MODEL-INDEPENDENT CONSTRAINTS ON REIONIZATION FROM LARGE-SCALE COSMIC MICROWAVE BACKGROUND POLARIZATION

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Received 2007 May 8; accepted 2007 September 26

ABSTRACT

On large angular scales, the polarization of the CMB contains information about the evolution of the average ionization during the epoch of reionization. Interpretation of the polarization spectrum usually requires the assumption of a fixed functional form for the evolution, e.g., instantaneous reionization. We develop a model-independent method where a small set of principal components completely encapsulates the effects of reionization on the large-angle E-mode polarization for any reionization history within an adjustable range in redshift. Using Markov chain Monte Carlo methods, we apply this approach to both the 3 year WMAP data and simulated future data. WMAP data constrain two principal components of the reionization history, approximately corresponding to the total optical depth and the difference between the contributions to the optical depth at high and low redshifts. The optical depth is consistent with the constraint found in previous analyses of WMAP data that assume instantaneous reionization, with only a slightly larger uncertainty due to the expanded set of models. Using the principal component approach, WMAP data also place a 95% confidence level upper limit of 0.08 on the contribution to the optical depth from redshifts $z > 20$. With improvements in polarization sensitivity and foreground modeling, approximately five of the principal components can ultimately be measured. Constraints on the principal components, which probe the entire reionization history, can test models of reionization, provide model-independent constraints on the optical depth, and detect signatures of high-redshift reionization.

Subject headings: cosmic microwave background — cosmology: theory — large-scale structure of universe

1. INTRODUCTION

The amplitude of the E-mode component of the cosmic microwave background (CMB) polarization on large scales provides the best current constraint on the Thomson scattering optical depth to reionization, $\tau$. Using the first 3 years of data from the Wilkinson Microwave Anisotropy Probe (WMAP) and making the simple assumption that the universe was reionized instantaneously, Spergel et al. (2007) find $\tau = 0.09 \pm 0.03$. Theoretical studies suggest that the process of reionization was too complex to be well described as a sudden transition (e.g., Barkana & Loeb 2001). Previous studies have examined how the constraint on $\tau$ depends on the evolution of the globally averaged ionized fraction during reionization, $x_e(z)$, for a variety of specific theoretical scenarios. If the assumed form of $x_e(z)$ is incorrect, the estimated value of $\tau$ can be biased; this bias can be lessened by considering a wider variety of reionization histories at the expense of increasing the uncertainty in $\tau$ (Kaplinghat et al. 2003; Holder et al. 2003; Colombo et al. 2005).

The angular scales on which CMB polarization from reionization is correlated depend on the horizon size at the redshift of the free electrons: the higher the redshift, the higher the multiple (e.g., Ng & Ng 1996; Zaldarriaga 1997; Hu & White 1997). Varying $x_e(z)$ changes the relative contributions to the polarization coming from different redshifts, and therefore changes the shape of the large-scale E-mode angular power spectrum, $C_{EE}$. Because of this dependence, measurements of the low-$\ell$ E-mode spectrum should place at least weak constraints on the global reionization history in addition to the constraint on the total optical depth. Recent studies suggest that WMAP data provide little information about $x_e(z)$ beyond $\tau$ (e.g., Lewis et al. 2006), but it is worth asking what we can ultimately expect to learn about reionization from CMB polarization.

Hu & Holder (2003) proposed using a principal component decomposition of the ionization history to quantify the information contained in the large-scale E-mode polarization. The effect of any ionization history on the E-modes can be described by a small number of eigenmode parameters, unlike a direct discretization of $x_e(z)$ in redshift bins. Here we extend the methods of Hu & Holder (2003) using Markov chain Monte Carlo (MCMC) techniques to find constraints on the principal components of $x_e(z)$ using both the 3 year WMAP observations and simulated future data.

Analytic studies and simulations indicate that reionization is an inhomogeneous process, and this inhomogeneity is expected to contribute to the small-scale CMB temperature and polarization anisotropies (e.g., Hu 2000; Iliev et al. 2006; Mortonson & Hu 2007; Doré et al. 2007). Here we focus on the large-scale E-modes only ($\ell \leq 100$), where such effects can be neglected, so we only consider the evolution of the globally averaged ionized fraction as a function of redshift.

In the following section we describe the principal component method for parameterizing the ionization history and show that the effects of $x_e(z)$ on large-scale E-mode polarization can be encapsulated in a small set of parameters. The method allows $x_e(z)$ to be a free function of redshift that is not bounded by physical considerations, so in §3 we derive limits that can be placed on the model parameters to eliminate most of the unphysical models where $x_e > 1$ or $x_e < 0$. We outline several ways to apply the principal component approach to constrain the reionization history with large-scale E-mode data in §4. Using MCMC methods, we examine some of these applications in more detail in §5 using...
both 3 year WMAP data and simulated future CMB polarization data. We summarize our findings and conclude in § 6.

2. IONIZATION HISTORY EIGENMODES

Models with similar total optical depth but different ionization histories can produce markedly different predictions for the E-mode power spectrum. In an instantaneous reionization scenario, the contribution to the optical depth from $x_r(z)$ is concentrated at the lowest redshifts possible for a given $r$, and the E-mode power spectrum for such a model is sharply peaked on large scales, at $\ell \lesssim 10$. The main effect of shifting some portion of the reionization history to higher redshifts while keeping $r$ fixed is to reduce the E-mode power on the largest scales and increase it on smaller scales.

This redistribution of power is illustrated in Figure 1 by the ionization histories and $C_1^{EE}$ for two models, one with nearly instantaneous reionization and the other with comparable optical depth but with $x_r(z)$ concentrated at higher $z$. In general, a flatter large-scale E-mode spectrum with power extending out to $\ell \sim 10-20$ is a sign of a large ionized fraction at high redshift. However, there is not a one-to-one correspondence between $\ell$ and $z$; the ionized fraction within any particular narrow redshift bin affects $C_1^{EE}$ over a wide range of angular scales. Ionized fractions in adjacent redshift bins have highly correlated effects on $C_1^{EE}$, which makes it difficult to extract from E-mode polarization data a constraint on $x_r(z)$ at a specific redshift.

As suggested by Hu & Holder (2003), one can use principal components of the reionization history as the model parameters instead of $x_r(z)$ in redshift bins. These components are defined to have uncorrelated contributions to the E-mode power; since each has a unique effect on $C_1^{EE}$, the amplitudes of the components can be inferred from measurements of the large-scale power spectrum. Principal component analysis of the reionization history as the model parameters can be determined best from the data. In this section we describe the principal component method and introduce the notation that we use throughout the paper.

Consider a binned ionization history $x_r(z_i), i \in \{1, 2, \ldots , N_z\}$, with redshift bins of width $\Delta z$ spanning $z_{\min} \leq z \leq z_{\max}$, where $z_1 = z_{\min} + \Delta z$ and $z_N = z_{\max} - \Delta z$ so that $N_z = (z_{\max} - z_{\min})/\Delta z$. Throughout this paper we assume that the ionized fraction is $x_r \approx 1$ for redshifts $z \leq z_{\min}$ and $x_r \approx 0$ at $z \geq z_{\max}$. We take $z_{\min} = 6$, consistent with observations of quasar and gamma-ray burst spectra (Fan et al. 2006; Toptani et al. 2006).

The principal components of $x_r(z_i)$ are eigenfunctions of the Fisher matrix, computed by taking derivatives of $C_1^{EE}$ with respect to $x_r(z_i)$:

$$ F_{ij} = \frac{1}{2} \sum_{\ell=2}^{\ell_{\max}} (\ell + \frac{1}{2}) \frac{\partial \ln C_1^{EE}}{\partial x_i(z)} \frac{\partial \ln C_1^{EE}}{\partial x_j(z)}, $$

assuming full sky coverage and neglecting noise. Since $x_r(z_i)$ only significantly contributes to the E-mode spectrum at small $\ell$, we typically truncate the sum in equation (1) at $\ell_{\max} = 100$, where $C_1^{EE}$ is dominated by the first acoustic peak. The derivatives are evaluated at a fiducial reionization history, $x_{rF}(z_i)$. Following Hu & Holder (2003) we typically choose $x_{rF}(z_i)$ to be constant during reionization, although other functional forms may be used. We compute the derivatives as finite differences with $\Delta x_r = 0.05$. The lowest variance principal components are robust with respect to small changes in this choice of $\Delta x_r$.

