Mathematical design optmization of wide-field x-ray telescopes: mirror nodal positions and detector tilts

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ABSTRACT

We describe a mathematical formalism for determining the mirror shell nodal positions and detector tilts that optimize the spatial resolution averaged over a field-of-view for a nested x-ray telescope, assuming known mirror segment surface prescriptions and known detector focal surface. The results are expressed in terms of ensemble averages over variable combinations of the ray positions and wavevectors in the flat focal plane intersecting the optical axis at the nominal on-axis focus, which can be determined by Monte-Carlo ray traces of the individual mirror shells. This work is part of our continuing efforts to provide analytical tools to aid in the design process for wide-field survey x-ray astronomy missions.

Keywords: X-ray astronomy, X-ray optics, ray trace, wide field-of-view optimization

1. INTRODUCTION

Since the pioneering work of Burrows, Burg, and Giaconni,[1] interest within the X-ray astronomy community has continued to increase in x-ray survey missions with improved spatial resolution over a wide field-of-view (say ∼30 arcmin). Aspects of a wide-field x-ray imaging survey mission were recently discussed by Murray *et al.*[2,3] Extensive reviews of the science and, to a lesser extent, the technology driving such a mission appear in the proceedings of the 2009 Bologna WFXT Workshop.[4] There is enormous potential for advances in the studies of stars, compact objects, galaxies, active galactic nuclei, galaxy clusters, and cosmology.

Monte-Carlo simulations[1,5–9] are currently extensively utilized to determine the design parameters for such optics. Since the number of mirror shells per telescope module is typically large (∼50—100), these procedures are computer intensive. While Monte-Carlo simulation will always be part of the design process, this and previous papers[10,11] are part of our continuing effort to develop analytic tools to restrict the required search ranges for design parameters and to further aid in the design of wide-field x-ray telescopes.

Here we provide a mathematical formalism for optimizing the placement of mirror shells along the optical axis and the tilt of a commonly employed detector configuration at the focus of a x-ray telescope consisting of nested mirror shells with known mirror surface prescriptions. We note that the geometric area available is constrained and essentially pre-determined by the diameter of the launch vehicle faring, the number of telescope modules (constrained by the desired FOV and the focal lengths permitted by the launch vehicle faring and available extendable optical benches), and the number of mirror shells per module allowed by mass and manufacturing constraints. We therefore adopt the spatial resolution averaged over the field-of-view as the figure of merit.

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2. VARIANCE IN RAY POSITION ON A FOCAL SURFACE

2.1 Focal surface

We adopt a coordinate system in which the positive z-axis points from the detector array to the telescope so that on an arbitrary focal surface S

$$z_S(x,y) \;=\; f_S(x,y), \tag{1}$$

and the optical axis lies along $x = y = 0$. In the flat plane perpendicular to the optical axis and passing through the on-axis focus of mirror shell j, any ray from that shell is completely characterized by its position (x_0, y_0, z_0) in that plane, its wavevector there (k_x, k_y, k_z), and the graze angles with which it reflected from the mirror segments of the shell. The coordinates of the ray on S are given by equation (1) and

$$x_S \;=\; x_0 \;+\; \left(\frac{k_x}{k_z}\right)(z_S - z_0) \;=\; x_0 \;+\; \left(\frac{k_x}{k_z}\right)[\; f_S(x_s, y_s) \;-\; z_0 \;], \tag{2}$$

$$y_S \;=\; y_0 \;+\; \left(\frac{k_y}{k_z}\right)(z_S - z_0) \;=\; y_0 \;+\; \left(\frac{k_y}{k_z}\right)[\; f_S(x_s, y_s) \;-\; z_0 \;]. \tag{3}$$

In practice the shape of the focal surface is highly constrained by detector technology.

2.2 Single mirror shell

In terms of the weighted ensemble average values defined in Appendix A.1, the positional variance of the multiply reflected rays from a single mirror shell, j, on an arbitrary focal surface S, is

$$\sigma^2_{j,S} \;=\; \frac{n_j}{n_j - 1}\,[\;(< x_j^2 >_S \;-\; < x_j >_S^2) \;+\; (< y_j^2 >_S \;-\; < y_j >_S^2) \;+\; (< z_j^2 >_S \;-\; < z_j >_S^2)\;]. \tag{4}$$

Here n_j is the number of multiply reflected rays from shell j.

