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# Computer Algebra Derivation of High-Order Optical Aberration Coefficients

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## Abstract

The use of computer algebra software enables a considerable simplification of the derivation of analytic expressions for the aberration coefficients of optical systems. In this paper, an algorithm for the symbolic computation of the intrinsic and extrinsic contributions of spherical surfaces to the higher-order aberration coefficients is described. This algorithm can be easily implemented in any major computer algebra language. As an example, two Mathematica programs producing the analytic expressions are given. With these programs, all aberration coefficients of third, fifth and seventh order have been obtained.

## 1 Introduction

Aberration theory has been used for a long time for gaining a deeper insight into the performances and limitations of optical systems throughout the lens design process. Even if presently only third-order (Seidel) coefficients are widely used in practical applications, it is known that for the design of high-quality optical systems higher order aberration coefficients can be a powerful tool.

Intuitively, optical systems are often designed in such a way that the ray paths inside the system are as "relaxed" as possible, i.e. the incidence angles, ray heights and slopes tend to be everywhere as small as permitted by the aperture and field requirements. Any surface for which these ray parameters are too large can be a major source of aberrations. The use of analytic expressions for the aberration coefficients can considerably facilitate optical system analysis by providing a tool for identifying the problematic surfaces in the system.

As will be shown in what follows, the various aberration coefficients are given by sums of surface contributions. For aberration coefficients of order higher than three each surface contribution consists of an intrinsic part, expressed in terms of paraxial marginal and chief ray data (incidence angles, ray heights and slopes) at the given surface, and an

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extrinsic part, due to lower order aberrations incoming from other surfaces. Thus, if the performances of a design are unsatisfactory, the surfaces which are the most important sources of aberrations can be identified by successively determining which aberration coefficients, which surface contributions of them and which marginal or chief ray data determining these surface contributions are too large. This information could be used e.g. for determining which element should be split.

Presently, several commercially available optical design programs can provide fifth-order aberration results. (For historical remarks about fifth order aberrations see e.g. [St].) In some cases, however, considering even higher-order effects might be important. For instance, Shafer has given an example of a system corrected for all third- and fifth-order aberrations, but where aberrations of seventh order and higher are so large that the system performs worse than a system which is not even corrected at third-order level ([Sh]).

Because the complexity of the aberration coefficients increases rapidly with each additional order, the derivation of analytic expressions for the coefficients of order higher than three is a difficult task. Computer algebra has been proven to be a powerful tool for the derivation of analytic expressions of aberration coefficients. (See e.g. Ref. [BK].) Therefore, analytic expressions for the aberration coefficients up to the seventh-order have been derived as part of the RIACA Optics Project. The derivation method used is an adaptation for computer algebra of an earlier method developed by Buchdahl ([Bu]).

For rotationally symmetric optical systems, Buchdahl has developed several decades ago a remarkably efficient technique for deriving high-order aberration coefficients. However, the effort made by its author to improve computational efficiency (i.e. to reduce the number of necessary calculations) has unfortunately obscured the elegant basic ideas of the method. Reading Buchdahl's work [Bu] is not an easy matter for the newcomer.

Nowadays, considering the capabilities of computer algebra software, computational efficiency is less important than insight into the derivation. For improving clarity, it becomes preferable to compute the aberration coefficients in a straightforward manner by adapting several basic ideas of Buchdahl to a form suitable for computer algebra and by translating them directly into computer algebra code. The principal aim of this paper is to give a detailed description of such a simplified version of Buchdahl's method. In the following, we consider only spherical surfaces.

It is assumed that the reader is familiar with paraxial optics and Seidel theory. (For the basics, see e.g. [We].) After developing the necessary prerequisites in the first five sections, the algorithm for the derivation of the analytic expressions of the aberration coefficients will be described in §6. As an example, two Mathematica programs generating these expressions will be given in Appendices A and B.