Since the effects on $C_1^{EE}$ of $x_r(z_i)$ in adjacent redshift bins are highly correlated, the Fisher matrix contains large off-diagonal elements. The principal components $S_\mu(z_i)$ are the eigenfunctions of $F_{ij}$.

$$ F_{ij} = (N_z + 1)^{-2} \sum_{\mu=1}^{N_z} S_\mu(z_i) S_\mu(z_j) \sigma_\mu^{-2}, $$

where the factor $(N_z + 1)^{-2}$ is included so that the eigenfunctions and their amplitudes have certain convenient properties. The inverse eigenvalues, $\sigma_\mu^{-2}$, give the estimated variance of each principal component eigenmode from the measurement of low-$\ell$ $E$-modes. We order the modes so that the best-constrained principal components (smallest $\sigma_\mu^{-2}$) have the lowest values of $\mu$, starting at $\mu = 1$. The noise level and other characteristics of an experiment can be included in the construction of the eigenfunctions, but since the effect on $S_\mu(z)$ is small, we always use the noise-free eigenfunctions here.

The eigenfunctions satisfy the orthogonality and completeness relations:

$$ \int_{z_{\min}}^{z_{\max}} dz S_\mu(z) S_\nu(z) = (z_{\max} - z_{\min}) \delta_{\mu\nu}, $$

$$ \sum_{\mu=1}^{N_z} S_\mu(z_i) S_\mu(z_j) = (N_z + 1) \delta_{ij}. $$

The normalization of $S_\mu(z)$ is chosen so that the eigenfunctions are independent of bin width as $\Delta z \rightarrow 0$. In equation (3) and elsewhere in this paper where there are sums over redshift, we assume the continuous limit, replacing $\sum_{\Delta z} f(z)$ by $\int dz$. As long as the bin width is chosen to be sufficiently small, the final results we obtain are independent of the redshift binning. We adopt $\Delta z = 0.25$ as the default bin width.

The three lowest variance eigenfunctions for two different fiducial models are shown in Figure 2. The lowest eigenmode ($\mu = 1$) is an average of the ionized fraction over the entire
redshift range, weighted at high $z$. The $\mu = 2$ mode can be thought of as the difference between the amount of ionization at high $z$ and at low $z$, and higher modes follow this pattern, with weighted averages of $x_r(z)$ that oscillate with higher and higher frequency in redshift. Eigenvectors of fiducial models with different values of $z_{\text{max}}$ have similar shapes with the redshift axis rescaled according to the width of $(z_{\text{max}} - z_{\text{min}})$. The eigenvectors are mostly insensitive to the choice of ionized fraction in the constant-$x_r$ fiducial histories.

An arbitrary reionization history can be represented in terms of the eigenvectors as

$$x_r(z) = x_r^{\text{fid}}(z) + \sum_\mu m_\mu S_\mu(z),$$

where the amplitude of eigenmode $\mu$ for a perturbation $\delta x_r(z) \equiv x_r(z) - x_r^{\text{fid}}(z)$ is

$$m_\mu = \frac{1}{z_{\text{max}} - z_{\text{min}}} \int_{z_{\text{min}}}^{z_{\text{max}}} dz \, S_\mu(z) \delta x_r(z).$$

[Note that our conventions for the normalization of $m_\mu$ and $S_\mu(z)$ differ from those of Hu & Holder (2003) by factors of $(N_\ell + 1)^{1/2}$.]

Any global ionization history $x_r(z)$ over the range $z_{\text{min}} < z < z_{\text{max}}$ is completely specified by a set of mode amplitudes $m_\mu$.

If perturbations to the fiducial history are small, $\delta x_r(z) \ll 1$, then the mode amplitudes are uncorrelated, with covariance matrix $\langle m_\mu m_\nu \rangle = \sigma_\mu^2 \delta_{\mu\nu}$. For a fixed fiducial model, however, arbitrary reionization histories generally have $\delta x_r \sim 1$, in which case the amplitudes of different modes can become correlated, as we discuss in § 5.3.

The main advantage of using the principal component eigenvectors of $x_r(z)$ instead of some other parameterization is that most of the information relevant for large-scale $E$-modes is contained in the first few modes. This means that if one constructs $x_r(z)$ from equation (5) keeping only the first few terms in the sum over $\mu$, then the $E$-mode spectrum of the resulting ionization history will closely match that of $x_r(z)$ with all modes included in the sum. The effect of each eigenmode on $C_{\ell}^{EE}$ becomes smaller as $\mu$ increases, as shown in Figure 3 for the first two modes. Hu & Holder (2003) demonstrated that for a specific fiducial ionization history $x_r^{\text{fid}}(z)$ and assumed true history, only the first three modes of $x_r(z)$ are needed to produce $C_{\ell}^{EE}$ indistinguishable from the true $E$-mode spectrum.

The ionization histories and corresponding $E$-mode spectra in Figure 4 demonstrate this completeness for a fairly extreme model in which the first 10 eigenmodes all have significant amplitudes. Even in the simplest case where a single eigenmode is used in place of the original $x_r(z)$, the error in $C_{\ell}^{EE}$ is only $\sim 10\%$. With three to five modes, the error is a few percent or less at all multipoles and safely smaller than the cosmic variance of $C_{\ell}^{EE}$.

$$\frac{\Delta C_{\ell}^{EE}}{C_{\ell}^{EE}} = \sqrt{\frac{2}{2\ell + 1}}.$$  

Note that with $N = 3 - 5$ the fractional error is small enough to be below cosmic variance even if deviations in $C_{\ell}^{EE}$ are correlated across wide bands in $\ell$.

Figure 4 (top) shows that completeness does not extend to the ionization history itself: $x_r(z)$ constructed from as many as five eigenmodes is a poor approximation to the full reionization history. The principal component method is not well suited to reconstructing the reionization history, since polarization data do not constrain the high-variance, rapidly oscillating modes of $x_r(z)$.

Instead, principal components are more useful for testing models of reionization or for constraining quantities such as the optical depth that are independent of the poorly constrained modes, as we discuss further in § 4.

From our tests on the completeness in $C_{\ell}^{EE}$ of the lowest variance eigenvectors, we conclude that the first three to five modes contain essentially all of the information about the reionization
history that is relevant for large-scale E-mode polarization. This fact is particularly useful for constraining the global reionization history with CMB polarization data using MCMC techniques. Since the number of parameters that must be added to a Monte Carlo chain to describe an arbitrary \(x_e(z)\) is relatively small, we can obtain constraints from the data that are independent of assumptions about the reionization history with minimal added computational expense (Hu & Holder 2003). The exact number of modes required varies depending on the true ionization history and the fiducial history, so when analyzing data it is a good idea to check that the results do not change significantly when the next modes are included in the sum in equation (5).

The main caveat to this model independence is that in practice we must set some maximum redshift for histories in any particular chain of Monte Carlo samples, ignoring any contribution of modes that retain the first one (thick curves), three (medium curves), and five (thick curves) eigenmodes; \(\tau\) for these models is 0.150, 0.147, and 0.148, respectively. The fiducial model used for the eigendecomposition has constant \(x_e = 0.15\) from \(z_{\text{min}} = 6\) up to \(z_{\text{max}} = 30\). In the bottom panel, the uncertainty due to cosmic variance is plotted as a dotted line.

The need to consider a limited range in redshift is shared by other methods, for example, those that constrain \(x_e(z)\) instead of the eigenmode amplitudes (Lewis et al. 2006). As already mentioned, the principal component approach has the unique advantages that results can be made independent of bin width and that relatively few extra parameters are required. However, this approach also has a unique difficulty in that the physicality of the reionization history \([0 \leq x_e(z) \leq 1]\) is not built into the method. Hence, constraints derived from measurements of the eigenmodes can be weaker than those from a method that enforces physicality. We can, however, place some prior constraints on the set of eigenmode amplitudes that must be satisfied by any physical model, as we discuss in the next section.

