Cosmic microwave background lensing with optimal convergence and shear estimators

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We present the optimal convergence and shear estimators for lensing reconstruction from the cosmic microwave background temperature field. This generalizes the deflection estimator, is sensitive to non-lensing modes, provides internal consistency checks, and is always at least as optimal. Previously, these estimators were only known in the squeezed limit. This paper decomposes convergence and shear fields into cosine and sine waves and the lensed correlation function is then Taylor expanded in the wave amplitudes. Maximizing the likelihood function gives the optimal estimators for the convergence and shear fields.

This method has the potential to improve the lensing reconstruction of the cosmic microwave background polarization field: the shear and convergence can be optimally combined to form a deflection estimator, or used separately to separate non-lensing modes, or utilize lensing of non-Gaussian secondary foregrounds.

I. INTRODUCTION

Gravitational lensing of the cosmic microwave background (CMB) has been recognized as a powerful probe of the large-scale structure of the Universe \cite{1,2}. Weak lensing has the advantage of directly tracing the matter distribution in the Universe and thus avoids the uncertainties with the relation between the galaxy and matter distributions. Precision measurements of the CMB lensing can be used to constrain the neutrino masses, dark energy, primordial non-Gaussianity, and the halo masses, etc\textsuperscript{2}. CMB lensing has been measured at high significance by current surveys (see e.g., Planck \cite{3}, ACT \cite{4}, SPTpol \cite{5}, and others) and future ground CMB experiments will continue to improve the measurements substantially (e.g., Simons Observatory \cite{6}, CMB-S4 \cite{7}).

The performance of CMB lensing reconstruction depends on the algorithms used to extract the lensing signal from the observed CMB map. The optimal quadratic deflection estimator is constructed by expanding the observed CMB temperature and polarization to linear order in the lensing deflection angle \cite{7,8}. Within this linear approximation, the quadratic estimator gives an optimal estimate for the lensing deflection field.

The deflection field reconstructs a displacement vector, i.e. two numbers at each point. In lensing, three numbers are observable: one convergence and two shears. In single plane lensing, all effects are a single scalar degree of freedom. In post-Born lensing, a curl, or B-mode can be generated. In contrast, gravitational waves are distinguishable from both scalar and B lensing\cite{9}, which illustrates information lost in the deflection estimation procedure. This paper will recover this lost information.

The quadratic estimator is constructed based on the linear order lensing effect on the CMB and thus can be biased and suboptimal due to the higher order terms \cite{10–12}. Therefore, the maximum likelihood estimator has been first proposed in Refs. \cite{10,11} and further explored in Refs. \cite{13,14}. However, the maximum likelihood estimators are generally very difficult to compute and have to be evaluated iteratively. In addition, the estimators based on the deflection angle are susceptible to the foreground contamination and can have a significant lensing bias for reconstruction with the CMB temperature \cite{15–18}.

The convergence and shear estimators have been proposed by considering the distortion of local CMB features from the large-scale lensing modes in Refs. \cite{19,20}, and the optimal weights in the long wavelength (squeezed) limit have been derived in Refs. \cite{21,22}. With the independence of convergence and shear and information, it is possible to separate the lensing signal from the lensing bias due to the extragalactic foregrounds \cite{18}. Unlike the optimal quadratic deflection estimator, the local convergence and shear estimators are only optimal on large scales and become non-optimal on smaller scales.

The multipole estimators can in principle reach the optimality of the quadratic deflection estimators \cite{18}, but it is also very difficult to apply to the real CMB data.

In this paper, we present the optimal convergence and shear estimators for the lensing reconstruction from CMB temperature map. We expand the lensed CMB correlation function to linear order in the convergence and shear fields in position space. The optimal estimators are given...
by the solution to the maximum likelihood function. The minimum variance combination of the convergence and shear estimators is equally optimal as the quadratic estimator on small scales and even better than the quadratic estimator on large scales, which is consistent with the results of the maximum likelihood analysis presented in Ref. [10].

This paper is organized as follows. In Sec. II we introduce the new formalism for describing CMB lensing. In Sec. III we describe the maximum likelihood estimator. In Sec. IV we test the performance of the estimators in simulations and show the numerical results. We discuss the future development and conclude in Sec. V.

II. FORMALISM

The convergence and shear describe the differential stretching of structures in the sky, analogous to the metric in general relativity. Lensing is a special case of a metric that results from a coordinate change of Euclidean space. In this case, one can describe the metric by a lensing transformation. An arbitrary metric can contain intrinsic curvature, making it unreducible to Euclidean space. This a full lensing estimator must be constructed in curvilinear space, an attribute which has slowed down attempts to implement this apart from the squeezed limit.

