MEASURING THE THREE-DIMENSIONAL SHAPE OF X-RAY CLUSTERS

JOHAN SAMSING, ANDREAS SKIELBOE, AND STEEN H. HANSEN

Dark Cosmology Centre, Niels Bohr Institute, University of Copenhagen, Juliane Maries Vej 30, 2100 Copenhagen, Denmark

Received 2011 October 24; accepted 2012 January 10; published 2012 March 1

ABSTRACT

Observations and numerical simulations of galaxy clusters strongly indicate that the hot intracluster X-ray-emitting gas is not spherically symmetric. In many earlier studies, spherical symmetry has been assumed partly because of limited data quality; however, new deep observations and instrumental designs will make it possible to go beyond that assumption. Measuring the temperature and density profiles are of interest when observing the X-ray gas; however, the spatial shape of the gas itself also carries very useful information. For example, it is believed that the X-ray gas shape in the inner parts of galaxy clusters is greatly affected by feedback mechanisms, cooling, and rotation, and measuring this shape can therefore indirectly provide information on these mechanisms. In this paper, we present a novel method to measure the three-dimensional shape of the intracluster X-ray-emitting gas. We can measure the shape from X-ray observations only, i.e., the method does not require combination with independent measurements of, e.g., the cluster mass or density profile. This is possible when one uses the full spectral information contained in the observed spectra. We demonstrate the method by measuring radiallly dependent shapes along the line of sight for CHANDRA mock data. We find that at least $10^6$ photons are required to get a $5\sigma$ detection of shape for an X-ray gas having realistic features such as a cool core and a double power law for the density profile. We illustrate how Bayes’ theorem is used to find the best-fitting model of the X-ray gas, an analysis that is very important in a real observational scenario where the true spatial shape is unknown. Not including a shape in the fit may propagate a possible radially dependent shape of an X-ray gas can be to a mass bias if the X-ray is used to estimate the total cluster mass. We discuss this mass bias for a class of spatial shapes.

Key word: X-rays: galaxies: clusters

Online-only material: color figures

1. INTRODUCTION

Galaxy clusters are the largest bound objects in the universe and they provide unique and independent information on the cosmological evolution. The standard LCDM parameters and a possible redshift varying dark energy component has accurately been measured and constrained from cluster observations in a variety of ways (Vikhlinin et al. 2009b, 2009a; Allen et al. 2008, 2011; Mantz et al. 2010). They reveal the distant universe behind them through gravitational magnification (Kneib et al. 2004; Amanullah et al. 2011; Bradley et al. 2011), and they are even sensitive to the initial perturbations of our universe (Fedeli et al. 2009; Chongchitnan & Silk 2011; Sartoris et al. 2010). Clusters not only serve as excellent laboratories for constraining the standard cosmology, but because of their relatively high mass and cosmological size they also provide a unique possibility to test general relativity itself in several independent ways, e.g., from measurements of cosmic growth (Rapetti et al. 2010) to gravitational redshift (Wojtak et al. 2011) and gravitational waves (Yoo et al. 2009). Other probes have also been suggested, such as lensing, cluster abundance, and the integrated Sachs–Wolfe effect (Jain & Zhang 2008). Despite their importance in modern cosmology, basic properties such as spatial shape is still not well measured for individual clusters. One reason is simply that the main part of a cluster is composed of dark matter which can only be measured indirectly by its gravitational interaction. The indirect measurements of the dark matter and its radial distribution are usually done using either lensing (Postman et al. 2011; Stark et al. 2007), by studying the dynamics of the intracluster galaxies (Wojtak & Łokas 2010; Łokas & Mamon 2003; Lemze et al. 2009), or by the hot baryonic X-ray-emitting gas located in the inner regions of all clusters (for a review of X-ray physics and applications; see, e.g., Sarazin 1988). Specifically, observations of the intracluster X-ray gas in terms of spatial shape, density, and temperature profiles play a key role in estimating local properties of the cluster. Many earlier studies assume a spherical shape of the gas (Pointecouteau et al. 2005; Host & Hansen 2011; Kaasra et al. 2004; Piffaretti et al. 2005; Hansen & Piffaretti 2007; Rapetti et al. 2010); however, there are several strong motivations why obtaining a precise estimation of the shape is interesting. One is the precise estimation of the cluster mass profile. This profile can directly be measured if the radial shape, temperature, and density profiles of the gas are known and the gas is in hydrostatic equilibrium (HE). Only recently it was shown that allowing the gas to have a triaxial shape is necessary for the estimated mass profile from the X-ray to agree with the mass estimated from lensing (Morandi et al. 2010, 2011; Sereno &Umetsu 2011), a result in good agreement with numerical simulations (Hayashi et al. 2007). This overall triaxiality is mostly due to the underlying shape of the dark matter potential. However, in the central cluster regions it is believed that a possible non-spherical X-ray shape is more affected by microphysical processes such as radiative cooling, turbulence, and different feedback mechanisms (Lau et al. 2011) than the dark matter potential shape is. These mechanisms change the gas shape into having relatively high ellipticity toward the center compared to the underlying dark matter potential shape. It is therefore possible to infer properties of these mechanisms if the shape of the gas, temperature, and density profiles are known to high precision.