2.3 Nested mirror shells

In terms of the weighted ensemble average values defined in Appendix A.2 the variance of the multiply reflected rays from a set of J nested shells on S is

$$\sigma^2_S \;=\; \frac{N}{N-1}\,[\;(< x^2 >_S \;-\; < x >_S^2) \;+\; (< y^2 >_S \;-\; < y >_S^2) \;+\; (< z^2 >_S \;-\; < z >_S^2)\;] \tag{5}$$

$$N \;=\; \sum_{j=1}^{J} n_j. \tag{6}$$

Using the definitions given in Appendices A.1 and A.2, equation (5) can be written in the form

$$\sigma^2_S \;=\; \sigma^2_{S,1} \;+\; \sigma^2_{S,2} \tag{7}$$

$$\sigma^2_{S,1} \;=\; \left(\frac{N}{W}\right) \sum_{j=1}^{J} \left(\frac{w_j}{n_j}\right) \left(\frac{n_j - 1}{N-1}\right) \sigma^2_{j,S} \tag{8}$$

$$\sigma^2_{S,2} \;=\; \left(\frac{N}{N-1}\right)\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)(\,<x_j>^2_S \;+\; <y_j>^2_S + <z_j>^2_S\,)$$
$$-\left(\frac{N}{N-1}\right)\left[\left(\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)\;<x_j>_S\right)^2 + \left(\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)\;<y_j>_S\right)^2 + \left(\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)\;<z_j>_S\right)^2\right] \tag{9}$$

Here we have defined

$$W \;\equiv\; \sum_{j=1}^{J} w_j \;=\; \sum_{j=1}^{J}\sum_{k=1}^{n_j} w_{j,k}, \tag{10}$$

where $w_{j,k}$ is the weight assigned in the ensemble average to the k-th multiply reflected ray from the j-th mirror shell (see Appendices A.1 and A.2). When $w_{j,k} = 1$, then $w_j = n_j$ and $W = N$. In order to account for dependence on energy E, for example for optics with two segments per mirror shell, the natural weight to use for doubly reflected rays is the product of the reflectivities from the primary, R_P, and secondary, R_S, mirror surfaces:

$$w_{j,k} \;=\; R_P(\alpha_{P,j,k}, E) \times R_S(\alpha_{s,j,k}, E), \tag{11}$$

where $\alpha_{P,j,k}$ and $\alpha_{S,j,k}$ are the primary and secondary graze angles for the k-th ray from the j-th mirror pair.

We see from equations (7)—(9) that σ^2_S is **not** a simple sum over the variances of the individual shells. We rewrite equation (9) for $\sigma^2_{S,2}$ in the forms

$$q_{ij,S} \;\equiv\; <x_i>_S<x_j>_S + <y_i>_S<y_j>_S + <z_i>_S<z_j>_S \tag{12}$$

$$\sigma^2_{S,2} \;=\; \left(\frac{N}{N-1}\right)\left[\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)q_{jj,S} \;-\; \sum_{i=1}^{J}\sum_{j=1}^{J}\left(\frac{w_i\,w_j}{W^2}\right)q_{ij,S}\right], \tag{13}$$

$$\sigma^2_{S,2} \;=\; \left(\frac{N}{N-1}\right)\left[\sum_{j=1}^{J}\left(\frac{w_j}{W}\right)\left(1 \;-\; \frac{w_j}{W}\right)q_{jj,S} \;-\; \sum_{i=1}^{J}\sum_{j\neq i}^{J}\left(\frac{w_i\,w_j}{W^2}\right)q_{ij,S}\right]. \tag{14}$$

2.4 Application to an inverted pyramid of detectors

We now consider a pyramid of four tilted detectors, with apex pointing away from the nested shells, and each occupying a quadrant with one corner on the diagonal intersecting the optical axis [see Figure 1)]. In this case, the focal surface $S \equiv S_D$ corresponds to the flat, but tilted, surfaces of the four detectors. The tilt angle we denote by ϑ. Let shell j be displaced along the optical axis so that the apex of the inverted pyramid is a distance δz_j from the on-axis focus for that shell (in our coordinate system, $\delta z_j < 0$ if the apex is further from the shell midplane than its on-axis focus). Then we have

$$\sigma^2_{j,S} \;=\; a_{j,0} \;+\; 2\;b_{j,0}\;\delta z_j \;+\; c_{j,0}\;\delta z_j^2 \;+2\;d_{j,0}\;\tan\vartheta \;+\; 2\;e_{j,0}\;\delta z_j\;\tan\vartheta \;+\; f_{j,0}\;\tan^2\vartheta. \tag{15}$$

Here the coefficients $a_{j,0}$, $b_{j,0}$, $c_{j,0}$, $d_{j,0}$, $e_{j,0}$ and $f_{j,0}$ are evaluated in the flat plane perpendicular to the optical axis and passing through the on-axis focus of shell j. Expressions for each coefficient in the first quadrant in terms