In this section, we introduce the nonlocal description for weak lensing where the relative deflection between two points is expressed as an integral over the convergence and shear fields along the unperturbed path. Then we can Taylor expand the lensed CMB temperature covariance using the convergence and shear to linear order with negligible higher order terms.

A. CMB lensing

Weak lensing of the CMB photons by the intervening matter distribution remaps the CMB temperature field by the deflection field $\alpha = \nabla \phi$ as

$$\tilde{T}(\theta) = T(\theta + \nabla \phi) = T(\theta) + \nabla \phi \cdot \nabla T(\theta) + \cdots,$$

where $\theta$ is the direction on the sky, $\tilde{T}$ is the lensed CMB temperature field, $T$ is the unlensed CMB temperature field, and $\phi$ is the lensing potential.

The transformation matrix for lensing remapping from the observed coordinate to the source coordinate, $\theta^S = \theta + \nabla \phi$, can be usefuly decomposed into convergence and shear as

$$M^S_{ij} = \frac{\partial \theta^S_i}{\partial \theta^S_j} = \begin{pmatrix} 1 - \kappa - \gamma_1 & -\gamma_2 \\ -\gamma_2 & 1 - \kappa + \gamma_1 \end{pmatrix},$$

where $\kappa = -(\phi_{,11} + \phi_{,22})/2$ is the convergence, $\gamma_1 = -(\phi_{,11} - \phi_{,22})/2$ and $\gamma_2 = -\phi_{,12}$ are the two components of the shear. Note that here $\phi_{,ij}$ denotes $\partial^2 \phi / \partial \theta^i \partial \theta^j$.

For weak gravitational lensing, the convergence and shear fields should be much smaller than unity; therefore, the transformation matrix $M$ is invertible everywhere.

The local transformation defined by $M$ describes the deformation of a feature on last scattering surface of infinitesimal angular size $d\theta$. The convergence and shear estimators can be constructed from local estimates of the anisotropic CMB power spectrum at the sky position $\theta$, but are only optimal in the long wavelength limit.

Therefore, instead of the differential variation of the deflection angle at a position $\theta$, we want to describe the relative deflection between two points at a finite distance on the sky. This describes the nonlocal effect of convergence and shear on the distance between two points on the last scattering surface instead of the deformation of a feature in the primary CMB temperature of infinitesimal angular size which is local on the sky.

B. Lensing metric

The lensing remapping from the observed coordinate to the source coordinate can be described by the matrix $M$ at the sky position. The invariant distance $ds$ between a point $\theta_S$ and a neighbouring point $\theta_S + d\theta_S$ on the last scattering surface is given by

$$ds^2 = \delta_{ij}d\theta^S_i d\theta^S_j,$$

which is invariant under the lensing remapping. In the observed coordinate, we have

$$ds^2 = g_{\mu\nu}d\theta^\mu d\theta^\nu,$$

where $g_{\mu\nu}$ is the lensing metric tensor. Combining Eq. (3) and Eq. (1), we have

$$\delta_{ij}d\theta^S_i d\theta^S_j = g_{\mu\nu}d\theta^\mu d\theta^\nu.$$

Using Eq. (2), we obtain

$$\delta_{ij}M^S_{1\mu} M^S_{2\nu} d\theta^\mu d\theta^\nu = g_{\mu\nu}d\theta^\mu d\theta^\nu,$$

for any $d\theta^\mu$ and $d\theta^\nu$, implying

$$g_{\mu\nu} = \delta_{ij} M^i_{\mu} M^j_{\nu}.$$

Keeping the linear order terms, we have

$$g_{\mu\nu} = \begin{pmatrix} 1 - 2\kappa - 2\gamma_1 & -2\gamma_2 \\ -2\gamma_2 & 1 - 2\kappa + 2\gamma_1 \end{pmatrix}.$$

In the regime of weak lensing where the lensing distortion is small, it should be a valid approximation to neglect the higher order terms in convergence and shear.

The distance between two points $A$ and $B$ on the last-scattering surface is given by

$$S_{AB} = \int_A^B ds = \int_A^B \sqrt{g_{\mu\nu}d\theta^\mu d\theta^\nu}.$$
We wish to write the distance between unlensed positions of $A$ and $B$ in terms of the observed coordinates with the lensing metric. However, this can not be integrated analytically if we do not know the form of convergence and shear fields in the lensing metric.