3. PRIORS FROM PHYSICALITY

Although the actual ionized fraction must be between 0 and 1 (neglecting helium reionization and the small residual ionized fraction after recombination), there is nothing in the construction of \(x_e(z)\) from the eigenmodes in equation (5) that ensures that the ionized fraction will obey these limits. Whether or not \(x_e\) has a physical value at a particular redshift depends on the amplitudes...
of all of the principal components. Even for a physical ionization history, the truncated sum up to mode \( N \),

\[
x_e^{(N)}(z) \equiv x_e^{\text{fid}}(z) + \sum_{\mu=1}^{N} m_{\mu} S_{\mu}(z),
\]

is not necessarily bounded by 0 and 1 at all redshifts. While formally it is possible to evaluate \( C_{EE}^{BB} \) for reionization histories with unphysical values of \( x_e \), we would like to eliminate as much as possible those models for which the full sum of the eigenmodes, \( x_e(z) = \lim_{N \to \infty} x_e^{(N)}(z) \), is unphysical.

We find the largest and smallest values of \( m_{\mu} \) that are consistent with \( x_e(z) \in [0, 1] \) for all \( z \) using the definition of \( m_{\mu} \) in equation (6). We are free to choose \( x_e^{\text{fid}}(z) \leq 1 \) so that \( -x_e^{\text{fid}}(z) \leq \delta x_e(z) \leq 1 - x_e^{\text{fid}}(z) \), where the lower limit is strictly negative or zero and the upper limit is positive or zero. For a particular mode \( \mu \), the choice of \( \delta x_e(z) \) that maximizes \( m_{\mu} \) is

\[
\delta x_e^{\text{max}}(z) = \begin{cases} 
-x_e^{\text{fid}}(z), & S_{\mu}(z) \leq 0, \\
1 - x_e^{\text{fid}}(z), & S_{\mu}(z) > 0.
\end{cases}
\]

Using this in equation (6) gives an upper limit on \( m_{\mu} \). Similarly, a lower limit can be obtained by reversing the signs of the inequalities in equation (9). The resulting physicality bounds are \( m_{\mu}^{(-)} \leq m_{\mu} \leq m_{\mu}^{(+)} \), where

\[
m_{\mu}^{(\pm)} = \int_{z_{\mu}}^{z_{\mu}^{\text{max}}} dz \frac{S_{\mu}(z)[1 - 2x_e^{\text{fid}}(z)] \pm |S_{\mu}(z)|}{2(z_{\mu}^{\text{max}} - z_{\mu}^{\text{min}})},
\]

If \( m_{\mu} \) violates these bounds for any \( \mu \), the reionization history is guaranteed to be unphysical for some range in redshift. The opposite is not true, however: even if all \( m_{\mu} \) satisfy equation (10), \( x_e(z) \) may still be unphysical for some \( z \).

The parameter space that physical models may occupy is restricted further by an inequality that must be satisfied by all eigenmodes simultaneously. Assume for simplicity that the fiducial model has a constant ionized fraction, \( x_e^{\text{fid}} \in [0, 1] \), for \( z_{\mu}^{\text{min}} < z < z_{\mu}^{\text{max}} \). Any physical reionization history \( x_e(z) \) must satisfy

\[
\int_{z_{\mu}^{\text{min}}}^{z_{\mu}^{\text{max}}} dz \left[ x_e(z) - x_e^{\text{fid}} \right]^2 \leq (z_{\mu}^{\text{max}} - z_{\mu}^{\text{min}}) f,
\]

where \( f \equiv \text{max} \{(x_e^{\text{fid}})^2, (1 - x_e^{\text{fid}})^2\} \). Using equation (5), the left-hand side of the inequality can also be written

\[
\int_{z_{\mu}^{\text{min}}}^{z_{\mu}^{\text{max}}} dz \left[ x_e(z) - x_e^{\text{fid}} \right]^2 = \int_{z_{\mu}^{\text{min}}}^{z_{\mu}^{\text{max}}} dz \left[ \sum_{\mu} m_{\mu} S_{\mu}(z) \right]^2 = (z_{\mu}^{\text{max}} - z_{\mu}^{\text{min}}) \sum_{\mu} m_{\mu}^2 f,
\]

where the second line follows from the orthogonality of the eigenfunctions (eq. [3]). Comparing equations (11) and (12) we obtain a constraint on the sum of the squares of the mode amplitudes,

\[
\sum_{\mu} m_{\mu}^2 \leq f,
\]

where 0.25 \( \leq f \leq 1 \), depending on the value of \( x_e^{\text{fid}} \). As with the physicality bounds of equation (10), this upper limit is a necessary but not sufficient condition for physicality.

Since in practice we can only constrain a limited set of eigenmodes, the uncertainty in modes higher than the first few prevents us from simply excluding all models where \( x_e < 0 \) or \( x_e > 1 \) at any redshift because the higher modes can have a significant effect on \( x_e(z) \). However, as shown in \$ 2 \$, the higher modes do not affect the polarization power spectrum, since the high-frequency oscillations in redshift of higher modes are averaged out.

Similarly, the high-variance eigenmodes have a small effect on the optical depth from a sufficiently large range in redshift. For the example in Figure 4, only 0.6% of the total optical depth comes from modes with \( \mu > 3 \); for \( \mu > 5 \) the contribution is less than 0.1% (see also Hu & Holder 2003). The effect of poorly constrained modes on the optical depth over more limited (but still wide) ranges in redshift is also small. From tests on a variety of ionization histories we find that the optical depth for \( 15 < z < 30 \) due to modes \( \mu > 5 \) subject to the physicality constraints of this section can be no larger than \( \sim 0.01 \), and is likely to be smaller for realistic reionization scenarios. Because of this, we assume that we can place priors on the optical depth that correspond to \( 0 \leq x_e \leq 1 \) over the relevant range in redshift. Reionization histories with an unphysical optical depth over a large range in redshift are considered to be unphysical models since the addition of higher modes cannot perturb the optical depth enough to give it a physical value.

4. APPLICATIONS OF THE PRINCIPAL COMPONENT METHOD

Once constraints on the principal components of the reionization history have been obtained from CMB polarization data, there are several ways to use those constraints to place limits on observables such as \( \tau \) or to test theories of reionization (Hu & Holder 2003). We describe some possible applications in this section, and in \$ 5 \$ we put these ideas into practice using the 3 year WMAP data and simulated future data.

As mentioned in \$ 1 \$, the constraint on the total optical depth to reionization depends on the assumed model for \( x_e(z) \). The principal component method allows us to explore all globally averaged ionization histories within a chosen redshift range, \( z_{\mu}^{\text{min}} < z < z_{\mu}^{\text{max}} \). For a given set of eigenmode amplitudes, \( \{m_{\mu}\} \), equation (5) yields the corresponding ionization history, which can then be integrated to find the optical depth between any two redshifts \( z_1 \) and \( z_2 \),

\[
\tau(z_1, z_2) = 0.0691 (1 - Y_p) \Omega_{bh} h \int_{z_1}^{z_2} dz \frac{(1 + z)^2}{H(z)/H_0} x_e(z).
\]

In particular, the total optical depth to reionization is

\[
\tau = \tau(0, z_{\mu}^{\text{min}}) + \tau(z_{\mu}^{\text{min}}, z_{\mu}^{\text{max}}),
\]

where \( \tau(0, z_{\mu}^{\text{min}}) \approx 0.04 \) for \( z_{\mu}^{\text{min}} = 6 \). The principal component approach provides a model-independent way to constrain \( \tau \), so we expect the results to be unbiased and the uncertainty in \( \tau \) to accurately reflect the present uncertainty about \( x_e(z) \). Moreover, the information about \( \tau(z_{\mu}^{\text{min}}, z_{\mu}^{\text{max}}) \) is encapsulated in the first few eigenmodes, i.e., the truncated ionization history of equation (8), \( x_e^{(N)}(z) \), with \( N = 3 \)–5 for typical fiducial models.

The total optical depth and the first principal component amplitude, \( m_1 \), are similar quantities in that they are both averages of \( x_e(z) \) weighted at high \( z \). As we show in the next section, CMB \( E \)-mode polarization data can constrain higher eigenmodes as well (\( \mu \geq 2 \)). In particular, the second mode should be the next
best constrained quantity since it is constructed to have the smallest variance after $m_i$. Since $m_2$ is related to the difference in $x_e$ between high redshift and low redshift (see Fig. 2), we might guess that besides total $\tau$ the data are mainly constraining the fraction of optical depth coming from high redshift versus low redshift. Given any set of mode amplitudes defining an ionization history, we can compute a low-$z$ optical depth, $\tau(z_{\text{min}}, z_{\text{mid}})$, and a high-$z$ optical depth, $\tau(z_{\text{mid}}, z_{\text{max}})$, for some choice of intermediate redshift, $z_{\text{mid}}$.