In this paper, we suggest and develop a method from which a possible radially dependent shape of an X-ray gas can be extracted from the X-ray observations only. We explicitly
Figure 1. Simplified description of how information propagates from three dimensions to a two-dimensional observation. The figure shows two free–free emission X-ray spectra (the two lowest spectra at 3 keV in black), the sum of these two spectra (second spectrum from the top at 3 keV in red), and a best-fit free–free spectrum to the red spectrum (upper spectrum at 3 keV in blue). This could correspond to a part of the gas with two temperature components (one spectrum for each component) projected along the line of sight (observed data). By comparing the blue and the red spectra one notices that the red spectrum cannot simply be fitted accurately with a free–free emission X-ray spectrum. This is true in the general case; a sum of free–free spectra cannot in general be fitted by another free–free spectrum. If the observed red spectrum is not correctly fitted one could incorrectly conclude the presence of either a non-thermal hard X-ray excess or non-thermal soft X-ray excess component, depending on the shape of the red spectrum. In our example one would report a hard excess component since the red spectrum is above the blue in the tail (see, e.g., Fusco-Femiano et al. 2005 for a hard excess discussion for A2256). (A color version of this figure is available in the online journal.)

demonstrate the possibilities of measuring the shape by fitting to CHANDRA mock data, and we estimate the mass bias if a shape is not treated correctly in the fitting. The method we use is a parameterized approach, i.e., we assume that the shape and profiles can be described by a set of well-defined functional forms. We also discuss the complications of choosing the best set of functions, i.e., a model, to describe the data.

The paper is organized in the following way. The method for measuring shape is explained in Section 2.1. We apply the method in Section 3 on CHANDRA mock data. We discuss how to quantify the goodness of fit in Section 3.3. Mass bias from not including the shape in the fitting is discussed in Section 4.

2. EXTRACTING 3D X-RAY INFORMATION FROM TWO-DIMENSIONAL OBSERVATIONS

An intracluster X-ray-emitting gas has a three-dimensional extension, spherical or not, but an observer will only see the two-dimensional projected image on the sky. Therefore, a given observed spectrum is the sum of all emission spectra along the line of sight through the gas (for a discussion; see Figure 1).

Each spectrum has a spectral shape determined by the local temperature and a scaling proportional to the local density squared (Sarazin 1988). Mathematically, no unique mapping can construct the true three-dimensional shape, density, and temperature profiles using only the observed two-dimensional image. However, if one makes prior assumptions, it can be done. For instance, by assuming that the gas is spherical, the density and temperature profiles can be found. From this assumption several previous groups have measured the temperature and density profiles of the X-ray gas using either projection or de-projection techniques (see, e.g., the XSPEC packages “deproject” and “project”).

The method we present in this paper for extracting three-dimensional information relies on the assumption that the X-ray gas shape, density, and temperature profiles can be described by parameterizations. This means that the shape and profiles are believed to be well described by a set of functions. In contrast to several previous studies we use the whole spectral information from the integrated observed picture of the X-ray gas. It means that we take into account that the actual observed spectra is a sum of spectra along the line of sight, and cannot simply be fitted by a single free–free spectrum. See Figure 1 for a discussion. We allow a radially dependent shape in contrast to previous studies. The tradeoff for including this extra freedom is that we limit our analysis to structures that are seen to be spherical on the sky. This is for purely practical reasons: in theory the fitting method we describe is not limited by this assumption, but with present day available data it is simply not possible to resolve a radially dependent shape if the three-dimensional shape and orientation of the gas is completely free to vary. In other words, the symmetry in the sky makes it possible to extract higher order corrections to the usual assumption about either sphericity or triaxiality with constant axis ratios. The method and procedure will be described in the following sections, and technical details are found in the Appendix together with illustrations of generated spectra and an X-ray structure.