Let us first consider the convergence field. In terms of the Fourier components, we have

$$\kappa(\theta) = \int \frac{d^2 \ell}{(2\pi)^2} \kappa(\ell)e^{i\ell \cdot \theta},$$  \hspace{1cm} (10)

where $\kappa(-\ell) = \kappa^*(\ell)$ since $\kappa(\theta)$ is a real scalar field. We only need to consider a half plane in Fourier space, $\ell > 0$ and $0 \leq \phi_\ell < \pi$. Thus

$$\kappa(\theta) = \int_{0 \leq \phi_\ell < \pi} \frac{d^2 \ell}{(2\pi)^2} \left[ \kappa(\ell)e^{i\ell \cdot \theta} + \kappa^*(\ell)e^{-i\ell \cdot \theta} \right].$$ \hspace{1cm} (11)

Decompose the complex exponentials into sine and cosine functions, we derive

$$\kappa(\theta) = \frac{1}{L^2} \sum_{0 \leq \phi_\ell < \pi} \left[ 2\kappa^*(\ell) \cos(\ell \cdot \theta) - 2\kappa^1(\ell) \sin(\ell \cdot \theta) \right],$$ \hspace{1cm} (12)

where $L$ is the size of the periodic box, $\kappa^*(\ell)$ and $\kappa^1(\ell)$ are real and imaginary parts of the complex Fourier coefficient $\kappa(\ell)$.

We write the convergence field as a linear combination of sine and cosine waves, with appropriate weights. We can easily estimate the magnitude of the coefficient from its variance

$$\langle (2\kappa^1(\ell)2\kappa^1(\ell)) \rangle = \frac{2C_{\kappa^1\kappa^1}}{L^4}.$$ \hspace{1cm} (13)

For a $10^6$ square patch of sky, $L = \pi/180 \approx 0.174$. Given that $C_{\kappa^1\kappa^1}$ has a maximum of approximately $2 \times 10^{-7}$, we find the standard deviation of about $2.57 \times 10^{-3}$, which is significantly less than one. The cumulative variance of convergence from all scales is given by $\langle \kappa(\theta)\kappa(\theta) \rangle = \int \langle \kappa(\ell) \rangle C_{\kappa^1\kappa^1}$. We find that the rms convergence to the last scattering surface is about 6% and 7% for $\ell_{\text{max}}$ = 3000 and 5000; therefore, the higher order term proportional to $O(k_2^2)$ is less than one percent. From this we verify that the linear order lensing Taylor expansion in convergence and shear is a good approximation [21].

For the lensing shear fields, we also have

$$\gamma_1 = \frac{1}{L^2} \sum_{0 \leq \phi_\ell < \pi} \left[ 2\gamma_1^1(\ell) \cos(\ell \cdot \theta) - 2\gamma_1^1(\ell) \sin(\ell \cdot \theta) \right],$$ \hspace{1cm} (14)

and

$$\gamma_2 = \frac{1}{L^2} \sum_{0 \leq \phi_\ell < \pi} \left[ 2\gamma_2^1(\ell) \cos(\ell \cdot \theta) - 2\gamma_2^1(\ell) \sin(\ell \cdot \theta) \right].$$ \hspace{1cm} (15)

In the following, we will use the dimensionless coefficients $\kappa^1(\ell) = 2\kappa^1(\ell)/L^2$ and $\kappa^1(\ell) = 2\kappa^1(\ell)/L^2$, similarly for the shear fields, where the superscript denote the weights of cosine and sine waves.

1. Convergence

Let us start with just one cosine wave of the convergence field, $\kappa(\theta) = \kappa^1(\ell) \cos(\ell \cdot \theta)$. Now the lensing metric tensor takes the form

$$g_{\mu\nu}(\theta) = \begin{pmatrix} 1 - 2\kappa(\theta) & 0 \\ 0 & 1 - 2\kappa(\theta) \end{pmatrix},$$ \hspace{1cm} (16)

and

$$S_{AB} = \int_{A}^{B} \sqrt{1 - 2\kappa(\theta)} \sqrt{d\theta^1}^2 + (d\theta^2)^2.$$ \hspace{1cm} (17)

Without loss of generality, we can take the wave vector $\ell = (\ell_1, 0)$ along the $\theta^1$ axis. Then we have the convergence field $\kappa(\theta) = \kappa^1(\ell_1, 0) \cos(\ell_1 \theta^1)$, varying only in the $\theta^1$ direction. We approximate the first term in the integral to linear order, $\sqrt{1 - 2\kappa(\theta)} \approx 1 - \kappa(\theta)$ and integrate along the unperturbed path connecting the lensed positions of $A$ and $B$ in the observed coordinates,

$$S_{AB} = \dot{\theta} \left[ 1 - \kappa^1(\ell) M_{\kappa^1}(\theta_A, \theta_B) \right],$$ \hspace{1cm} (18)

where $\dot{\theta}$ is the magnitude of the relative position vector $\theta = \theta_B - \theta_A$, the relative distance between the lensed positions of points $A$ and $B$, and the matrix

$$M_{\kappa^1}(\theta_A, \theta_B) = \frac{\sin(\ell_1 \theta_b^1) - \sin(\ell_1 \theta_A^1)}{\ell_1 \theta_B^1 - \ell_1 \theta_A^1}.$$ \hspace{1cm} (19)