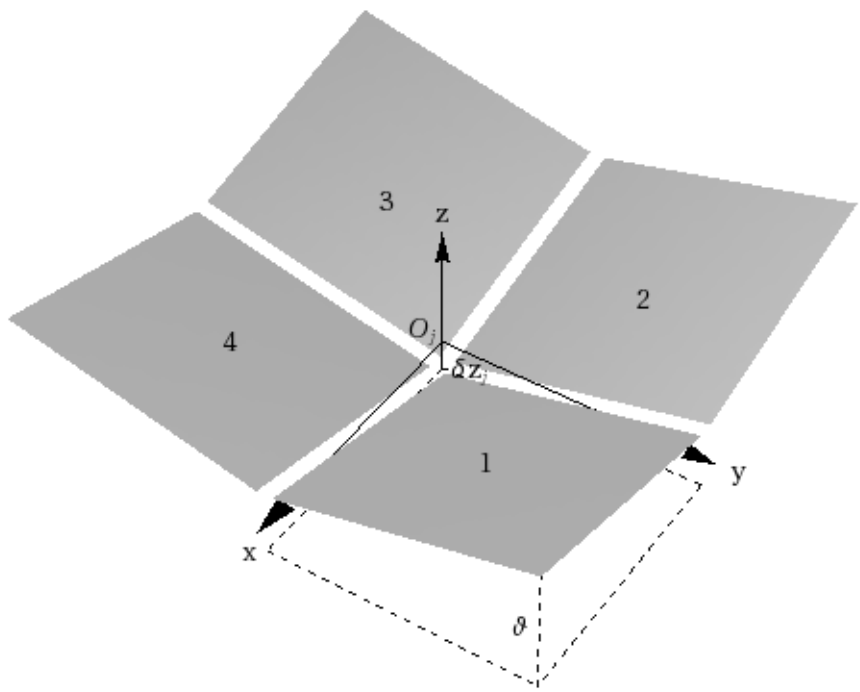

Figure 1. Illustration of the inverted pyramid detector setup discussed in the text. Each of four detectors lies within a numbered quadrant, with gaps between the detector edges. The corner of each detector diagonally opposite from the z-axis is tilted up by an angle ϑ. The positive z-axis points toward the optic and is the optical axis. The point O_j on the z-axis is the on-axis focus for shell j. The apex of the pyramid lies a distance δz_j from the point O_j on the optical axis. In our coordinate system the case shown satisfies $\delta z_j < 0$. Thus the midplane for a two segment optic would be placed a distance $f - \delta z_j = f + |\delta z_j|$ away from the apex, where f is nominal focal length for the shell.

of the weighted ensemble average for the appropriate combination of ray position vectors and ray wavevectors are given in Appendix B.1.

To second order in the δz and in $\tan\vartheta$, we also have

$$\begin{aligned} q_{ij,S} &= a_{ij,0} + (b_{ij,0}\ \delta z_i + b_{ji,0}\ \delta z_j) + c_{ij,0}\ \delta z_i\ \delta z_j \\ &\quad + (d_{ij,0} + d_{ji,0})\tan\vartheta + (e_{ij,0}\ \delta z_i + e_{ji,0}\ \delta z_j)\tan\vartheta + \left(\frac{1}{2}\right)(f_{ij,0} + f_{ji,0})\tan^2\vartheta. \end{aligned} \tag{16}$$

Again the coefficients $a_{ij,0}$, $b_{ij,0}$, $c_{ij,0}$, $d_{ij,0}$, $e_{ij,0}$, and $f_{ij,0}$ are evaluated in the flat plane perpendicular to the optical axis and passing through the on-axis focus of shell j. Expressions for each coefficient in the first

quadrant in terms of the weighted ensemble average for the appropriate combination of ray position vectors and ray wavevectors are given in Appendix B.2.

Using the notation introduced in Appendix B.3, we can express $\sigma^2_{S_D}$ compactly as

$$\begin{aligned}\sigma^2_{S_D} \;=\; & A_0 \;+\; 2\,D_0\,\tan\vartheta \;+\; F_0\,\tan^2\vartheta \;+\; \sum_{j=1}^{J}\left(\,2\,B_{j,0}\,\delta z_j + C_{j,0}\,\delta z_j^2 + 2\,E_{j,0}\,\delta z_j\,\tan\vartheta\,\right) \\ & -\sum_{i=1}^{J}\sum_{j\neq i}^{J}\left[\,(B_{ij,0}\,\delta z_i + B_{ji,0}\,\delta z_j) + C_{ij,0}\,\delta z_i\,\delta z_j + (E_{ij,0}\,\delta z_i + E_{ji,0}\,\delta_j)\tan\vartheta\,\right].\end{aligned} \tag{17}$$

3. MERIT FUNCTION

For X-ray survey applications one desires a large effective collecting area over a broad energy range combined with good spatial resolution over a wide FOV. The geometric area available is essentially pre-determined by the diameter of the launch vehicle faring, the number of desired telescope modules (which are constrained by the desired FOV and, in the absence of extendable optical benches, the focal lengths permitted by the launch vehicle faring), and the number of mirror shells per module allowed by mass and manufacturing constraints. In our work, we have therefore concentrated on optimizing the spatial resolution averaged over the FOV, by minimizing the merit function:

$$M \;=\; (\sigma^2_S)_M \;\equiv\; \frac{\int_{\phi=0}^{2\pi}\,d\phi\,\int_{\theta=0}^{\theta_{FOV}}\,\theta\,d\theta\,w_{FOV}(\theta,\phi)\,\sigma^2_S(\theta,\phi)}{\int_{\phi=0}^{2\pi}\,d\phi\,\int_{\theta=0}^{\theta_{FOV}}\,\theta\,d\theta\,w_{FOV}(\theta,\phi)}, \tag{18}$$

where θ is the polar off-axis angle for the incident X-rays, ϕ is the azimuthal angle for the incident X-rays, and $w_{FOV}(\theta,\phi)$ is a viewing angle weighting factor. The quantity $\sigma^2_S(\theta,\phi)$ is the variance in the position of multiply reflected rays reaching the focal surface S. We remind the reader that our previous expressions for σ^2_S already include weights for the reflectivity of multiply reflected rays from the mirror surfaces of the shell [see equation (11)].

For the inverted pyramid of detectors described in §2.4, by symmetry the average in Eq. (18) may be restricted to $\phi \in [0, \pi/4]$. This statement neglects any repositioning of the apex of the pyramid to place the on-axis aim point on one of detectors. However, such relocation of the on-axis aim point is not necessary when optimizing a survey instrument since the best-focus will not be on-axis.

Substituting equation (17) for the inverted pyramid configuration into equation (18), we find

$$\begin{aligned}(\sigma^2_{S_D})_M \;=\; & (A_0)_M + 2(D_0)_M\tan\vartheta + (F_0)_M\tan^2\vartheta + \sum_{j=1}^{J}\left[\,2(B_{j,0})_M\delta z_j + (C_{j,0})_M\delta z_j^2 + 2(E_{j,0})_M\delta z_j\tan\vartheta\,\right] \\ & -\sum_{i=1}^{J}\sum_{j\neq i}^{J}\left\{\,[(B_{ij,0})_M\delta z_i + (B_{ji,0})_M\delta z_j] + (C_{ij,0})_M\delta z_i\,\delta z_j + [(E_{ij,0})_M\delta z_i + (E_{ji,0})_M\delta z_j]\tan\vartheta\,\right\},\end{aligned} \tag{19}$$

where $(Q)_M$ denotes an average of the quantity Q over the FOV just as in equation (18).

4. FINDING THE OPTIMUM VALUES FOR THE OPTIC DISPLACEMENTS AND FOR THE DETECTOR TILT

4.1 Known mirror prescriptions

When the prescriptions for the mirror surfaces are known in advance, the minimum value for $(\sigma^2_{S_D})_M$, and hence the best values for the optic displacements $\{\delta z_k, (k = 1, J)\}$ and for the detector tilt angle ϑ, may be found by setting the derivatives of $< \sigma^2_{S_D} >_M$ with respect to each displacement δz_k and with respect to $\tan\vartheta$ equal to zero and solving the resulting equations for the δz_k and $\tan\vartheta$. We find

$$\frac{\partial(\sigma^2_{S_D})_M}{\partial \delta z_k} \;=\; 2 \left[(B'_{k,0})_M + (E'_{k,0})_M \;\tan\vartheta \;+\; (C_{k,0})_M \;\delta z_k - \sum_{j\neq k}^{J} (C_{jk,0})_M \;\delta z_j \right] \;=\; 0, \tag{20}$$

$$\frac{\partial(\sigma^2_{S_D})_M}{\partial \tan\vartheta} \;=\; 2 \left[(D_0)_M + \tan\vartheta \;(F_0)_M + \sum_{k=1}^{J} (E'_{k,0})_M \;\delta z_k \right] \;=\; 0. \tag{21}$$

The coefficients $(B'_{k,0})_M$, $(E'_{k,0})_M$ and $(E'_{jk,0})_M$ (needed below) are defined in Appendix B.3. These expressions are linear in the δz_k and $\tan\vartheta$, and so their simultaneous solution is in principle accessible via well-known methods.

Solving equation (21) for $\tan\vartheta$, we find

$$\tan\vartheta \;=\; -\left[(D_0)_M + \sum_{k=1}^{J} (E'_{k,0})_M \;\delta z_k \right] / \;(F_0)_M. \tag{22}$$

Substituting equation (22) for $\tan\vartheta$ into equation (20), and rearranging terms, leads to a system of linear equations for the δz_k which we express in linear algebra form:

$$\overline{\overline{\beta}} \cdot \vec{\delta z} \;=\; \vec{Y}, \tag{23}$$

where the column vectors $\vec{\delta z}$ and $\vec{Y}$ are given by

$$\vec{\delta z} \;=\; \{\; \delta z_k,\; (k = 1, J)\; \}, \tag{24}$$

$$\vec{Y} \;=\; \left\{\; (D_0)_M \;(E'_{k,0})_M - (F_0)_M \;(B'_{k,0})_M,\; (k = 1, J)\; \right\}. \tag{25}$$