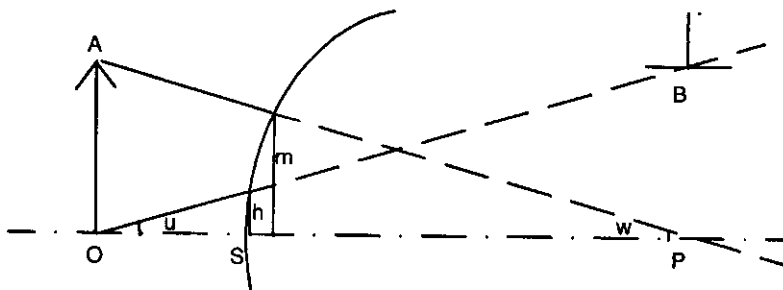


Figure 1: Ray Parameters of the Marginal and Chief Rays at the First Surface of the System

## 2 Paraxial approximation

Consider a rotationally symmetric optical system. We denote the object plane by  $\mathcal{P}$ , the paraxial image plane by  $\mathcal{Q}$  and the stop plane by  $\mathcal{S}$ . We define an arbitrary ray through the system by its normalized coordinates in the object plane  $(\tau_x, \tau_y)$ —the field coordinates and in the stop plane  $(\sigma_x, \sigma_y)$ —the aperture coordinates. Thus, if the stop radius is  $r_S$  and the maximal object height is  $r_P$ , then the Cartesian coordinates are related to the normalized coordinates, at the stop plane by

$$x_S = r_S \sigma_x, \quad y_S = r_S \sigma_y \quad (1)$$

and at the object plane by

$$x_P = r_P \tau_x, \quad y_P = r_P \tau_y. \quad (2)$$

(The special case when the object is at infinity will be discussed in the next section.)

At each surface, the position and direction of a ray passing through the system are fully determined by the  $x$  and  $y$  coordinates of its point of intersection with the surface and by the optical direction cosines  $\xi$  and  $\eta$ , corresponding to  $x$  and  $y$ . (The optical direction cosines are the direction cosines multiplied by the refractive index.)

It can be shown ([Bo], [Ho]) that in the paraxial approximation (the lowest order approximation in  $\sigma_x, \sigma_y, \tau_x, \tau_y$ )  $x, y, \xi$  and  $\eta$  are for all surfaces of the system given by linear combinations of the aperture and field coordinates. The coefficients are then height and slope of the paraxially traced marginal and chief rays at that surface. If we denote paraxial coordinates by a tilde, we thus have

$$\begin{aligned} \tilde{x} &= m\tau_x + h\sigma_x, & \tilde{\xi} &= -nw\tau_x - nu\sigma_x, \\ \tilde{y} &= m\tau_y + h\sigma_y, & \tilde{\eta} &= -nw\tau_y - nu\sigma_y. \end{aligned} \quad (3)$$

Here, the refractive index is denoted by  $n$ , the paraxial marginal and chief ray heights are denoted  $h$  and  $m$  and the corresponding marginal and chief ray slopes are denoted  $u$  and  $w$ . (See Figure 1.) The sign convention adopted here for  $u$  and  $w$  is that their signs are the opposite of those of the corresponding direction cosines. (This is why we have minus signs in the equations for  $\xi$  and  $\eta$ .)

We will also use that  $h, m, u, w$  are not independent. In fact, the quantity  $H$  defined by

$$H = mnu - hnw \quad (4)$$

retains the same value throughout the system. (See e.g. [Ho].) For this reason  $H$  is called the *paraxial system invariant*. It plays an essential role in Buchdahl's deductions.

Generally, we adopt the following notation: Quantities after refraction are denoted by a prime whereas quantities before refraction are left unprimed. Thus, in Eqs (3),  $n, u, w, \xi$  and  $\eta$  are quantities prior to refraction. Of course, similar relations exist for the corresponding primed quantities.

### 3 Quasi-invariants

For an arbitrary ray, consider the two components of the transverse aberration vector of the ray. As usual, these components are defined at the paraxial image plane by

$$\Xi_x = x_Q - \tilde{x}_Q, \quad \Xi_y = y_Q - \tilde{y}_Q. \quad (5)$$

Our aim in this work is to compute the coefficients of the power series expansions of  $\Xi_x$  and  $\Xi_y$  with respect to  $\sigma_x, \sigma_y, \tau_x, \tau_y$ .