To illustrate how convergence changes the relative deflection between two points, we can consider a few extreme examples. When the amplitude of the cosine wave $\kappa^1(\ell_1, 0)$ equals zero, we have $S_{AB} = \dot{\theta}$; the relative distance between the lensed positions of $A$ and $B$ is the same as the unlensed positions. When $\kappa^1 = 2\pi n/\ell_1$ and $n$ is an integer, $M_{\kappa^1}(\theta_A, \theta_B)$ is zero; here the convergence effect cancels since it is a sinusoidal function. When $\kappa^1$ is much smaller than the wavelength $2\pi/\ell_1$, $M_{\kappa^1}(\theta_A, \theta_B)$ approaches $\cos(\ell_1 \theta_A^1)$, i.e., the value of convergence at position $A$. When $\kappa^1$ is much larger than the wavelength $2\pi/\ell_1$, we have $M_{\kappa^1}(\theta_A, \theta_B) \ll 1$, where a near cancellation occurs between the two positions.

For a cosine convergence wave $\kappa(\theta) = \kappa^1(\ell) \cos(\ell \cdot \theta)$ in any direction, we have

$$M_{\kappa^1}(\theta^A, \theta^B) = \frac{\sin(\ell \cdot \theta_B^1) - \sin(\ell \cdot \theta_A^1)}{\ell \cdot \theta_B^1 - \ell \cdot \theta_A^1},$$ \hspace{1cm} (20)

where the difference is just replacing $\ell_1 \theta^1$ by $\ell \cdot \theta$. The inner product $\ell \cdot \theta$ is the product of the wavenumber $\ell$ and the projection of the vector $\theta$ in the direction of the wave vector $\ell$.

Similarly, for a sine wave $\kappa(\theta) = -\kappa^1(\ell) \sin(\ell \cdot \theta)$, we obtain

$$S_{AB} = \dot{\theta} \left[ 1 - \kappa^1(\ell) M_{\kappa^1}(\theta_A, \theta_B) \right],$$ \hspace{1cm} (21)

where

$$M_{\kappa^1}(\theta_A, \theta_B) = \frac{\cos(\ell \cdot \theta_B) - \cos(\ell \cdot \theta_A)}{\ell \cdot \theta_B - \ell \cdot \theta_A}.$$ \hspace{1cm} (22)
2. Shear 1

For the $\gamma_1$ component of the lensing shear field, the lensing metric can be written as

$$g_{\mu\nu}(\theta) = \begin{pmatrix} 1 - 2\gamma_1(\theta) & 0 \\ 0 & 1 + 2\gamma_1(\theta) \end{pmatrix},$$

and the unlensed distance between $A$ and $B$ is given by the observed coordinates,

$$S_{AB} = \int_A^B \sqrt{(1 - 2\gamma_1(\theta))(d\theta^1)^2 + (1 + 2\gamma_1(\theta))(d\theta^2)^2}. \tag{24}$$

For a cosine or sine wave of the $\gamma_1$ shear field, $\gamma_1(\theta) = \gamma_1^c(\theta) \cos(\ell \cdot \theta)$ or $\gamma_1(\theta) = \gamma_1^s(\theta) \sin(\ell \cdot \theta)$, we have

$$S_{AB} = \vartheta \left[ 1 - \gamma_1^{c/s}(\ell) M_{\gamma_1^{c/s}}(\theta_A, \theta_B) \right], \tag{25}$$

where

$$M_{\gamma_1^c}(\theta_A, \theta_B) = \frac{(\vartheta^1)^2 - (\vartheta^2)^2 \sin(\ell \cdot \theta_B) - \sin(\ell \cdot \theta_A)}{(\vartheta^1)^2 + (\vartheta^2)^2} \ell \cdot \theta_B - \ell \cdot \theta_A, \tag{26}$$

and

$$M_{\gamma_1^s}(\theta_A, \theta_B) = \frac{(\vartheta^1)^2 - (\vartheta^2)^2 \cos(\ell \cdot \theta_B) - \cos(\ell \cdot \theta_A)}{(\vartheta^1)^2 + (\vartheta^2)^2} \ell \cdot \theta_B - \ell \cdot \theta_A. \tag{27}$$

The factor before the sinusoidal part accounts for the anisotropic nature of the $\gamma_1$ shear field. When the slope of $\vartheta$ is 1 or $-1$, $\vartheta^1 = \vartheta^2$ or $\vartheta^1 = -\vartheta^2$, the distance between $A$ and $B$ is invariant under the mapping by $\gamma_1$ shear field. The $\gamma_1$ shear does not induce variation along these two directions.