Note that if either of the redshift ranges $[z_{\text{min}}, z_{\text{mid}}]$ or $[z_{\text{mid}}, z_{\text{max}}]$ is too narrow, constraints on the partial optical depths will be influenced by the physically priors (since $0 \leq x_e \leq 1$ sets limits on $\tau$ in redshift intervals as discussed in § 3) and by the uncertainty in modes higher than those included in the chain, which have greater effect on the optical depth in narrower redshift intervals. For these reasons, $z_{\text{mid}}$ should be chosen to be not too close to either $z_{\text{min}}$ or $z_{\text{max}}$.

Given an appropriately chosen value of $z_{\text{mid}}$, constraints on the principal components can be converted into constraints on the optical depths at high and low redshift. These partial optical depths are observables in the sense that high-$z$ and low-$z$ optical depth affect the large-scale $E$-modes over different ranges of multipoles. For example, compare the two reionization models in Figure 1. Both have similar total optical depth, but in one case $\tau$ only comes from $z < 15$, resulting in more power at $l < 8$ and less power at $l > 8$ than the other model, in which the optical depth primarily comes from $z > 15$.

Besides learning about the relative amount of ionization at $z < z_{\text{mid}}$ and $z > z_{\text{mid}}$, the partial optical depth constraints also provide a way to empirically set the maximum redshift, $z_{\text{max}}$. If some set of data is found to place a tight upper bound on $\tau(z_{\text{mid}}, z_{\text{max}})$ for fairly conservative (i.e., large) values of $z_{\text{max}}$ and $z_{\text{mid}}$, then for analyses of future data this value of $z_{\text{mid}}$ can be used as a new, lower value for $z_{\text{max}}$ since optical depth from higher redshifts is small. This approach assumes that there is essentially no reionization earlier than the original $z_{\text{max}}$, but as long as this initial maximum redshift is taken to be large, the presence or absence of high-$z$ ionization can be tested in this way over a wide range of redshifts. We explore this idea further in § 5.

While we do not examine constraints on specific reionization models in this paper, the principal component approach is well suited to model testing. Consider a model of the global reionization history, $x_e(z; \theta)$, parameterized by $\theta$. This could be a simple toy model (for example, instantaneous reionization where $\theta$ is a single parameter, the redshift of reionization) or a more physical model where $\theta$ might include parameters that govern properties of the ionizing sources. For a particular choice of $x_e(z; \theta)$, the principal component amplitudes of the reionization model follow from equation (6), giving a set of mode amplitudes that depend on the model parameters, $\{m_i(\theta)\}$. Then constraints on the mode amplitudes from CMB polarization data (defined using the same fiducial history) can be mapped to constraints on the parameters of the reionization model.

Applying this method to a model that has as one of its parameters a maximum redshift allows one to obtain constraints on $z_{\text{max}}$ within a class of theoretical models. Although obtaining good constraints on model parameters does not necessarily imply validation of the model class, this procedure provides a straightforward method by which different model classes can be tested and falsified within a single analysis.

Generating Monte Carlo chains to find constraints on $\{m_i\}$ as described in the next section can be a somewhat time-consuming process, but it only needs to be done once per redshift range, after which any model of the global reionization history within this range $z_{\text{min}} < z < z_{\text{max}}$ can be tested using the same parameter chains. In cases where constraints from the data turn out to be close to Gaussian, the covariance matrix of the principal components can be used in place of the full Monte Carlo chains, reducing the amount of information needed for model testing from $\sim 10^6$ numbers in chains of Monte Carlo samples to only $N(N + 3)/2$ numbers when $N$ eigenmodes are included in the chains [$N$ mean values plus $N(N + 1)/2$ entries in the covariance matrix, $(m_i, m_j)$]. However, near-Gaussian constraints on $\{m_i\}$ are likely to be possible only for certain realizations of future data, as discussed in the next section.

5. MARKOV CHAIN MONTE CARLO

CONSTRAINTS ON EIGENMODES

We find reionization constraints from CMB polarization data using MCMC techniques to explore the principal component parameter space (see, e.g., Christensen et al. 2001; Kosowsky et al. 2002; Dunkley et al. 2005). Chains of Monte Carlo samples are generated using the publicly available code CosmoMC4 (Lewis & Bridle 2002), which includes the code CAMB (Lewis et al. 2000) for computing the theoretical angular power spectrum at each point in the $(m_1, \ldots, m_N)$ parameter space. We have modified both codes to allow specification of an arbitrary reionization history calculated from a set of mode amplitudes using equation (5).

The principal component amplitudes are the only parameters allowed to vary in the chains. Since nearly all the information in $C_{EE}$ from reionization is contained within the first few eigenmodes of $x_e(z)$, we include the modes $\{m_1, \ldots, m_N\}$ in each chain with $3 \leq N \leq 5$. We use only the $E$-mode polarization data for parameter constraints, and assume that the values of the standard $\Lambda$CDM parameters (besides $\tau$) are fixed by measurements of the CMB temperature anisotropies. Keeping the set of parameters in the Monte Carlo chains as small as possible enables faster exploration of effects related to the fiducial history (e.g., $z_{\text{max}}$ and $N$), assumptions about priors, and various data sets, both real and simulated. This simplification leads to a slight underestimate of the error in $\tau$, as we discuss below, but to a good approximation the effect of $x_e(z)$ on the large-scale $E$-modes is independent of the other parameters. We have checked that our parameter constraints are not strongly affected by this assumption by comparing with the results of a set of 10-parameter chains using WMAP TT, TE, and EE spectra to constrain $\Omega_b h^2$, $\Omega_c h^2$, $\theta$, $A_s$, $e^{-2z}$, and $n_s$ in addition to the first five principal component amplitudes. We describe these results at the end of § 5.1.

For the Markov chains in which all cosmological parameters besides the principal component amplitudes are fixed (i.e., all chains used here except for the 10-parameter chains mentioned above), we take $\Omega_b h^2 = 0.0222$, $\Omega_c h^2 = 0.106$, $100\theta = 1.04$ (corresponding to $h = 0.73$), $A_s e^{-2z} = 1.7 \times 10^{-5}$, and $n_s = 0.96$, consistent with results from the most recent version of the WMAP 3 year likelihood code. When computing the optical depth to reionization we take the primordial helium fraction to be $Y_p = 0.24$. We also assume that $z_{\text{min}} = 6$, so that the optical depth contributed at lower redshifts is fixed at $\tau(z_{\text{min}}) = 0.04$. The remaining total optical depth from reionization, $\tau(z_{\text{min}}, z_{\text{max}})$, is determined by the values of $\{m_i\}$ for each sample in the chains. The default bin width for our fiducial models $x_e^f(z) = \Delta z = 0.25$, which is small enough that numerical effects related to binning should be negligible.

To get accurate results from MCMC analysis, it is important to make sure that the parameter chains contain enough independent samples covering a sufficient volume of parameter space that the

\[4 \text{ See http://cosmologist.info/cosmomc/} \]
density of the samples converges to the actual posterior probability distribution. For each scenario that we study, we run four separate chains until the Gelman and Rubin convergence statistic $R$, corresponding to the ratio of the variance of parameters between chains to the variance within each chain, satisfies $R - 1 < 0.01$ (Gelman & Rubin 1992; Brooks & Gelman 1998). The convergence diagnostic of Raftery & Lewis (1992) is used to determine how much each chain must be thinned to obtain independent samples. Both of these statistics and other diagnostic measures are computed automatically by CosmoMC.

To help the chains converge even in the presence of parameter degeneracies, we make use of CosmoMC’s ability to propose steps in the parameter space along directions determined by the covariance matrix, which we compute from previous trial runs for each scenario. Since $x_r(z)$ during reionization must match $x_r \approx 1$ at $z = z_{\text{min}}$ and $x_r \approx 0$ at $z = z_{\text{max}}$, there are often sharp transitions at these redshifts, since nothing in equation (5) forces $x_r(z)$ to satisfy these boundary conditions. To avoid problems with the time integration in CAMB, we smooth the reionization history by convolving $x_r(z)$ with a Gaussian of width $\sigma_z = 0.5$.

