$-modes variance when compared to the no-leakage case. The reionization survey $BB$ uncertainty at low noise levels is particularly impacted by the polarization mixing, with a maximum of 80% increase for large angular scales at 0.1 - 1 $\mu K \text{arcmin}$. Since the xQML method minimizes bins correlations as well as polarization mixing, the resulting error bars thus correspond to the minimal uncertainty achievable when aiming to polarization variance leakage reduction.

Comparison with the pure pseudo-spectrum formalism shows a significant improvement of the error bars and correlations for both $BB$ and $EB$ when using the xQML method. The particular advantage relative to pure methods is that it does not require any special masks apodization processing. However, due to its higher computational cost ($O(N_d^3)$ operations) relative to pseudo-spectra ($O(N_d^{3/2})$ operations), the xQML cannot be run on as many modes as for the pseudo-spectra. For those reasons, the xQML estimator is particularly suited for large and intermediate angular scales analysis.

As a forecast analysis, we show on Fig. 11 the uncertainty on $r$, obtained from each method introduced previously, as a function of the noise level. We also proceed with a comparison with the mode-counting formula\(^4\), which gives a naive estimate of the lowest achievable variance, neglecting correlations and leakage induced by the sky coverage. We use the spectrum-based likelihood presented in [29], which is a cross-spectrum extended version of the low-multipoles Hamimeche&Lewis likelihood [30]. The pure method covariance matrix is computed as de-

\(^4\) i.e. \[2\hat{C}_\ell + 2\hat{C}_\ell (N^A_\ell + N^B_\ell) + N^A_\ell N^B_\ell / [(\ell+1)\Delta \ell J_{\ell \ell'}],\]
where $\hat{C}_\ell$ is the power spectrum fiducial model, $N_\ell = n_\ell/B_\ell$ is the noise spectrum of the dataset convolved by the corresponding beam functions $B_\ell$. 

\[W_{\ell\ell'} = \left[ \begin{array}{ccc} W_{EE} & W_{EB} & W_{BB} \\ W_{BE} & W_{BB} & W_{EB} \\ W_{EB} & W_{BB} & W_{EE} \end{array} \right] \]
scribed in Sec. [IV.C] We consider only two datasets, no foreground contamination and/or residual, nor de-lensing. For low SNR, the impact of the polarization mixing is small, and both pseudo-spectrum methods give the same error on \( r \). For high SNR, the uncertainty on \( r \) is cosmic variance limited, which corresponds to the plateau from \( \sigma_n = 0.1 \) to \( \sigma_n = 1 \mu K.arcmin \). At this regime, the \( q \)QLM produces \( \sim 30\% \) lower uncertainty on \( r \) than the \( PpCl \) method.

![FIG. 11: Error on the tensor-to-scalar ratio with a fiducial \( r = 10^{-3} \), for the reionization (up) and recombination (bottom) surveys. We compare the uncertainty obtained from the standard pseudo-spectrum (blue stars), the pure pseudo-spectrum (orange triangles), the cross quadratic pixel based (green dots), and the mode-counting formula (red squares), with respect to noise levels \( 0.1 \leq \sigma_n \leq 50 \mu K.arcmin \).](image)

**Acknowledgments**

The authors would like to thank G. Efstathiou and J. Grain for the helpful discussions about the \( q \)QLM method. We also thank H. Taeter for his help leading to the identification of the Sylvester equation. Some of the results in this paper have been derived using the HEALPix [37] package and the NaMaster [38] package.
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