3. Shear 2

For the $\gamma_2$ component of the shear field, we have the lensing metric tensor

$$g_{\mu\nu}(\theta) = \begin{pmatrix} 1 & -2\gamma_2(\theta) \\ -2\gamma_2(\theta) & 1 \end{pmatrix},$$

and the unlensed distance between $A$ and $B$ written in the observed coordinates,

$$S_{AB} = \int_A^B \sqrt{(d\theta^1)^2 + (d\theta^2)^2 - 2 \times 2\gamma_2(\theta))d\theta^1d\theta^2}. \tag{29}$$

For a cosine or sine wave of the $\gamma_2$ shear field, $\gamma_2(\theta) = \gamma_2^c(\theta) \cos(\ell \cdot \theta)$ or $\gamma_2(\theta) = \gamma_2^s(\theta) \sin(\ell \cdot \theta)$, we have

$$S_{AB} = \vartheta \left[ 1 - \gamma_2^{c/s}(\ell) M_{\gamma_2^{c/s}}(\theta_A, \theta_B) \right], \tag{30}$$

where

$$M_{\gamma_2^c}(\theta_A, \theta_B) = \frac{2\vartheta^1\vartheta^2}{(\vartheta^1)^2 + (\vartheta^2)^2} \frac{\sin(\ell \cdot \theta_B) - \sin(\ell \cdot \theta_A)}{\ell \cdot \theta_B - \ell \cdot \theta_A}, \tag{31}$$

and

$$M_{\gamma_2^s}(\theta_A, \theta_B) = \frac{2\vartheta^1\vartheta^2}{(\vartheta^1)^2 + (\vartheta^2)^2} \frac{\cos(\ell \cdot \theta_B) - \cos(\ell \cdot \theta_A)}{\ell \cdot \theta_B - \ell \cdot \theta_A}. \tag{32}$$

Here, the prefactor of the sinusoidal part reflects the anisotropic nature of the $\gamma_2$ shear field. When $\theta$ is along the $\theta^1$ axis or $\theta^2$ axis, the distance between $A$ and $B$ is invariant under the mapping by $\gamma_2$ shear.

C. CMB correlation function

Lensing remap the CMB temperature field on the sky and thus changes the correlation function. The lensed CMB temperature correlation function is given by

$$C_{TT}^\sim(\theta_A, \theta_B) = C_{TT}(S_{AB}), \tag{33}$$

where $C_{TT}$ is the correlation function of the unlensed CMB temperature, which only depends on the separation between points. Combining all the convergence and shear waves, the distance between the unlensed positions of $A$ and $B$ is

$$S_{AB} = \vartheta \left( 1 - \sum_\alpha p_\alpha M_\alpha(\theta_A, \theta_B) \right), \tag{34}$$

where $\vartheta$ is the observed distance between two points on the sky, and $p_\alpha$ denotes the lensing parameters, $\kappa^c(\ell)$, $\kappa^s(\ell)$, $\gamma_1^c(\ell)$, $\gamma_1^s(\ell)$, $\gamma_2^c(\ell)$, $\gamma_2^s(\ell)$. Here we include the $\ell$ dependence in $p_\alpha$ for brevity. We can approximate the covariance of the lensed CMB temperature to linear order in convergence and shear:

$$C_{TT}^\sim(\theta_A, \theta_B) = C_{TT}(\vartheta) + \sum_\alpha p_\alpha C_{TT}^\alpha(\theta_A, \theta_B), \tag{35}$$

where the first derivative

$$C_{T}^\alpha(\theta_A, \theta_B) = -\frac{\partial C_{TT}(\vartheta)}{\partial \ln \vartheta} M_\alpha(\theta_A, \theta_B) \tag{36}$$

Lensing breaks the spherical symmetry and translation invariance and the lensed correlation becomes anisotropic and position dependent on the sky. The $O(\kappa^2)$ terms in the lensed covariance is at the percent level. Thus the lensed covariance is well approximated by the linear order Taylor expansion in convergence and shear.

III. LIKELIHOOD ANALYSIS

The likelihood function for gravitational lensing retains all the information provided by the observations. The optimal estimator is given by maximizing the likelihood function to the lensing parameters, the values of the lensing potential or the convergence and shear fields. However, the maximum likelihood estimator $\hat{\phi}$ for the lensing
potential $\phi$ is very difficult to compute since it is a nonlinear function of the lensing potential and has to be solved iteratively [10].