As described in previous sections, we assume that $0 \leq x_r \leq 1$ between $z_{\text{min}}$ and $z_{\text{max}}$. This assumption neglects helium reionization, which can make $x_r$ slightly larger than unity, and the small residual ionized fraction remaining after recombination that prevents $x_r$ from ever being exactly zero. These are relatively small effects, especially since we are not placing constraints on $x_r(z)$ directly but rather on weighted averages of $x_r$ over redshift. The residual ionized fraction at $z > z_{\text{max}}$ is accounted for in the Monte Carlo exploration of reionization histories.

In § 5.1 we examine the current constraints from the 3 year WMAP data. We then propose forecasts for principal component constraints with idealized, cosmic-variance-limited, simulated data in § 5.2. In each case the likelihood computation includes only the $E$-mode polarization data, up to $\ell = 100$ for simulated data and $\ell = 23$ for WMAP, the likelihood code for WMAP does not use $C_{\ell}^{EE}$ at smaller scales due to low signal-to-noise ratio. At multipoles $\ell \gtrsim 100$ the global reionization history only affects the amplitude of the angular power spectra, which we fix by setting $A_1 e^{2\tau}$ constant in the Monte Carlo chains. A comparison of the MCMC results with the Fisher matrix approximation follows in § 5.3.

5.1. Constraints from WMAP

In our analysis of WMAP data we use the 3 year WMAP likelihood code, with settings chosen so that likelihoods include only contributions from the low-$\ell$ $E$-mode polarization. In this regime, the code computes model likelihoods with a pixel-based method instead of using the angular power spectrum (Page et al. 2007). Since the maximum redshift at which there is still a significant ionized fraction is uncertain, we generate Monte Carlo chains using different fiducial models with $10 \leq z_{\text{max}} \leq 40$. To avoid possible bias due to neglecting the possibility of high-redshift reionization, we focus here on the results obtained using the more conservative values of $z_{\text{max}} = 30$ and 40.

The MCMC constraints on the first three principal components from WMAP are shown in Figure 6 using fiducial models with $z_{\text{max}} = 30$ and 40. The marginalized constraints are plotted within the physicality bounds of equation (10), $m_{\mu}^{(-)} \leq m_{\mu} \leq m_{\mu}^{(+)}$, so the size of the contours inside each box gives an idea of the constraining power of the data within the space of potentially physical models. For both fiducial histories, the data place a strong upper limit on $m_1$ and weakly constrain $m_2$. It is important to note that although the parameters $\{m_1, m_2, m_3\}$ have the same names in both the $z_{\text{max}} = 30$ and 40 plots, they are defined with respect to different fiducial models, and so we do not expect the contours in the left and right plots in Figure 6 to agree exactly. The qualitative similarity between the contours simply reflects the fact that the eigenfunctions for different $z_{\text{max}}$ have similar shapes (Fig. 2).

Since $m_1$ and $\tau$ are both averages of $x_r$ from $z_{\text{min}}$ to $z_{\text{max}}$ with more weight at high $z$ than low $z$, the strong constraint on $m_1$ mostly reflects the ability of the data to constrain the total optical depth to reionization. Indeed, $m_1$ and $\tau$ are strongly correlated in the Monte Carlo chains, as shown in Figure 7, while the correlations between $\tau$ and higher principal components of $x_r(z)$ are weaker.
The uncertainty in $\tau$ from the Monte Carlo chains is slightly underestimated because we fix all cosmological parameters that are not directly related to reionization. To estimate the effect of this assumption, we compare constraints on $\tau$ in two cases where instantaneous reionization is assumed instead of using the model-independent principal component approach: one in which the non-reionization parameters are fixed as in the rest of our Monte Carlo chains, and the other, from the 3 year WMAP analysis of Spergel et al. (2007), in which these parameters are allowed to vary. These constraints, listed in rows 6 and 7 of Table 1, suggest that fixing $\Lambda$CDM parameters besides $\tau$ reduces $\sigma_\tau$ by $\sim 10\%$. This 10\% difference in the error on $\tau$ is confirmed by our single set of 10 parameter chains described earlier in which several additional $\Lambda$CDM parameters are allowed to vary (row 5 of Table 1).

For all analyses of the 3 year WMAP data listed in Table 1, the uncertainty in $\tau$ is similar regardless of whether we use principal components to explore a variety of reionization histories or restrict the analysis to instantaneous $x_r(z)$. This is somewhat surprising, since in general one would expect that expanding the model space for $x_r(z)$ would increase the estimated error on $\tau$. The physicality priors may be responsible for reducing $\sigma_\tau$ slightly—top-hat priors on $\{m_{1}\}$ induce a prior on $\tau$ that is flat over a certain range but falls off approximately linearly at the edges—but even after accounting for priors, the optical depth constraint is robust to replacing the instantaneous reionization assumption with a model-independent analysis.

Plotting the trajectory of instantaneous reionization models through the space of principal components helps illustrate why the WMAP constraint on $\tau$ is insensitive to the set of models considered. In the left panel of Figure 8 we show the set of instantaneous models as a curve in the $m_1-m_2$ plane, since the first two eigenmodes have the greatest effect on $\tau$.

As described in § 4, principal component constraints from MCMC yield model-independent constraints on the total optical depth. For each Monte Carlo sample of the principal components we compute $\tau$ using equation (15). The constraints on $\tau$ are listed in Table 1 for various values of $z_{\text{max}}$ and $N$, the number of modes in the Monte Carlo chains.

### Table 1

| Data\(^a\) | Use PCs of $x_r (z)$$^{b, c}$ | $z_{\text{max}}$ | $N$ | Fix Other Parameters?\(^d\) | $\tau$ |
|----------|-----------------------------|----------------|-----|-----------------------------|-----|
| WMAP-3 | Yes | 20 | 3 | Yes | 0.098 ± 0.025 |
| | Yes | 30 | 3 | Yes | 0.104 ± 0.027 |
| | Yes | 30 | 5 | Yes | 0.106 ± 0.027 |
| | Yes | 40 | 5 | Yes | 0.107 ± 0.029 |
| | Yes | 30 | 5 | No | 0.109 ± 0.030 |
| | No | ... | ... | Yes | 0.096 ± 0.027 |
| | No | ... | ... | No | 0.089 ± 0.030\(^d\) |
| CV (1) | Yes | 20 | 3 | Yes | 0.103 ± 0.004 |
| | Yes | 30 | 5 | Yes | 0.108 ± 0.005 |
| | No | ... | ... | Yes | 0.108 ± 0.003 |
| | No | ... | ... | Yes | 0.135 ± 0.005 |
| CV (D) | Yes | 30 | 5 | Yes | 0.103 ± 0.007 |
| | No | ... | ... | Yes | 0.135 ± 0.005 |

\(^{a}\) WMAP-3: WMAP 3 year data; CV (1): cosmic-variance-limited simulated data assuming the true history is instantaneous reionization with $\tau = 0.105$ using the realization of $C_{l}^{EE}$ in Fig. 10 (left); CV (D): cosmic-variance-limited realization of $C_{l}^{EE}$ taking the true history to be the double-reionization model with $\tau = 0.090$.\n
\(^{b}\) If not using principal components, reionization is assumed to occur instantaneously.

\(^{c}\) “Other” parameters are $\Omega_{b}h^2$, $\Omega_{c}h^2$, $h$, $A_s$, and $n_s$. Other nonreionization parameters are always fixed.

\(^{d}\) From Spergel et al. (2007).
probability distribution $P(\tau)$. The result is that the probability distributions for $\tau$ are similar for both instantaneous reionization models and the more general class of models, as shown in the right panel of Figure 8.

We use two methods to find the posterior distribution for $\tau$ in the instantaneous reionization case: one is the usual approach of varying the optical depth (or reionization redshift) in a Monte Carlo chain, and the other involves computing $P(\tau)$ for a subset of samples from chains in which principal components of proposed ionization histories and comparing the one-parameter instantaneous reionization model with a $z_{\text{min}} = 6$ prior (thick curve). The sharp cutoff at low $\tau$ in $P(\tau)$ for instantaneous reionization models comes from our $z_{\text{min}} = 6$ prior.