2.1. Fitting Shape and Profiles using the Parameterization Approach

The procedure needed in order to measure spatial shape, temperature, and density profiles of an observed X-ray gas using the parameterization approach is as follows. First we choose a model, i.e., a set of parameterizations that are believed to generally describe the form of density, temperature, and spatial shape (along the line of sight), for the observed structure. The chosen parameterizations must be sufficiently general to accurately describe observations of real and simulated structures. We then calculate the agreement between an artificial generated data set (see Appendix A.1 for how we generate artificial data sets and mock data) created from the chosen model given a specific combination of parameter values and the observed data set. In our case we quantify the agreement by a simple $\chi^2$ statistic which simply can be related to a probability by $\exp(-\chi^2/2)$ when the noise is Gaussian. This routine of comparing artificial generated data sets with the observed data set is then repeated for a wide range of parameter value combinations until a good estimate of the underlying probability distribution function (PDF) for our model has been made. For this we use standard Monte Carlo techniques as described in Appendix A.2. From the parameter combination having the maximum PDF value, the best estimate for profiles and shape, given our prior input parameterizations, can then be made. The overall procedure can then be repeated for different models, until the best model is found. We will discuss this in more detail in Section 3.3.

3. RESULTS FROM FITTING SHAPE AND PROFILES OF SELECTED X-RAY MODELS

In the following, we show the possibilities of measuring the radial profiles of non-spherical X-ray structures with varying radially dependent shapes along the line of sight. As briefly discussed in the end of Section 2, we only consider structures that are spherical on the sky. We consider two simulated structures in our analysis: first, a simple toy model to clearly illustrate the method and second, a more realistic model with features such as a cool core and a double power law for the density profile. The shape parameterizations are described later.
In this part of the analysis we fit for profiles and shape using the same set of parameterizations that are used to generate the data. In this way we get the cleanest picture of how a shape signal propagates to observables.

We present results in terms of a virial radius \( r_v \). The shape, temperature, and density profiles we use are consistent with a virial radius similar to \( r_{500} \) (Vikhlinin et al. 2006).

### 3.1. A Simple Toy Model

We consider a data set denoted by “shM1” where the density and temperature profiles are modeled by simple broken power laws,

\[
\begin{align*}
\rho(r) &= n_0 (1 + (r/r_c)^2)^{-3\beta/2} \\
T(r) &= T_0 (1 + (r/r_t)^3)^{-\alpha/2},
\end{align*}
\]

known as beta-models. The parameter \( n_0 \) acts as a normalization factor and is regulated such that the artificial data set has a fixed number of total (photon) counts. The shape parameterization we consider is a simple linear function for ellipticity,

\[
\epsilon_1(r) = s_2 \cdot r + s_1,
\]

where \( \epsilon \equiv b/a \) is defined as the ratio between the radius perpendicular to the observer (b) and the radius along the line of sight (a) of the observer. The parameter values for shM1 are listed in Table 1, and Figure 2 shows the corresponding shape and profiles. The chosen parameters for the density and temperature profiles are in fair agreement with typical observed values. The priors on the shape parameterization we use in this example are: (1) \( 0.2 < b/a \leq 1 \) and (2) \( \epsilon_1(r/r_1) > 0.5 \). In general, a structure could naturally have an axis ratio \( b/a \geq 1 \) and still be spherical on the sky, and therefore in a scenario where no prior shape information is available, shapes with \( b/a \geq 1 \) must be included in the fit as well.

The left plot of Figure 3 shows the maximized PDFs for the fitted density, temperature, and shape parameters for a total of \( 3 \times 10^5 \) photon counts (\( \approx 10 \) ks CHANDRA observation of A1689). The width of the projected PDFs, i.e., a measure of the fitting error for each parameter, is simply related to the number counts by \( \approx 1/\sqrt{N} \), where \( N \) is the number of photons. The right plot of Figure 3 shows the corresponding correlation matrix defined in the usual way as \( \text{CORR}(X, Y) = \left((X - \mu_X)(Y - \mu_Y)\right)/(\sigma_X \sigma_Y) \) where \( X, Y \) are random variables with expectation values \( \mu_X, \mu_Y \) and standard deviations \( \sigma_X, \sigma_Y \). In our case, to find, e.g., the correlation coefficient \( \text{CORR}(p_1, p_1) \) the structure and therefore “allows” more mass along the line of sight. This is simply because an ellipticity “stretches” the structure and therefore is related to the shape and density, but assuming spherical symmetry.