Lensing of CMB breaks the statistical isotropy, which is manifested in real space by an orientation and position dependent correlation function $C^{TT}(\theta_A, \theta_B)$. Maximizing the likelihood to the lensing parameters, in this case the amplitudes of sine and cosine waves ($\kappa^c, \kappa^s, \gamma^c_1$, etc.), we have the optimal estimators for convergence and shear fields. Within the linear approximation, Eq. (35), the maximum likelihood estimator reduces to a set of linear algebra operations, for example the matrix multiplication, matrix inverse, matrix trace computation, etc. which are more computational tractable, instead of the maximum likelihood estimator $\hat{\phi}$ where higher order terms in the covariance are important [10].

In Sec. III A we introduce the likelihood function for CMB lensing. In Sec. III B we maximize the likelihood function and derive the estimators for convergence and shear. In the derivations below, we will largely follow Ref. [10].

A. Likelihood function

We consider a data set of the measured temperature $\tilde{T}(\theta_i)$ at $N$ positions $\theta_i$ ($i = 1, \ldots, N$). The measured temperature is the sum of the lensed temperature $\hat{T}$ and the instrument noise $\epsilon$:

$$\tilde{T}(\theta_i) = \hat{T}(\theta_i) + \epsilon(\theta_i).$$

(37)

The probability distribution for the measured CMB temperature is describe by a density function $P(\tilde{T}|\kappa)$, where $\kappa$ is the lensing parameters. Here, we use the abbreviated notation $\kappa$ for the amplitudes of sine and cosine waves. The covariance matrix of the measured temperature is

$$C^{TT}[\kappa] = C^{TT}[\kappa] + C^{\epsilon \epsilon},$$

(38)

where $C^{TT}$ is the lensed covariance matrix and $C^{\epsilon \epsilon}$ is the noise covariance matrix. Here, we assume that both the CMB temperature fluctuations and the instrument noises are Gaussian. Then the probability density of $\tilde{T}$ for a lens configuration $\kappa$ is related to its covariance by a Gaussian function:

$$P(\tilde{T}|\kappa) = \frac{1}{(2\pi)^{N/2}\sqrt{\det C^{TT}}} \exp\left(-\frac{1}{2} \tilde{T}^T C^{-1}^{TT} \tilde{T}\right).$$

(39)

For simplicity, we will use the negative logarithm $L$ of the likelihood function in the derivation,

$$L[\kappa] = -\ln P(\tilde{T}|\kappa) = \frac{1}{2} \tilde{T}^T \left( C^{TT}[\kappa] \right)^{-1} \tilde{T} + \frac{1}{2} \ln \det C^{TT}[\kappa].$$

(40)

B. Likelihood-based estimators

We wish to find a set of lensing parameters $p_\alpha$, which maximize the likelihood function, $\partial L/\partial p_\alpha = 0$. Differentiating Eq. (40) and using Eq. (35), we obtain

$$\hat{p}_\alpha = F^{-1}_{\alpha\beta} \hat{T}^T C^{-1}_{\beta\gamma} C^{-1}_{\gamma\delta} \hat{T} - \text{Tr}[C^{-1} C^{TT}]$$

(41)

where the Fisher matrix

$$F_{\alpha\beta} = \frac{1}{2} \text{Tr} \left[ C^{-1} C^{TT} \right] \left( C^{-1} C^{TT} \right)^{-1} C^{TT},$$

(42)

The maximum likelihood estimator becomes a quadratic estimation process in the linear approximation. In terms of the maximum likelihood iteration, it corresponds to an initial guess $\kappa = 0$, with the covariance evaluated in the case of no lensing. The estimator converges after a single iteration. This is only valid when the maximum likelihood point is close to the initial guess $\kappa = 0$, which is indeed the case for weak gravitational lensing where the convergence and shear are much smaller than unity. However, we can still iterate the estimator to get better performance when the nonlinear terms are important.

Remember that the lensing parameters $\kappa^c(\ell)$, $\kappa^s(\ell)$, $\gamma^c_1(\ell)$, ..., are real and imaginary parts of the lensing fields by the factor $2/L^2$. Then the Fourier modes of the convergence field is simply

$$\kappa(\ell) = \kappa^c(\ell) + i\kappa^s(\ell) = \kappa^c(\ell)L^2/2 + i\kappa^s(\ell)L^2/2,$$

(43)

and similarly for the shear fields $\gamma_1(\ell)$ and $\gamma_2(\ell)$.

From the two shear components, we can construct the two following linear combinations in Fourier space:

$$\gamma_E(\ell) = \gamma_1(\ell) \cos 2\phi_\ell + \gamma_2(\ell) \sin 2\phi_\ell,$$

(44)

and

$$\gamma_B(\ell) = -\gamma_1(\ell) \sin 2\phi_\ell + \gamma_2(\ell) \cos 2\phi_\ell,$$

(45)

where $\cos \phi_\ell = \ell/l$ and $\sin \phi_\ell = \ell^2/l$. The parity-even $\gamma_E$ gives an estimate of the lensing convergence $\kappa$, while the parity-odd $\gamma_B$ estimates the curl part in the lensing remapping, which is usually very small.