Note that the fact that the instantaneous reionization curve passes through the middle of the 68% confidence region indicates that models with rapid reionization are not at all disfavored by the 3 year WMAP data. This intersection of instantaneous models with WMAP constraints on more general models parameterized by principal components is perhaps not too surprising, considering that the current data only weakly constrain the principal components and are consistent with a wide variety of reionization histories. We expect that this will not be the case with future polarization data; tighter constraints on $\{m_i\}$ mean that any particular class of simple models is less likely to pass through the parameter space that fits the data well. With improved polarization measurements, then, the posterior distribution for $\tau$ assuming instantaneous reionization should in general differ from the model-independent $P(\tau)$ computed using MCMC with principal components, as we show explicitly in § 5.2.

The weak $m_2$ constraint visible in Figure 6 suggests that in addition to determining the total optical depth, WMAP data may provide useful limits on high-$z$ and low-$z$ optical depth as defined in the previous section. The 68% and 95% posterior probability contours for the partial optical depths from WMAP are shown in Figure 9 for $z_{\text{min}} = 20$ and $z_{\text{max}} = \{30, 40\}$. The $x_e = 0$ physicality prior cuts off the contours at $\tau(z_1, z_2) = 0$; in both panels, the upper limits set by $x_e = 1$ are outside the plotted area, so the contours are not strongly influenced by those priors. The error “ellipses” are narrowest in the direction along which the total optical depth is constrained, as shown by dashed lines of constant total optical depth at $\tau = 0.06$ and 0.12 (approximately the upper and lower 1 $\sigma$ limits from the 3 year WMAP analysis of Spergel et al. [2007]).

Comparison of the two panels in Figure 9 reveals that the choice of $z_{\text{min}}$ does not have a large effect on constraints on the optical depth above and below $z = 20$. This suggests that $\tau(20, z_{\text{max}})$ should be interpreted as $\tau(z > 20)$. We provide further justification for this interpretation in § 5.2.

The 95% upper limits on the high-redshift optical depth, $\tau(z > 20)$, are 0.076 and 0.078 for $z_{\text{max}} = 30$ and 40, respectively, after marginalizing over all other parameters. This is not a particularly strong constraint, since this result is only marginally inconsistent with all of the optical depth from reionization coming from $z > 20$, but with future data it should be possible to either reduce the upper limit on high-$z$ optical depth or detect the presence of a substantial ionized fraction at high redshift (see § 5.2).

Models of reionization can be tested by computing the principal components of proposed ionization histories and comparing with constraints on $\{m_i\}$ from Monte Carlo chains. The WMAP constraints in Figure 6 are non-Gaussian, in part because the physicality priors on $\{m_i\}$ intersect the posterior probability contours where the likelihood is large. Because the constraints do not have a simple Gaussian form, it appears that the full parameter chains are necessary for accurate model testing, although the viability of various models can be estimated by comparing their eigenmode amplitudes with marginalized constraints such as those in Figure 6, keeping in mind that models favored by marginalized
constraints could be disfavored in the full $N$-D parameter space.

As mentioned earlier, our single 10 parameter MCMC run (varying five principal components, $\Omega_m h^2, \Omega_b h^2, \theta, A_s e^{-2\tau}$, and $n_s$, and using TT and TE data, as well as EE) constrains the optical depth to $\tau = 0.109 \pm 0.030$. The uncertainty in $\tau$ is 10% larger than in our standard Monte Carlo chains with the same fiducial model, for which $\tau = 0.106 \pm 0.027$ (compare rows 3 and 5 in Table 1). This is the result of a slight widening of the constraints on principal components in directions orthogonal to surfaces of constant $\tau$. Other than this difference, the main effect of including additional parameters and temperature data is a small reduction in the posterior probability of models in certain corners of the region of parameter space bounded by physicality requirements [e.g., in the $m_2$-$m_3$, plane, models with $(m_2, m_3) \approx (m_2^{\text{true}}, m_3^{\text{true}})$.]

For such models, the Doppler effect from a large optical depth over a narrow slice in redshift at $z \approx z_{\text{max}}$ generates additional power in $C_{TT}^\ell$ at $\ell \sim 10$–100, so these models are disfavored when the likelihood includes the TT power spectrum. Since this is a small effect, our usual assumption that reionization constraints from polarization data can be considered separately from temperature constraints on other parameters is fairly good. With improved polarization measurements, this assumption should be even better since the relative contribution of temperature data to constraints on reionization will be even less than it is with the WMAP data.

5.2. Cosmic-Variance-Limited Data

To forecast how well principal components of the reionization history could be measured by future CMB polarization experiments, we repeat the analysis of § 5.1 using simulated realizations of the full-sky, noiseless $E$-mode angular power spectrum instead of WMAP data. Any real experiment will of course involve sky cuts, noise, foregrounds, and other complications, so the results presented here represent an optimistic limit on what we can learn about the global reionization history from low-$\ell$ $E$-mode polarization. At the end of this section, we estimate how much the constraints might be degraded from this idealized case for an experiment with characteristics similar to those proposed for the Planck satellite.

We generate simulated realizations of $C_{EE}^\ell$ drawn from $\chi^2$ distributions with cosmic variance determined by the theoretical angular power spectra that we compute using CAMB. For the $j$th sample in a chain, the likelihood including only $E$-mode polarization is

$$-\ln L_{(j)} = \sum_{\ell} \left( \ell + \frac{1}{2} \right) \left( \frac{\hat{C}_{EE}^{(j)}}{C_{EE}^{\text{true}}} + \ln \frac{C_{EE}^{(j)}}{C_{EE}^{\text{true}}} - 1 \right),$$

where $\hat{C}_{EE}^{(j)}$ is the spectrum of the simulated data and $C_{EE}^{\text{true}}$ is the theoretical spectrum calculated with the parameter values at step $j$ in the chain.

We have run Monte Carlo chains for multiple realizations of $C_{EE}^\ell$ drawn from spectra computed assuming a variety of “true” reionization histories, $x_e^{\text{true}}(z)$. We start by taking the true history to be a model with nearly instantaneous reionization and $\tau = 0.105$. As a contrasting model for comparison we also use an extended, double-reionization model with $\tau = 0.090$. Figure 1 shows $C_{EE}^\ell$ and $x_e(z)$ for each of these models.

Since parameter constraints derived using a single draw of $C_{EE}^\ell$ from the underlying power spectrum may contain features unique to that realization, we generated Monte Carlo chains for 10 random realizations of the instantaneous reionization power spectrum. Two of these realizations are plotted as points in Figure 10, along with the theoretical spectrum with cosmic-variance bands. The thick curves in Figure 10 are spectra of the best-fit models from the Monte Carlo chains for each realization. The overall best-fit models are similar for the two realizations, and both agree closely with the theoretical $C_{EE}^\ell$. The dashed curve in the right panel of Figure 10 shows an “alternative” best-fit model that we discuss later.

The 2D marginalized MCMC constraints on principal components for these two realizations are shown in Figure 11. The plotted regions are bounded by the physical top-hat priors on $\{m_\nu\}$.\n
Fig. 10.—$E$-mode spectra of the best-fit models from two Monte Carlo chains (thick curves), each using a different realization of simulated cosmic-variance-limited data (circles). The realizations are drawn from the same $C_{EE}^\ell$ of the instantaneous reionization model in Fig. 1, plotted as thin curves with shaded regions showing the 1 $\sigma$ cosmic-variance limits. The dashed curve in the right panel shows the best-fit model within the high-$m_2$ peak in the posterior probability (see Fig. 11).
as in Figure 6, but the eigenmodes are different here, with $z_{\text{max}} = 20$ instead of 30 or 40 for the fiducial history. Since we have constructed $x^{\text{true}}(z)$ to have no ionization at $z \gtrsim 15$, we know that $z_{\text{max}} = 20$ should be a large enough maximum redshift; this choice of $z_{\text{max}}$ also reflects the fact that improved empirical determination of $z_{\text{max}}$ will allow it to be set at lower redshift for future data analysis, assuming that high-$z$ reionization is not detected.