(A color version of this figure is available in the online journal.)

### Table 1

| Model | Equation | \( n_0 \) | \( r_c \) | \( \beta \) | \( \alpha/2 \) | \( T_0 \) | \( a \) | \( b \) | \( r_t \) | \( s_1 \) | \( s_2 \) |
|-------|----------|-----------|-----------|-----------|--------------|-----------|---|---|---|---|---|
| shM1  | 1, 2, 3  | \cdots | 0.11 | 0.6 | 0 | 5.0 | 0 | 0.14 | 0.99 | 0.3 | 0.83 |
| shM2  | 4, 6, 7  | \cdots | 0.15 | 0.76 | 1.2 | 4.3 | 2.45 | 0.7 | 0.13 | 0.94 | 0.2 |

\[ \text{CORR}(X, Y) \]

Figure 2. Shape and profiles for data set shM1 (red, solid lines) and shM2 (blue, dashed lines). Left: ellipticity of the X-ray gas along the line of sight. Middle: X-ray gas density profile. Right: X-ray gas temperature profile. Black, dotted lines: best estimate from an MCMC fitting to shM2 using the true parameterizations for temperature and density, but assuming spherical symmetry.
of sight. This is exactly how $n_0$ affects the projected data set, too. So, if we increase the overall scaling (increasing $n_0$) we can compensate by decreasing the ellipticity (increasing $s_1$). That means the lower truncation of $s_1$ also shows up as a lower truncation on $n_0$. In fact, a constant ellipticity along the line of sight $\epsilon$ is completely degenerate with the overall density scaling $\rho_0$ by $\rho_0^2\epsilon$. This is an intrinsic degeneracy and can only be broken by including other observations, e.g., SZ observations, which effectively trace $\rho_0\epsilon T$ (see, e.g., Planck Collaboration et al. 2011; De Filippis et al. 2005; Conte et al. 2011; Sereno et al. 2011).

The overall conclusion from the fitting results is that the parameter values specifying the true shape as well as temperature and density are exactly reconstructed. This is an ideal case, but it is clearly showing that temperature, density, and shape in principle can be separated.

From the correlations we can conclude that the temperature profile is well and almost independently fitted. In the perspective of optimizing the fit for shape, this also implies that independent measurements of the density will directly result in a better fit for the shape.

### 3.2. A More Realistic Model

We now perform an analysis on a data set, denoted by “shM2,” describing a structure with a cool core and a double power law for the density profile. The inclusion of these features is motivated by real observations (Vikhlinin et al. 2006). The temperature and density profiles are now parameterized as

$$\rho(r) = n_0 \frac{(r/r_c)^{-\alpha/2}}{(1 + (r/r_c)^2)^{3\beta/2 - \alpha/4}} \quad (4)$$

$$T(r) = T_0 \frac{1 + a(r/r_c)}{(1 + (r/r_c)^2)^{\beta}} \quad (5)$$

and the shape is parameterized by

$$\epsilon_2(r) = s_2 \cdot \log_{10}(r) + s_1. \quad (6)$$

This shape parameterization approximately describes the gas shape seen in the inner parts ($r \lesssim r_{500}$) of the clusters in numerical simulations (Lau et al. 2011). We use the same shape priors as used in the previous toy model example. A list of temperature and density parameterizations are found in Vikhlinin et al. (2006).

The true parameter values for “shM2” are listed in Table 1 and the corresponding shape and profiles are plotted in Figure 2. Figure 4 shows the PDF and the correlation matrix for the 10 parameter model fitting.

An inner density slope captured by $\alpha$ is now one of the new parameters compared to the toy model. Since both the shape and this inner slope have a logarithmic dependence, there is a strong correlation between $\alpha$ and $s_2$. This is clearly seen in the correlation matrix and the PDF plot where the lower cut on $s_2$ directly relates to the skewness in the $\alpha$ distribution. This freedom in the inner slope is the main reason for the fitting to require many more photons than the toy model. This is discussed in more detail in Section 3.3 below.

The overall conclusion is that the true parameter values are reconstructed, but to keep down the statistical errors a relatively high number of photons is required. This is mostly due to the similar parameterizations for shape and density. In agreement with intuition, we see that it is much harder to extract a logarithmic shape when the density is varying logarithmically, too, compared to, e.g., a linearly dependent shape. From the correlation matrix we see that the temperature fitting is nearly unaffected as we also concluded in the previous toy model example.