The Fisher matrix for the $\kappa$ and $\gamma_E$ estimator is

$$F = \begin{pmatrix} F_{\kappa\kappa} & F_{\kappa\gamma_E} \\ F_{\gamma_E\kappa} & F_{\gamma_E\gamma_E} \end{pmatrix}.$$  

(46)

Its inverse gives the variance of the $\kappa$ and $\gamma_E$ estimator,

$$N = \begin{pmatrix} N_{\kappa\kappa} & N_{\kappa\gamma_E} \\ N_{\gamma_E\kappa} & N_{\gamma_E\gamma_E} \end{pmatrix},$$

(47)

where $\langle \hat{\kappa}(\ell)\hat{\kappa}(\ell') \rangle = (2\pi^2)\delta^D(\ell + \ell')|C^{\kappa\kappa}_{\ell} + N_{\ell}^{\kappa\kappa}|$ and similarly for $\langle \hat{\gamma}_E(\ell)\hat{\gamma}_E(\ell') \rangle$ and the covariance between them.

In Fig. 1, we plot the noise power spectrum for $\hat{\kappa}$, $\hat{\gamma}_E$ and the covariance between $\hat{\kappa}$ and $\hat{\gamma}_E$, for experiments.
FIG. 1. The noise power spectrum for the convergence estimator $N^{\kappa\kappa}$ (solid lines), shear estimator $N^{\gamma E\gamma E}$ (dashed lines), and the covariance between these two estimators $N^{\kappa\gamma E}$ (dotted lines), for experiments with a beam of 1 arcmin and three noise levels 10 $\mu$K arcmin, 6 $\mu$K arcmin, and 1 $\mu$K arcmin (from left to right). The thick solid lines show the lensing convergence power spectrum $C_{\ell}^{\kappa\kappa}$. Notice that the shear and convergence estimators are nearly independent on large scales and gradually correlated on smaller scales.

A. Numerical simulations

We generate the CMB lensing simulations on a $10^\circ \times 10^\circ$ path with pixels of 0.5 arcmin square on the sky. The primary CMB temperature field is lensed using the method described in Ref. [24]. We consider experiments with three noise levels, 10, 6, and 1 $\mu$K arcmin, and a beam of 1 arcmin, which roughly corresponds to the noise levels of the ACT experiment [4], Simons Observatory [6] and CMB-S4 [2]. In the analysis, we use the multipole range from $\ell_{\text{min}}$ = 36 to $\ell_{\text{max}}$ = 2500. The results are averaged over ten independent simulations and the error bars are the 1$\sigma$ uncertainty of the scatter between the simulations.

B. Results

Figure 2 shows the noise power spectrum of the minimal variance combination of the convergence and shear estimators for three different white noise levels. We also plot the noise power spectrum of the quadratic deflection estimator for comparison. The convergence map errors are measured by computing the difference between input and reconstructed convergence maps, $\hat{\kappa}_{\text{MV}} - \kappa$. The power spectra of the error in the convergence reconstruction are shown in Fig. 2. We find that the numerical results agree well with the theoretical noise curves computed using the Fisher matrix. The theoretical noise power spectrum of the $\hat{\gamma}_B$ estimator is also plotted and the numerical results are consistent with the theoretical predictions as well.

Therefore, the minimal variance combination of the convergence and shear estimators is equally optimal as the quadratic deflection estimators on smaller scales and is even better on larger scales, which is consistent with the results of the maximum likelihood analysis of the

IV. IMPLEMENTATION AND RESULTS

To test the performance of the new estimators, we apply the convergence and shear estimators to CMB lensing simulations. In this section, we consider the power spectrum of the error in the convergence reconstruction and present the convergence power spectrum estimated from the simulated CMB maps.
lensing deflection field (see Fig. 4 of Ref. [10]). This confirms the validity of the linear approximation made in the lensed covariance Eq. (35). However, keep in mind that the convergence and shear estimators can still be iterated to obtain better performance, although for weak lensing we find that the linearized version of the maximum likelihood estimator suffices.

In Fig. 3 we plot the power spectrum of the input and reconstructed convergence fields and the cross power spectrum between them. The data points are displaced slightly to avoid overlapping. We find that the cross power spectrum agrees very well with the input power spectrum on all scales, even small scales where the reconstruction noises dominate. The reconstructed convergence power spectrum agrees well with the input power on large scales and still consistent with the input power within the 1σ uncertainty. This is due to the large reconstruction noise on small scales, where the noise is higher than the signal by orders of magnitude.