The contours in Figure 11 show that cosmic-variance-limited data can constrain models within the physically allowed parameter space much better than current data can. The chains used for the results shown here vary the first three eigenmodes; by running chains with $N > 3$ we find that cosmic-variance-limited data can provide $2 \sigma$ constraints that are tighter than the physicality bounds for the first four eigenmodes of a $z_{\text{max}} = 20$ fiducial model and for at least five eigenmodes when $z_{\text{max}} = 30$.

Although the only difference in the MCMC setup for the left and right panels of Figure 11 is the realization of $C_{EE}^{\ell}$ (Fig. 10), there are some significant differences in the resulting eigenmode constraints, particularly in the $m_2$-$m_3$ plane. Despite the multimodality visible in the constraints on the right, the chain is in fact well converged according to the criteria listed previously (e.g., $R - 1 < 0.01$), and multiple independent Markov chains using this realization of $C_{EE}^{\ell}$ all produce the same constraints on the principal components. Furthermore, the differences between the left and right panels of Figure 11 can be explained by comparing $C_{EE}^{\ell}$ for specific reionization histories with these realizations of the polarization power spectra.

Differences in the principal component constraints among realizations of the simulated data are related to whether features in the theoretical $C_{EE}^{\ell}$ remain intact with the inclusion of cosmic variance. The relevant features in the spectrum are the small oscillations in the low-power “valley” in $C_{EE}^{\ell}$ on scales $10 \lesssim \ell \lesssim 30$. In the example shown here, the feature that matters most is the bump in the theoretical spectrum at $\ell \approx 13$. In the left panel of Figure 10, the $C_{EE}^{\ell}$ realization retains this bump, while in the right panel the bump is washed out by cosmic variance. The result is that the left realization is better able to pick out those reionization models in Monte Carlo chains that reproduce the true $C_{EE}^{\ell}$, leading to the tight constraints in the left panel of Figure 11. The realization in the right panel of Figure 10 lacks this important “fingerprint” for identifying models that match the theoretical $C_{EE}^{\ell}$, so the data allow a wider variety of models, as reflected in the constraints in the right panel of Figure 11. In this case, there are two best-fit models corresponding to the two 68% contours separated in the $m_2$ direction. The spectrum of the overall best-fit model (with smaller $m_2$), which is close to the theoretical spectrum, is plotted as a thick solid curve in the right panel of Figure 10, while the other best-fit model (at larger $m_2$) is plotted as a dashed curve. These two models have significantly different spectra, but because of the scatter in the random draw of $C_{EE}^{\ell}$, they are each able to fit the data better at some multipoles and worse at others in such a way that the high-$m_2$ best-fit model is only a slightly worse fit than the low-$m_2$ best-fit model. Note that for both models, $C_{EE}^{\ell}$ is within the 68% cosmic-variance band around the spectrum of the true reionization history.

Among the realizations of simulated data that we explored with MCMC methods, constraints like those in the right panel of Figure 11 are a fairly extreme case, occurring about 10%–20% of the time. In general, the realizations form a sort of continuum between the two presented here, with about half showing some displacement of the 95% contour toward larger $m_2$, but not as much as in the second realization that we show as an example. In particular, the constraints for most of the realizations do not have multimodal contours at the 68% confidence level (CL). The extent to which differences between realizations show up in principal component constraints depends on $x^{\text{true}}(z)$. For example, the $C_{EE}^{\ell}$ values for the double-reionization model (Fig. 1) have more pronounced oscillations at $\ell \sim 10$–30 than the instantaneous reionization spectrum, so they are not as easily erased by cosmic variance or noise, and the resulting principal component constraints tend to be more consistent from one realization to the next and more like the left panel of Figure 11.

The differences between constraints from various realizations of simulated data suggest the interesting possibility that our
ability to learn about the reionization history from large-scale $E$-mode polarization may ultimately depend on the luck of the draw of $C_{EE}^{C}$ at our particular vantage point. In an unlucky draw, cosmic variance can distort subtle features in the power spectrum in a way that would limit constraints on reionization eigenmodes to be worse than we might expect from the Fisher approximation or a more typical draw. The good news is that even a realization like the one in the right panels of Figures 10 and 11 would permit constraints that are far better than what is currently possible. It is also important to note that although such constraints are weaker than in the best-case scenario, they are still consistent with the true parameter values and in general would not lead us to rule out the true reionization history based on a principal component analysis of the data.

As with the principal components of $x_e(z)$, MCMC analysis indicates that constraints on the total optical depth to reionization would be greatly improved with cosmic-variance-limited data: $\sigma_\tau \approx 0.005$, down a factor of 6 from the 3 year $WMAP$ value, $\sigma_\tau \approx 0.03$. The constraints on $\tau$ using the realization of instantaneous reionization $C_{EE}^{C}$ in the left panel of Figure 10 are listed in Table 1 for two fiducial models with $z_{\text{max}} = 20$ and 30. Optical depth constraints from the other draw of $C_{EE}^{C}$ are similar, so estimates of $\tau$ and $\sigma_\tau$ appear not to be biased for atypical realizations. It makes sense that differences in realizations do not significantly affect $\tau$, since the optical depth constraint comes mainly from the peak in $C_{EE}^{C}$ on the largest scales, whereas differences in principal component constraints between realizations arise from the low-power part of the spectrum at higher $\ell$.

The model-independent constraints on $\tau$ are neither biased nor significantly weaker relative to the constraint obtained assuming instantaneous reionization (bottom row in Table 1), as is true for the $WMAP$ data. This should not be surprising, since we have assumed that $x_e^{\text{true}}(z)$ is an instantaneous reionization model. However, if $x_e^{\text{true}}(z)$ is in fact very different from the instantaneous model, the estimate of $\tau$ obtained under the assumption of instantaneous reionization will be incorrect. For example, if we take $x_e^{\text{true}}(z)$ to be the double-reionization model of Figure 1, the model-independent approach yields an optical depth constraint consistent with the true value of $\tau = 0.090$. On the other hand, MCMC analysis restricted to instantaneous reionization histories gives a significantly biased estimate, $\tau = 0.135 \pm 0.005$. As Figure 12 shows, in this case the 1D curve of instantaneous reionization models in the space of eigenmodes never lies near the principal component values favored by the data, so any analysis that only considers such models will never find a good fit to the data. This illustrates the importance of a model-independent approach: although results from current data may not be significantly affected by the assumption of a specific form of $x_e(z)$, future data will be sensitive enough to the reionization history that the choice of a specific model can greatly impact the results (Holder et al. 2003; Colombo et al. 2005).

Although constraints on the contributions to $\tau$ from high and low $z$ are currently limited to weak upper bounds, future polarization data will likely enable more definitive detections of high-$z$ reionization if it is present, or tighter upper limits if absent. The left and right panels of Figure 13 show these constraints from Monte Carlo chains using the $C_{EE}^{C}$ plotted in the left and right panels of Figure 10, respectively. The true ionization history has zero ionized fraction at $z > 15$, and the MCMC analysis places a 95% CL upper limit on $\tau(z > 15)$ of $\tau < 0.03$. Figure 14 shows MCMC constraints on the same partial optical depths using simulated data where the true model is instead taken to be the extended, double-reionization history plotted as a thin curve in the inset of Figure 1. In this case, most of $\tau(z_{\text{min}}, z_{\text{max}})$ comes from $z > 15$, and using the principal components of $x_e(z)$ the high-$z$ optical depth can be detected at a high level of confidence and measured to an accuracy of $\sim 0.01$. Note that the constraints in both Figures 13 and 14 are consistent with the $WMAP$ constraints in Figure 9.

As with $WMAP$ data, most of the constraints from simulated data in Figures 13 and 14 do not appear to depend strongly on the choice of $z_{\text{max}}$. For the instantaneous reionization model used for Figure 13, this is to be expected, since we know that the simulated $C_{EE}^{C}$ have no contribution from $z \gtrsim 20$. Each set of contours in Figure 13 is consistent with the values of $\tau(6, 15)$ and $\tau(15, z_{\text{max}})$ for $x_e^{\text{true}}(z)$. The constraints in the second panel in Figure 13 extend to larger high-$z$ optical depth than those in the first panel because the effect of the physicality priors is not as strong at larger $z_{\text{max}}$, as noted in § 5.1; the leftmost $z_{\text{max}} = 20$ contours would stretch to larger $\tau(15, 20)$ and smaller $\tau(15, 15)$ if we did not apply the physicality bounds. The two panels on the right side of Figure 13 show weaker constraints on the partial optical depths because the principal component constraints for that realization of $C_{EE}^{C}$ are weaker.