### 3.3. Quantifying the Goodness of Fit

In this section, we will discuss how to quantify the goodness of fit for the parameters within a given model, as well as the goodness of fit for the model itself relative to other competitive models.

#### 3.3.1. Individual Parameters within a Model

The best-fit parameter values for a given model are located at the likelihood maximum or the minimum $\chi^2$ if the measurement noise is Gaussian. To quantify the goodness of fit is not unique. To quantify this one must often combine statistical estimators...
Figure 4. Fitting results for data set “shM2.” Left: maximized PDFs along each of the 10 parameters in the model. Right: correlation matrix for the 10 parameters in the model. The lower left part of the matrix shows the absolute value of the correlation coefficient where the upper right corner shows the sign of the coefficient in black (negative) and white (positive). The results are based on a data set scaled to have a total of $1 \times 10^6$ photon counts.

(A color version of this figure is available in the online journal.)

Figure 5. Plot shows the ratio $\hat{\pi}_i / \sigma_i$ for the most difficult parameters to estimate when fitting for structure “shM1” (left figure) and “shM2” (right figure) in black lines. The worst estimated parameter in terms of $n$ when fitting to “shM1” is $r_t$ and $s_2$ when fitting to “shM2.” The red dashed line in the left plot shows the ratio for parameter $s_1$ which is the worst determined of the two shape parameters when fitting to “shM1.” It can be read from the figure that $\approx 4.2 \times 10^6$ number total photon counts are required for a minimum 5$\sigma$ detection on all parameters when fitting to “shM2.” The radial and spectral binning is kept constant in the plot.

(A color version of this figure is available in the online journal.)

with prior knowledge. An often used estimator is the reduced chi square, $\chi^2_{\text{red}} = \chi^2 / K$, where $K$ is the number of degrees of freedom. However, this estimator has two major problems. First, the $\chi^2$ itself has a significant noise due to random noise of the data, and second, the number of degrees of freedom is not in general well defined (Andrae et al. 2010). Another, maybe more intuitive, estimator is the ratio $\hat{\pi}_i / \sigma_i$, where $\hat{\pi}_i$ is the best estimate for parameter $\pi_i$ and $\sigma_i$ is the associated standard deviation. If we denote this ratio by $n$ we can quantify the goodness of fit by reporting $n$ for each parameter or the minimum $n$ for the whole model. For the fitting examples we presented above, it is then of interest to know the number of photons required for, e.g., a minimum $5\sigma$ detection for all parameters. We will investigate this in the following. Figure 5 shows the ratio $\hat{\pi}_i / \sigma_i$ as a function of total photon counts for the parameter that has the largest ratio, i.e., the parameter which is the most difficult to estimate for the two structures “shM1” (left plot) and “shM2” (right plot). In the “shM1” example the most difficult parameter to estimate in terms of $n$ is $r_t$; to reach a minimum 5$\sigma$ detection of this (and thereby for each parameter of the whole model) we find from the figure that more than $\approx 2.5 \times 10^5$ photons are required. If we instead only require that the shape parameters must be estimated with a minimum 5$\sigma$ each, we find a limit of $\approx 1.4 \times 10^5$ photons or roughly a factor of two less compared to an overall 5$\sigma$ detection. Following the same procedure for the more realistic example “shM2” we find that a minimum of $\approx 4.2 \times 10^6$ photons is required for a minimum 5$\sigma$ detection on all parameters. The same number of photons are required for the shape fitting because $s_2$ is the most difficult parameter to estimate in terms of $n$. 

(A color version of this figure is available in the online journal.)
3.3.2. Model Comparison

Assuming that the quantities we try to measure for a gas can be parameterized, we still have the problem that we have no idea of how the “true” or best parameterization for the gas looks like in a real observation. This means, e.g., that a set of shape parameters defined in a specific gas parameterization do not have to describe a real shape at all. The parameters could in principle just capture higher order corrections to the density profile because of the generally tight correlation between shape and density. In this case, the real problem is to realize that your model does not return information about the system in the way you believe. The question is therefore how to quantify how a specific model performs relative to one or several other competitive models. A useful measure of this can be found using Bayes’ theorem. From this theorem it is possible to calculate the relative probability, also known as the posterior odds, of two competing models (Jenkins & Peacock 2011; Trotta 2008). In the case where we assume flat parameter and model priors, the posterior odd ratio reduces to the simple ratio