The element of the matrix $\overline{\overline{\beta}}$ in the k-th row and j-th column is given by

$$\beta_{kj} \;=\; \delta_{kj} \left[\; (F_0)_M (C_{k,0})_M - (E'_{k,0})^2_M \;\right] \;-\; (1-\delta_{kj}) \left[\; (F_0)_M (C_{jk,0})_M - (E'_{k,0})_M \;(E'_{jk,0})_M \;\right], \tag{26}$$

where δ_{kj} is the Kronecker delta equal to 1 when $k \;=\; j$ and 0 otherwise. Thus we have arrived at a system of J linear equations (23)—(26) for the δz_k and an equation (22) for $\tan\vartheta$ in terms of the δz_k. We suggest that the system of linear equations (23)—(26) ought to be linearly independent in the sense that the determinant $|\,\overline{\overline{\beta}}\,| \neq\; 0$. However, even if this is true in principle, current wide field telescope designs approach 100 closely nested mirror shells, so that numerical precision and convergence may be issues for any computer implementation of the solution of these equations.

4.2 Single mirror shell

For a single mirror shell j with $J = j = 1$, the conditions (20) and (21) reduce to

$$(b_{1,0})_M + \tan\vartheta\ (e_{1,0})_M \ + \ \delta z_1\ (c_{1,0})_M \ = \ 0, \tag{27}$$

$$(d_{1,0})_M + \tan\vartheta\ (f_{1,0})_M + \delta z_1\ (e_{1,0})_M s \ = \ 0, \tag{28}$$

with solution

$$\delta z_1 \ = \ \frac{(d_{1,0})_M (e_{1,0})_M \ - (b_{1,0})_M (f_{1,0})_M}{(c_{1,0})_M (f_{1,0})_M \ - (e_{1,0})_M^2}, \tag{29}$$

$$\tan\vartheta \ = \ \frac{(b_{1,0})_M (e_{1,0})_M \ - (c_{1,0})_M (d_{1,0})_M}{(c_{1,0})_M (f_{1,0})_M \ - (e_{1,0})_M^2}. \tag{30}$$

4.3 Optimizing mirror prescriptions

When optimization of the mirror prescriptions is desired the above procedure becomes more complex. For example consider the case of so-called polynomial x-ray optics[1] assuming the two mirror segment surfaces and J mirror shells, for which $M - 1$ higher order polynomial terms $p_{m,j,s}(z - z_{mid})^m$, with $m = (2, M)$, $j = (1, J)$, and $s = (1, 2)$, are added to a Wolter I prescription for the mirror segment radius squared. Then derivatives with respect to each of the $p_{m,j,s}$ must be set to zero and simultaneously solved in addition to the conditions for δz_j and $\tan\vartheta$. Assuming the $p_{m,j,s}$ are small enough to permit linearization of the new conditions, the linear system to be solved now consists of ($M \times J \ + 1$) equations (including the equation for $\tan\vartheta$).

5. CONCLUDING REMARKS

Monte-Carlo ray traces will continue to play a big role in the design of x-ray telescopes suitable for wide-field survey missions. The ultimate goal of our studies is to provide analytical tools to aid in the design process and reduce its complexity. In this paper we have provided a mathematical formalism for determining the mirror shell nodal positions and detector tilts for a set of nested mirror shells with known surface prescriptions and detector focal surface, expressed in terms of ensemble averages over variable combinations of the ray positions and wavevectors in the flat focal intersecting the optical axis at the nominal on-axis focus.

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APPENDIX A. WEIGHTED ENSEMBLE AVERAGES

A.1 Single mirror shell

For a single mirror shell, designated with the subscript j, we define weighted ensemble average values of the ray positions (x, y, z) for a set of multiply reflected rays on an arbitrary focal surface S as

$$\begin{aligned} < x_j >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ x_{(j,k),S} \\ < y_j >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ y_{(j,k),S} \\ < z_j >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ z_{(j,k),S}. \end{aligned} \tag{A.1-1}$$

Here n_j is the number of multiply reflected rays from shell j, and $(x_{(j,k),S}, y_{(j,k),S}, z_{(j,k),S})$ are the (x, y, z) coordinates of the k-th ray on the surface S given by $z_S = f(x_S, y_S)$. In addition, $w_{s,k}$ is the weight assigned to the k-th ray from shell j and

$$w_j \equiv \sum_{k=1}^{n_j} w_{s,k}. \tag{A.1-2}$$

Similarly

$$\begin{aligned} < x_j^2 >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ x^2_{(j,k),S} \\ < y_j^2 >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ y^2_{(j,k),S} \\ < z_j^2 >_S &= \frac{1}{w_j} \sum_{k=1}^{n_j} w_{s,k}\ z^2_{(j,k),S}. \end{aligned} \tag{A.1-3}$$

We define weighted ensemble average values of the ray wavevectors (k_x, k_y, k_z), or any combination of ray positions and ray wavevectors, in precisely the same way.