![Graph](image)

**FIG. 2.** The noise curves for the quadratic deflection estimator (dashed lines) and the minimal variance estimator (solid lines). The convergence power spectrum is shown in thick solid lines. The noise power for the \( \hat{\gamma}_B \) estimator is also plotted in dotted lines. The data points show the results from simulations. The measured power spectra are averaged over ten simulations and the error bars show the rms error between the simulations. The minimal variance estimator is slightly better on large scales and equally optimal as the quadratic deflection estimator on smaller scales.

V. DISCUSSION

In this paper we present the optimal convergence and shear estimators, which improves upon the previous convergence and shear estimators which are only optimal in the long wavelength limit [21,23]. This is achieved by decomposing the convergence and shear fields using the sine and cosine waves and then expanding the lensed correlation function to linear order in convergence and shear. Maximizing the likelihood function gives the estimator for the lensing fields.

The methodology to calculate the lensed correlation function is similar to the method to compute the lensed CMB power spectrum, where the lensed correlation is computed in configuration space, ensemble averaged over both the primary CMB temperature fluctuations and the lens configurations, and then computing the inversion to the power spectrum [23]. After averaged over an ensemble of lens configurations, the lensed correlation function only depends on the separation between two points; the linear order terms \( \sim O(\kappa) \) vanish as the expectation value of \( \kappa \) is zero and the \( O(\kappa^2) \) terms contribute at the leading order. However, we are expanding the lensed correlation function for a given lens realization and the lensed correlation function is both anisotropic and position dependent, which is a manifestation of the linear order effect of lensing. A related discussion is presented in Ref. [27], but is still based on the deflection field instead of the convergence and shear fields considered here. From the analysis in this paper, we find that the lensing reconstruction from the CMB temperature field is limited by the maximum multipole \( \ell_{\text{max}} \) included in the analysis instead of the experimental noise level. Increasing the maximum multipole \( \ell_{\text{max}} \) in the analysis will induce lensing biases due to the extragalactic foregrounds [15,18]. The shear estimator is less susceptible to the foregrounds and thus can use a higher \( \ell_{\text{max}} \) [18]. It is also possible to separate the lensing signal from the foreground biases with the independent shear and convergence information which we plan to explore in the future.

The maximum likelihood method is the same as the previous maximum likelihood analysis for the lensing potential [10,11]. The difference is that we write the lensed covariance using the convergence and shear fields instead of the deflection angle or the lensing potential as in the previous studies. Since the linear approximation neglects the second-order and higher order terms in the covariance, the new estimators can still be biased and non-optimal due to terms beyond the linear order. There is still possibilities to obtain more information from higher order correlation functions. The new estimators here can be write in the iterative form to perform a nonlinear analysis. The bias and optimality of the new estimators need
FIG. 3. The power spectrum of the input and reconstructed convergence fields and the cross power spectrum between them. The solid curves show the theoretical convergence power spectrum. The data points in each $\ell$ bin are displaced for clarity. The measured power spectra are averaged over the ten simulations and the error bars show the scatter between the ten simulations. The cross power spectra $C_{\kappa\kappa}$ agree very well with the input power $C_{\kappa\kappa}^{\text{in}}$. The reconstructed convergence power spectrum $C_{\kappa\kappa}^{\hat{\kappa}\hat{\kappa}}$ agree well with the input power spectrum $C_{\kappa\kappa}^{\text{in}}$ on large scales and are still consistent with $C_{\kappa\kappa}^{\text{in}}$ within the $1\sigma$ uncertainty on all scales. This is mostly due to the very large noise power in lensing reconstruction on smaller scales, where the noise power is tens of times higher than the convergence power spectrum.

to be tested with simulations to assess the validity of the linear approximation as the tests for quadratic deflection estimator (see e.g., Refs. 28–50 for recent discussions). We defer a more careful analysis to a future work. The estimators are constructed in position space instead of Fourier space and can be directly generalized to the analysis with boundaries and inhomogeneous noises.

For non-Gaussian lensing sources, e.g., 21cm[21] or CIB, or non-Gaussian noise, the convergence and shear estimators will exhibit non-Gaussian variances. The separate construction allows an optimal combination, which improves optimality relative to deflection estimator, and provides an intrinsic consistency check.

Equipped with a generalized lensing estimator, one might ask how to generate a non-trivial non-displacement field. The simplest case is a non-Gaussian foreground, e.g., KSZ, CIB, for which this decomposition provides a broader noise matrix. In the Gaussian case, say with a primordial gravitational wave, one would need to specify the metric. The geodesic distance given by Eq. 9 describes the distance between pairs of points, and one would need to diagonalize Eq. 33 to generate random numbers. This diagonalization would no longer be an FFT or spherical harmonic transform. Nevertheless, it implements a (non-stationary) Gaussian Random field.

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