$$F(H_1, H_0) = \int \mathcal{L}(D \mid H_1, \beta) d\beta / \int \mathcal{L}(D \mid H_0, \alpha) d\alpha, \quad (7)$$

where $\mathcal{L}(D \mid H, \beta)$ is the likelihood for getting the data $D$ given the model $H$ which depends on the parameter set $\beta$. This ratio $F$ is often denoted the evidence ratio between model $H_1$ and $H_0$. Model $H_0$ is often a “null” or default model where $H_1$ is a competing and often more complicated model. In our case, $H_0$ could be a model assuming spherical symmetry and $H_1$ a model allowing the shape to vary. The evidence threshold, or critical threshold, between rejecting or accepting a competitive model is often taken to be the Jeffrey’s threshold 1:148 (Jenkins & Peacock 2011). We now go through a few examples.

First suppose we want to compare two models, $M_1$ and $M_2$, given the data set shM2. Both models are using the correct parameterizations for temperature and density, but not the same parameterization for shape; model $M_1$ includes the true parameterization of shape in the fitting, but model $M_2$ assumes the spherical symmetry. We can now use Bayes’ theorem to show whether, e.g., a 5 × 10^4 photon exposure carries enough information to distinguish between $M_1$ and $M_2$. Performing the two integrals in Equation (7) for a 5 × 10^4 photon exposure we find $F \sim 900$, i.e., we can correctly conclude that $M_1$ is strongly favored over $M_2$. The slightly biased estimations for the density and temperature when shM2 is fitted assuming $M_2$ is seen in Figure 2.

Another scenario could be when we fit the shape with a parameterization that is different from the true one. In that case, suppose we fit data set shM1 with two models $M_1$ and $M_2$. Both of them are using the true temperature and density parameterizations, but model $M_1$ is using Equation (3) for the shape parameterization in contrast to model $M_2$, which is using Equation (6). For a 3 × 10^4 photon exposure we find $F \sim 6700$, concluding correctly that $M_1$ is strongly favored over $M_2$.

The last example is a case where the true structure has temperature and density profiles as “shM2,” but has a spherical shape. We now make a fit including shape, but we use Equation (1), i.e., a simple beta-model, to describe the density instead of the true Equation (4), which has one extra degree of freedom. The interesting thing is now that the best fit using the beta-model will show a clear detection of shape away from spherical. This is seen in Figure 6. The under-fitted density profile is simply compensated by allowing a non-spherical shape in the inner parts.

This is a false detection. In a real case where the true shape of the gas is not known, this can be very hard to realize. Comparing this fit using Bayes’ theorem with a fit using the more general density profile in Equation (4) we find $F \sim 300$ for a 6 × 10^4 photon exposure, which correctly means a spherical model is favored.

It is possible to write up a simple scaling relation between the number photons and the evidence ratio given that the PDF can approximately be described by a multidimensional Gaussian near its peak: assuming from an $N_2$ photon exposure we have calculated the evidence ratio $F_{N_2}$ between two models $M_1$ and $M_2$, from that we can simply calculate the ratio $F_{N_1}$ for an $N_1$ photon exposure by $F_{N_1} \approx F_{N_2}(P_{M_1}^* / P_{M_2}^*)^{(N_1/N_2)-1}$, where $P^*$ is the value of the PDF at its maximum for the $N_2$ photon exposure. Here, we have used the analytical solution to Equation (7) (see, e.g., Jenkins & Peacock 2011, Equation (8)). This scaling relation can be useful for forecasting the case where a correct integration is limited by, e.g., computational power. However, this estimator can be relatively noisy because of its dependence on the value at the PDF maximum. One way to reduce this scatter could be to fit a Gaussian to the PDF near its peak.

4. X-RAY GAS SHAPE AND CLUSTER MASS BIAS

By knowing the three-dimensional X-ray gas temperature and density profiles one can calculate the underlying total cluster density, and hence mass, by combining the HE equation:

$$\nabla (\rho_{\text{gas}} T_{\text{gas}}) = -\rho_{\text{gas}} \nabla \Phi_{\text{total}} \quad (8)$$

with the Poisson equation

$$\nabla^2 \Phi = 4\pi G \rho_{\text{total}}. \quad (9)$$

where the index “total” indicates that the contribution is from both gas and dark matter. When X-ray observations are possible for a cluster and the X-ray gas is in HE, this method is one of the most precise ways to estimate the cluster mass as a function of radius within the visible X-ray region. However, as we can
see, the estimated cluster mass will be wrong if the gas is not in HE or if $\rho_{\text{gas}}$ and $T_{\text{gas}}$ are not correctly known. One way of misestimating $\rho_{\text{gas}}$ and $T_{\text{gas}}$ is fitting a spherical model to data for an intrinsic non-spherical gas structure. Depending on the shape, this assumption will propagate to a bias in the estimated total cluster mass. In this section, we will study the cluster mass bias as a function of different shapes along the line of sight.