A.2 Nested mirror shells

For a set of J nested shells, the corresponding definitions are

$$\begin{aligned} < x >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ x_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < x_j >_S \\ < y >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ y_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < y_j >_S \\ < z >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ z_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < z_j >_S \\ W &= \sum_{j=1}^{J} w_j = \sum_{k=1}^{n_j} w_{s,k}. \end{aligned} \tag{A.2-1}$$

Similarly

$$\begin{aligned} < x^2 >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ x^2_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < x_j^2 >_S \\ < y^2 >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ y^2_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < y_j^2 >_S \\ < z^2 >_S &= \frac{1}{W} \sum_{j=1}^{J} \sum_{k=1}^{n_j} w_{s,k}\ z^2_{(j,k),S} = \sum_{j=1}^{J} \left(\frac{w_j}{W}\right) < z_j^2 >_S . \end{aligned} \tag{A.2-2}$$

Again, we define average values of the ray wavevectors (k_x, k_y, k_z) in precisely the same way.

APPENDIX B. COEFFICIENT DEFINITIONS

B.1 $\sigma^2_{j,S}$

We let the subscript 0 denote a quantity evaluated in the flat plane perpendicular to the optical axis and intersecting that axis at the on-axis focus. We let the subscript j denote shell j. We let (x, y, z) be the ray position vector and (k_x, k_y, k_z) be the ray wavevector. The coefficients in equation (15) are

$$a_{j,0} \equiv (< x^2 >_{j,0} - < x >^2_{j,0}) + (< y^2 >_{j,0} - < y >^2_{j,0}). \tag{B.1-1}$$

$$b_{j,0} \equiv \left[< x \left(\frac{k_x}{k_z}\right) >_{j,0} - < x >_{j,0} < \left(\frac{k_x}{k_z}\right) >_{j,0} \right] + \left[< y \left(\frac{k_y}{k_z}\right) >_{j,0} - < y >_{j,0} < \left(\frac{k_y}{k_z}\right) >_{j,0} \right], \tag{B.1-2}$$

$$c_{j,0} \equiv \left[< \left(\frac{k_x}{k_z}\right)^2 >_{j,0} - < \left(\frac{k_x}{k_z}\right) >^2_{j,0} \right] + \left[< \left(\frac{k_y}{k_z}\right)^2 >_{j,0} - < \left(\frac{k_y}{k_z}\right) >^2_{j,0} \right]. \tag{B.1-3}$$

The expression for $z(x, y)$ on the surface of the flat tilted detector varies with quadrant. For the first quadrant, we have $z = x + y$, and therefore in that quadrant

$$\begin{aligned} d_{j,0} \equiv & \left[< x \left(\frac{k_x}{k_z}\right) (x+y) >_{j,0} - < x >_{j,0} < \left(\frac{k_x}{k_z}\right) (x+y) >_{j,0} \right] \\ & + \left[< y \left(\frac{k_y}{k_z}\right) (x+y) >_{j,0} - < y >_{j,0} < \left(\frac{k_y}{k_z}\right) (x+y) >_{j,0} \right]. \end{aligned} \tag{B.1-4}$$

$$e_{j,0} = e_{j,01} + e_{j,02} \tag{B.1-5}$$

$$\begin{aligned} e_{j,01} \equiv & \left[< \left(\frac{k_x}{k_z}\right)^2 (x+y) >_{j,0} - < \left(\frac{k_x}{k_z}\right) >_{j,0} < \left(\frac{k_x}{k_z}\right) (x+y) >_{j,0} \right] \\ & + \left[< \left(\frac{k_y}{k_z}\right)^2 (x+y) >_{j,0} - < \left(\frac{k_y}{k_z}\right) >_{j,0} < \left(\frac{k_y}{k_z}\right) (x+y) >_{j,0} \right] \end{aligned} \tag{B.1-6}$$

$$\begin{aligned} e_{j,02} \equiv & \left[< x \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} - < x >_{j,0} < \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \right] \\ & + \left[< y \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} - < y >_{j,0} < \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \right]. \end{aligned} \tag{B.1-7}$$

$$f_{j,0} = f_{j,01} + 2\, f_{j,02} + f_{j,03} \tag{B.1-8}$$

$$
\begin{aligned}
f_{j,01} \quad \equiv \quad & \left[< \left(\frac{k_x}{k_z}\right)^2 (x+y)^2 >_{j,0} - < \left(\frac{k_x}{k_z}\right)(x+y) >^2_{j,0} \right] \\
& + \left[< \left(\frac{k_y}{k_z}\right)^2 (x+y)^2 >_{j,0} - < \left(\frac{k_y}{k_z}\right)(x+y) >^2_{j,0} \right]
\end{aligned}
\tag{B.1-9}
$$

$$
\begin{aligned}
f_{j,02} \quad \equiv \quad & \left[< x \left(\frac{k_x}{k_z}\right)(x+y)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} - < x >_{j,0} < \left(\frac{k_x}{k_z}\right)(x+y)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \right] \\
+ & \left[< y \left(\frac{k_y}{k_z}\right)(x+y)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} - < y >_{j,0} < \left(\frac{k_y}{k_z}\right)(x+y)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \right].
\end{aligned}
\tag{B.1-10}
$$

$$
\begin{aligned}
f_{j,03} \quad \equiv \quad & < (x+y)^2 >_{j,0} - < (x+y) >^2_{j,0} \\
= \quad & a_{j,0} \; + \; 2 \; (\; < x \; y >_{j,0} \; - \; < x >_{j,0} < y >_{j,0} \;).
\end{aligned}
\tag{B.1-11}
$$