In the extended, double-reionization model used for Figure 14, reionization actually starts at $z = 23$, so the choice of $z_{\text{max}} = 20$ is not appropriate for this model. The result of such an error is that the constraint on $\tau(15, 20)$ is inconsistent with the true value, marked by a cross in the left panel of Figure 14. The $z_{\text{max}} = 30$ constraints in the right panel are consistent with the expected value, although not in perfect agreement due to cosmic variance. It is interesting that although the value chosen for $z_{\text{max}}$ in the left panel is too low for this model, the constraints on $\tau(z > 15)$ for $z_{\text{max}} = 20$ and 30 are still consistent with each other. This supports the interpretation of constraints on $\tau(z_{\text{min}}, z_{\text{max}})$ as $\tau(z > z_{\text{min}})$ in § 5.1.

While the cosmic-variance-limited simulated data are useful for determining how well the reionization history could possibly be constrained by large-scale $E$-mode polarization measurements, it is also interesting to ask how well we can do with future
experiments that fall somewhat short of the idealized case that we have considered so far. In particular, the upcoming Planck satellite is expected to improve our knowledge of the large-scale $E$-mode spectrum substantially (Planck Collaboration 2006); what does this imply for constraints on $x_e(\tau)\? To estimate what might be possible with Planck data, we assume that after subtracting foregrounds a single foreground-free frequency channel remains for constraining the low-$\ell$ $E$-mode polarization. We take this to be the 143 GHz channel with a white noise power level of $w_p^{1/2} = 81 \mu$K arcmin and beam size $\theta_{FWHM} = 7.1'$, and we assume that the sky coverage is $f_{sky} = 0.8$ after cutting out the Galactic plane (Planck Collaboration 2006; Albrecht et al. 2006). We compute the likelihood of Monte Carlo samples using the routines provided in CosmoMC and analyze parameter chains with the principal component method as described for WMAP and cosmic-variance-limited data.

For various choices of $x_e^{\text{fid}}(\tau)$ and $x_e^{\text{true}}(\tau)$, we find that going from full-sky cosmic-variance-limited data to Planck-like data increases the uncertainty in $x_e(\tau)$ principal components, $\sigma_1$, and in the optical depth, $\sigma_\tau$, by roughly a factor of 2. Based on these results, it should be possible to constrain about three eigenmodes at $\sim 2 \sigma$ within the space of physical models, and we expect $\tau$ to be determined to an accuracy of about $\pm 0.01$. This is consistent with previous estimates of the Planck optical depth uncertainty when considering more general reionization models than instantaneous reionization (e.g., Holder et al. 2003; Hu & Holder 2003).

5.3. Fisher Matrix Predictions versus MCMC Results

The Fisher matrix analysis of § 2 predicts that the principal components of $x_e(\tau)$ should be uncorrelated, with errors given by $\sigma_\mu$ from equation (2) (in the idealized limit of full sky, noiseless observations). These characteristics rely on the assumption that the difference between the true and fiducial reionization histories is small: $\delta x_e^{\text{true}}(\tau) = x_e^{\text{true}}(\tau) - x_e^{\text{fid}}(\tau) \ll 1$. Clearly this assumption will not hold for any single fiducial history if one wants to consider a variety of possible true histories, and the consequence is that $\langle m_\mu m_\nu \rangle$ differs from $\sigma_\mu^2$.

As an example of the difference between the Fisher approximation and the full Monte Carlo analysis, in Figure 15 the marginalized constraints in the $m_1$-$m_2$ plane from the left panel of Figure 11 are compared with the Fisher matrix error ellipses, centered on the true $(m_1, m_2)$ for the same choices of $x_e^{\text{true}}(\tau)$ (instantaneous reionization with $\tau = 0.105$) and $x_e^{\text{fid}}(\tau)$ (constant $x_e = 0.15$ out to $z_{\text{max}} = 20$). The MCMC constraints have correlated values of $m_1$ and $m_2$ with somewhat larger uncertainties than the
The principal components of the reionization history are a promising tool for extracting as much of that information as possible from the data. We have shown that the principal component method can be usefully applied to real, currently available data, and forecasts from simulated data suggest that there is room to substantially improve constraints on the reionization history using this method as measurements of the large-scale $E$-modes improve.

We find that the key features of the principal component analysis put forward by Hu & Holder (2003) continue to apply when we go from the Fisher matrix approximation to an exploration of the full likelihood surface using Markov chain Monte Carlo methods. For fairly conservative choices of the maximum redshift of reionization ($z_{\text{max}} \sim 30-40$), only the first five principal components at most are needed for a complete representation of the $E$-mode angular power spectrum to within cosmic variance. To account for arbitrary reionization histories in the analysis of CMB data, only a few additional parameters must be included in chains of Monte Carlo samples if those parameters are taken to be the lowest variance principal components of $x_e(z)$.

Specific models of reionization can be tested easily by computing their eigenmode amplitudes and comparing with constraints on the eigenmodes from the data. The principal component decomposition of $x_e(z)$ also provides a convenient way to reduce CMB polarization data so that it may be combined with additional probes of reionization such as planned future observations of the $21$ cm line of neutral hydrogen, which are expected to yield complementary information about the late stages of reionization (see Furlanetto et al. 2006 for a review). Principal component constraints could be mapped onto the $21$ cm parameter space for analysis of the joint constraints from CMB polarization and $21$ cm data on the reionization history. Constraints on derived parameters, such as total optical depth or the optical depth from a certain range in redshift, represent other applications of the MCMC constraints on principal components of $x_e(z)$.

Often, estimates of the optical depth to reionization are computed assuming instantaneous reionization or some other simple form for $x_e(z)$. Here we extend the analysis of the $3$ year WMAP data to allow a more general set of models of the global reionization history. We find that expanding the model space does not significantly widen the uncertainty in $\tau$ beyond the instantaneous reionization value of $\sigma_\tau = 0.03$. Robust $\tau$ constraints are important for tests of the dark energy based on the growth of structure, since they control the uncertainty on the amplitude of the initial spectrum.

Moreover, even with current data the principal component constraints are beginning to show the possibility of determining properties of reionization in addition to $\tau$. By comparing the optical depth from high $z$ with that from low $z$, we obtain an upper limit on the contribution to the optical depth from high redshift: $\tau(z > 20) < 0.08$ at $95\%$ confidence, assuming that there is no significant episode of reionization at $z \gg 40$.

Due to the limitations of noise and foreground contamination, only the first two eigenmodes of the reionization history, $m_1$ and $m_2$, can be determined with present polarization data to any reasonable degree of accuracy. Constraints on these two modes come primarily from the main, broad peak in $E$-mode power at low $\ell$ from reionization.

As measurements of the $E$-mode polarization improve, for example, from additional WMAP data or through planned future experiments such as Planck, better knowledge of the low-power "trough" in $C^{EE}_\ell$ between the main reionization peak and the first acoustic peak should enable constraints on the third and higher principal components, up to about $m_5$ for near-cosmic-variance-limited data. Since constraints on these higher modes rely on the ability to identify subtle features in the trough of $C^{EE}_\ell$, the ultimate accuracy to which the eigenmodes can be determined may depend on whether or not the necessary features are well reproduced in the particular random draw of $C^{EE}_\ell$ that is available to us. However, even if we are unlucky enough to have a realization...
in which some of the important features of the spectrum are washed out by randomness, it should still be possible to measure several of the principal components to better accuracy than is currently possible. Knowledge of the $\mu \geq 3$ eigenmodes of $x_i(z)$, along with improved constraints on $m_1$ and $m_2$, will allow more stringent tests of reionization models and a better understanding of the global reionization history.

We thank Cora Dvorkin, Gilbert Holder, Dragan Huterer, Hiranya Peiris, and Jochen Weller for useful discussions. M. J. M. was supported by a National Science Foundation Graduate Research Fellowship. W. H. was supported by the Kavli Institute for Cosmological Physics through the grant NSF PHY-0114422, the Department of Energy through contract DE-FG02-90ER-40560, and the David and Lucile Packard Foundation.

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