4.1. Mass Bias

The upper plot in Figure 7 shows the shape along the line of sight for four different X-ray structures. We take the four structures to have temperature and density profiles similar to shM2, but different spatial shapes. Fitting temperature and density profiles to these four structures assuming spherical symmetry will result in biased mass profiles. The ratio between the biased and the true mass profiles is shown in the lower plot. We have only included the mass contribution within $r_v$. Taking the rest of the mass of the cluster into account requires an extrapolation of the dark matter potential form beyond the visible X-ray region. This is necessary when combining or comparing with other mass probes such as lensing.

As seen on the plot, the shapes we are considering lead to small biases at the 10% level, dependent on the radius. This difference can be important for doing future precision cosmology using clusters. However, at this level the degree of hydrostatic equilibrium may lead to higher uncertainties in the mass estimation (Lau et al. 2009; Piffaretti & Valdarnini 2008; Cavaliere et al. 2011).

5. CONCLUSIONS

We have presented a new method for measuring a radially dependent shape along the line of sight of the intracluster X-ray-emitting gas. The method uses the assumption that the shape, temperature, and density profiles can be described by parameterized functions. Compared to several previous studies, we use the whole spectral information. Using this method we have demonstrated the possibilities of measuring shape on CHANDRA mock data.

We find that around $10^6$ photons are required to get a $5\sigma$ shape detection when fitting to a model showing realistic features of the gas, such as a cool core and a double power law for the density profile. We have seen, by presenting correlation matrices, that density and shape have a strong correlation, whereas temperature is essentially uncorrelated. This strong correlation indicates that independent measurements of the density profile can strongly improve the estimation of the shape.

We demonstrated that Bayes’ theorem can be very effectively used to compare different prior input models for our approach. This is of great importance since the actual science one extracts in the end has to be read off from the input model.

Finally, we showed the effect of assuming spherical symmetry on the mass profile estimation when fitting structures with non-spherical shapes. Within our considered class of shapes, we found the mass estimation to be biased at the 10% level.

In a future paper, we will use our framework on real data.

We warmly thank Martina Zamboni for useful discussions. The Dark Cosmology Centre is funded by the Danish National Research Foundation.

APPENDIX

A.1. Creating Artificial Observations of an X-Ray Gas

In our analysis we have two different situations where we need to simulate a data set. The first is as input to the MCMC routine when fitting to a given data set. The second is where we actually simulate the data set that has to be fitted, i.e., the mock data. The first steps for both are the same and are described in the following; given a set of parameterized profiles and shape we create a three-dimensional X-ray gas on a grid. The local spectral information is calculated by XSPEC’s (see, e.g., Arnaud 1996; Schafer 1991) model mekal (http://heasarc.nasa.gov/xanadu/XSPEC/manual/XSmodelMekal.html and references therein) at redshift zero including galactic absorption. We use five times higher spatial resolution in the inner regions compared to the outer parts to make sure no resolution effects propagate into the results. We then project all the spectral information onto the two-dimensional observational plane defined such that the X-gas structure is spherically symmetric in that plane. The projected data are then convolved in XSPEC with an instrumental response function, here chosen to be from CHANDRA, to create a final observed picture. In an ideal world this is the picture read out from the instrument assuming pixelation from the CCD is unimportant. In a real world, spatial and spectral rebinning is done at this step. When we create a data set as input to the MCMC routine, the binning is done so that it matches the binning of the observed data set. When generating a mock data set
Figure 8. Left: a generated X-ray gas map with no noise added in the plane along the line of sight for structure “shM2” introduced in Section 3.2. The color indicates the temperature in keV. Right: upper plot shows two spectra generated from the region between the two black lines shown in the left plot. The spectrum in red is a free–free spectrum generated with the mean X-ray temperature from the region between the two black lines in the left plot and the spectrum in blue is the true projected spectrum, i.e., the sum of many free–free spectra each generated locally in the X-gas. The lower plot shows the ratio between the red and the blue spectra.