On the surface of the detector in the second quadrant we have $z = -x + y$, in the third quadrant $z = -x - y$, and in the fourth quadrant $z = x - y$. The expressions for $d_{j,0}$, $e_{j,0}$ and $f_{j,0}$ are easily modified accordingly. However, because we place the apex of the inverted detector pyramid on the optical axis, the configuration is symmetric with respect to reflection about the x and y axes and about the straight lines running at 45° with respect to those axes.

We see from equations (B.1-1)—(B.1-11) that to evaluate the coefficients above we need for each shell j the values of the weighted ensemble averages

$$
\begin{array}{ccc}
< x >_{j,0} & & < y >_{j,0} \\
< x^2 >_{j,0} & < x\ y >_{j,0} & < y^2 >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) >_{j,0} & & < \left(\frac{k_y}{k_z}\right) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)^2 >_{j,0} & & < \left(\frac{k_y}{k_z}^2\right) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) x >_{j,0} & & < \left(\frac{k_y}{k_z}\right) y >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) (x+y) >_{j,0} & & < \left(\frac{k_y}{k_z}\right) (x+y) >_{j,0} \\
< x\ \left(\frac{k_x}{k_z}\right) (x+y) >_{j,0} & & < y\ \left(\frac{k_y}{k_z}\right) (x+y) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)^2 (x+y) >_{j,0} & & < \left(\frac{k_y}{k_z}\right)^2 (x+y) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} & & < \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \\
< x\ \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} & & < y\ \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)^2 (x+y)^2 >_{j,0} & & < \left(\frac{k_y}{k_z}\right)^2 (x+y)^2 >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) (x+y) >_{j,0} & & < \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) (x+y) >_{j,0} \\
< x\ \left(\frac{k_x}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) (x+y) >_{j,0} & & < y\ \left(\frac{k_y}{k_z}\right) \left(\frac{k_x+k_y}{k_z}\right) (x+y) >_{j,0}\ .
\end{array}
\tag{B.1-12}
$$

B.2 $< x_i >_S < x_j >_S + < y_i >_S < y_j >_S + < z_i >_S < z_j >_S$

To second order in the δz and in $\tan\vartheta$, the coefficients, for the detector in the first quadrant, in equation (16) are

$$a_{ij,0} \equiv < x >_{i,0} < x >_{j,0} + < y >_{i,0} < y >_{j,0} \tag{B.2-1}$$

$$b_{ij,0} \equiv < x >_{j,0} < \left(\frac{k_x}{k_z}\right) >_{i,0} + < y >_{j,0} < \left(\frac{k_y}{k_z}\right) >_{i,0} \tag{B.2-2}$$

$$c_{ij,0} \equiv < \left(\frac{k_x}{k_z}\right) >_{i,0} < \left(\frac{k_x}{k_z}\right) >_{j,0} + < \left(\frac{k_y}{k_z}\right) >_{i,0} < \left(\frac{k_y}{k_z}\right) >_{j,0} \tag{B.2-3}$$

$$d_{ij,0} \equiv < \left(\frac{k_x}{k_z}\right) (x+y) >_{i,0} < x >_{j,0} + < \left(\frac{k_y}{k_z}\right) (x+y) >_{i,0} < y >_{j,0} \tag{B.2-4}$$

$$
\begin{aligned}
e_{ij,0} \;\equiv\; & \left[< \left(\frac{k_x}{k_z}\right) >_{i,0} < \left(\frac{k_x}{k_z}\right)(x+y) >_{j,0} + < \left(\frac{k_y}{k_z}\right) >_{i,0} < \left(\frac{k_y}{k_z}\right)(x+y) >_{j,0} \right] \\
& + \left[< \left(\frac{k_x}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right) >_{i,0} < x >_{j,0} + < \left(\frac{k_y}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right) >_{i,0} < y >_{j,0} \right]
\end{aligned}
\tag{B.2-5}
$$

$$
f_{ij,0} \;\equiv\; f_{ij,01} \;+\; 2\, f_{ij,02} \;+\; f_{ij,03} \tag{B.2-6}
$$

$$
f_{ij,01} \;\equiv < \left(\frac{k_x}{k_z}\right)(x+y) >_{i,0} < \left(\frac{k_x}{k_z}\right)(x+y) >_{j,0} + < \left(\frac{k_y}{k_z}\right)(x+y) >_{i,0} < \left(\frac{k_y}{k_z}\right)(x+y) >_{j,0} \tag{B.2-7}
$$

$$
f_{ij,02} \;\equiv < \left(\frac{k_x}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right)(x+y) >_{i,0} < x >_{j,0} + < \left(\frac{k_y}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right)(x+y) >_{i,0} < y >_{j,0} \tag{B.2-8}
$$

$$
\begin{aligned}
f_{ij,03} \;\equiv\; & (\, < x >_{i,0} + < y >_{i,0} \,)\,(\, < x >_{j,0} + < y >_{j,0} \,) \\
=\; & a_{ij,0} + (\, < x >_{i,0} < y >_{j,0} \;+\; < x >_{j,0} < y >_{i,0} \,).
\end{aligned}
\tag{B.2-9}
$$