(A color version of this figure is available in the online journal.)

we perform the binning such that the radial bins have the same number photon counts and the spectral bins have more than a given threshold. This ensures equal statistical weights for each bin. For the fits in this paper, we fixed the number of radial bins to 12 for all data sets. Because an X-ray gas density profile usually has a logarithmic shape, the radial bins are therefore also approximately logarithmically linearly spaced. Our spectral threshold is chosen such that the number of new spectral bins is around 200 of originally 1024. This corresponds to a threshold of 20 counts per spectral bin for a $6 \times 10^4$ number photon observation. It was not computationally possible to scan over different binning strategies, but the chosen binning is believed to match a real case scenario fairly well.

Figure 8 (left) illustrates a noise-free generated X-ray gas map with a non-spherical shape and its temperature profile. The shape and the temperature profile is the one used for “shM2” introduced in Section 3.2. The right plot in Figure 8 shows two spectra generated from the region between the two black lines shown in the left plot. The spectrum in red is a free–free spectrum generated with XSPEC using the mean projected temperature and the spectrum in blue is the true projected spectrum, i.e., the sum of many free–free spectra, each generated locally in the X-gas. The difference seen in the lower part of the right plot is basically what gives us information about the shape and profiles.

A.2. Monte Carlo Techniques Used in This Paper

We wrote an MCMC algorithm for fitting to a data set. The MCMC uses a Metropolis–Hastings sampling (Chib & Greenberg 1995) with a flat and symmetric proposal density. The size of this proposal density was tuned to reach an acceptance rate of around 0.2–0.3, which has been shown to be the most optimal for sampling higher dimensional distributions. The width of the proposal density along each parameter axes was tuned in units of the root mean square for the individual PDF for each parameter. For all runs the sampling space was limited by bounds on each parameter axis and realizations with a temperature profile exceeding 15 kev or going below 0.5 kev was given zero probability. Among numerous tests of possible resolution, boundary, or sampling effects we tested that the codes reproduced the theoretically expected degeneracy between an overall density scaling and a fixed axis ratio along the line of sight. We tested this up to a total number of 300,000 photons. A sample of tests was also done against an independently written code which generates artificial X-ray data using the “shell binning” approach (see, e.g., http://cxc.harvard.edu/contrib/deproject/).

We tested convergence by starting chains at random places and with different scalings (number photons) of the PDF. All distributions shown in the paper are based on $5 \times 10^5$ samplings. The fitting results presented are based on one realization of data, marginalizing over several realizations was not computationally possible. We assumed a diagonal covariance matrix for the observed photon measurements and the noise to be Gaussian.

REFERENCES

Allen, S. W., Evrard, A. E., & Mantz, A. B. 2011, ARA&A, 49, 409
Allen, S. W., Rapetti, D. A., Schmidt, R. W., et al. 2008, MNRA, 383, 879
Amanullah, R., Goobar, A., Clement, B., et al. 2011, arXiv:1109.4740
Andrae, R., Schulze-Hartung, T., & Melchior, P. 2010, arXiv:1012.3754
Arnaud, K. A. 1996, in ASP Conf. Ser. 101, Astronomical Data Analysis Software and Systems V, ed. G. H. Jacoby & J. Barnes (San Francisco, CA: ASP), 17
Bradley, L. D., Bouwens, R. J., Zitrin, A., et al. 2011, arXiv:1104.2035
Cavaliere, A., Lapi, A., & Fusco-Femiano, R. 2011, A&A, 525, A110
Chib, S., & Greenberg, E. 1995, J. Amer. Stat., 49, 327
Chongchitnan, S., & Silk, J. 2011, arXiv:1107.5617
Conte, A., de Petris, M., Comis, B., Lamagna, L., & de Gregori, S. 2011, A&A, 532, A14
De Filippis, E., Sereno, M., Bautz, M. W., & Longo, G. 2005, ApJ, 625, 108
Fedeli, C., Moseidini, L., & Matarrese, S. 2009, MNRA, 397, 1125
Fusco-Femiano, R., Landi, R., & Orlandini, M. 2005, ApJ, 624, L69
Hansen, S. H., & Piffaretti, R. 2007, A&A, 476, L37
Hayashi, E., Navarro, J. F., & Springel, V. 2007, MNRA, 377, 50
Host, O., & Hansen, S. H. 2011, ApJ, 736, 52