The same comments from the end of Appendix B.1 about modifications for the other quadrants and about symmetry again apply. We see from equations (B.2-1)—(B.2-9) that to evaluate the coefficients above we need for each shell j the values of the weighted ensemble averages

$$
\begin{array}{cc}
< x >_{j,0} & < y >_{j,0} \\
< \left(\frac{k_x}{k_z}\right) >_{j,0} & < \left(\frac{k_y}{k_z}\right) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)(x+y) >_{j,0} & < \left(\frac{k_y}{k_z}\right)(x+y) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} & < \left(\frac{k_y}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right) >_{j,0} \\
< \left(\frac{k_x}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right)(x+y) >_{j,0} & < \left(\frac{k_y}{k_z}\right)\left(\frac{k_x+k_y}{k_z}\right)(x+y) >_{j,0} .
\end{array}
\tag{B.2-10}
$$

Each of these is included in the list given in equation (B.1-12).

B.3 Additional notation to provide compact expressions for σ_S^2 and its derivatives

We introduce additional notation in order to reduce the space required for the equations expressing σ_S^2 and its derivatives. We define

$$
\begin{aligned}
A_{j,0} \;\equiv\; & \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) a_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) a_{jj,0}, \\
A_{ij,0} \;\equiv\; & \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) a_{ij,0}.
\end{aligned}
\tag{B.3-1}
$$

$$
\begin{aligned}
B_{j,0} &\equiv \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) b_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) b_{jj,0}, \\
B_{ij,0} &\equiv \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) b_{ij,0}.
\end{aligned} \tag{B.3-2}
$$

$$
\begin{aligned}
C_{j,0} &\equiv \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) c_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) c_{jj,0}, \\
C_{ij,0} &\equiv \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) c_{ij,0}.
\end{aligned} \tag{B.3-3}
$$

$$
\begin{aligned}
D_{j,0} &\equiv \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) d_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) d_{jj,0}, \\
D_{ij,0} &\equiv \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) d_{ij,0}.
\end{aligned} \tag{B.3-4}
$$

$$
\begin{aligned}
E_{j,0} &\equiv \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) e_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) e_{jj,0}, \\
E_{ij,0} &\equiv \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) e_{ij,0}.
\end{aligned} \tag{B.3-5}
$$

$$
\begin{aligned}
F_{j,0} &\equiv \left(\frac{N}{W}\right)\left(\frac{w_j}{n_j}\right)\left(\frac{n_j-1}{N-1}\right) f_{j,0} \;+\; \left(\frac{N}{N-1}\right)\left(\frac{w_j}{W}\right)\left(1-\frac{w_j}{W}\right) f_{jj,0}, \\
F_{ij,0} &\equiv \left(\frac{N}{N-1}\right)\left(\frac{w_i w_j}{W^2}\right) f_{ij,0}.
\end{aligned} \tag{B.3-6}
$$

We also define

$$
A_0 \;\equiv\; \sum_{j=1}^{J} A_{j,0} \;-\; \sum_{i=1}^{J}\sum_{j\neq i}^{J} A_{ij,0}, \tag{B.3-7}
$$

$$
D_0 \;\equiv\; \sum_{j=1}^{J} D_{j,0} \;-\; \left(\frac{1}{2}\right)\sum_{i=1}^{J}\sum_{j\neq i}^{J} \left(D_{ij,0} \;+\; D_{ji,0}\right), \tag{B.3-8}
$$

$$
F_0 \;\equiv\; \sum_{j=1}^{J} F_{j,0} \;-\; \left(\frac{1}{2}\right)\sum_{i=1}^{J}\sum_{j\neq i}^{J} \left(F_{ij,0} \;+\; F_{ji,0}\right). \tag{B.3-9}
$$

Finally we define

$$B'_{k,0} \;\equiv\; B_{k,0} \;-\; \sum_{i\neq k}^{J} B_{ki,0}, \tag{B.3-10}$$

$$E'_{k,0} \;\equiv\; E_{k,0} \;-\; \sum_{i\neq k}^{J} E_{ki,0}, \tag{B.3-11}$$

$$E'_{jk,0} \;\equiv\; E_{j,0} \;-\; \sum_{i\neq (j,k)}^{J} E_{ji,0}, \tag{B.3-12}$$