Consider first Eqs (3), which hold for the paraxial approximations of the ray parameters. For a reason which will become apparent in §6, we start by seeking certain quantities which can be related to the given ray such that relations similar to Eqs (3) hold exactly for them. More precisely, we look for eight quantities  $\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\tau}_x, \hat{\tau}_y$  such that at every surface of the system we have

$$\begin{aligned} \hat{x} &= m\hat{\tau}_x + h\hat{\sigma}_x, & \hat{\xi} &= -nw\hat{\tau}_x - nu\hat{\sigma}_x, \\ \hat{y} &= m\hat{\tau}_y + h\hat{\sigma}_y, & \hat{\eta} &= -nw\hat{\tau}_y - nu\hat{\sigma}_y. \end{aligned} \quad (6)$$

The first requirement for determining the new quantities is that in the paraxial approximation Eqs (6) reduce to Eqs (3). Thus, the paraxial approximations of  $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\tau}_x, \hat{\tau}_y$  must be the quantities  $\sigma_x, \sigma_y, \tau_x, \tau_y$  which, by definition ((1) and (2)) are surface-independent. Following Buchdahl, any quantity which reduces to such an invariant in the paraxial limit will be called a quasi-invariant. Clearly,  $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\tau}_x, \hat{\tau}_y$  are such quantities.

The basic idea is now to relate the aberrations produced by each surface to the changes of the quasi-invariants at that surface. Therefore, we require that the quasi-invariants associated to the field and aperture coordinates are free of aberrations at the object and stop planes, i.e. that they reduce to the corresponding ray coordinates,

$$\hat{\tau}_{xp} = \tau_x, \quad \hat{\tau}_{yp} = \tau_y \quad (7)$$

and

$$\hat{\sigma}_{xs} = \sigma_x, \quad \hat{\sigma}_{ys} = \sigma_y. \quad (8)$$

Since at the object plane we have  $m = r_p$  and  $h = 0$  and at the stop plane we have  $h = r_s$  and  $m = 0$ , it follows by comparing Eqs (6) with Eqs (1) and (2) that at these two planes we have

$$\hat{x} = x, \quad \hat{y} = y. \quad (9)$$

We now require that Eqs (9) must be valid at each plane surface.

The components  $\Xi_x$  and  $\Xi_y$  of the transverse aberration can be expressed through the quasi-invariants. By denoting the maximal paraxial image height by  $r_Q$ , it follows from Eqn (5) that

$$\Xi_x = x_Q - \tilde{x}_Q = r_Q(\hat{\tau}_{x_Q} - \tau_x). \quad (10)$$

A similar relation is valid for the  $y$ -component. Let us however consider for the moment only the  $x$ -component. Obviously, the total change of  $\hat{\tau}_x$  from the object to the image plane can be written as sum of all individual changes in the system.

$$\hat{\tau}_{x_Q} - \tau_x = \hat{\tau}_{x_Q} - \hat{\tau}_{x_p} = \sum \Delta \hat{\tau}_x. \quad (11)$$

For determining the expressions of the quasi-invariants, consider Eqs (6) as systems of linear equations with unknowns  $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\tau}_x, \hat{\tau}_y$ . It follows from Eqs (6) and (4) that at each surface of the system we have

$$\hat{\tau}_x = \frac{1}{H}(nu\hat{x} + h\hat{\xi}) \quad (12)$$

and

$$\hat{\sigma}_x = -\frac{1}{H}(nw\hat{x} + m\hat{\xi}). \quad (13)$$

Let us now determine the precise form of  $\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}$ . The usual assumption in aberration theory is that transfer through an homogeneous medium does not contribute to the aberrations. Therefore, we simply require that the change of  $\hat{\tau}_x$  vanishes at transfer through a homogeneous medium.

Consider first the case of the transfer between two planes separated by the distance  $z$ . It can be easily verified that the transfer contributions vanish for

$$\hat{\xi} = \frac{n\xi}{\zeta}, \quad \hat{\eta} = \frac{n\eta}{\zeta}, \quad (14)$$

where  $\zeta$  is the optical direction cosine with respect to the  $z$ -axis,

$$\zeta = \sqrt{n^2 - \xi^2 - \eta^2}. \quad (15)$$

In fact, at transfer,  $n, u, \xi$ , and  $\zeta$  remain unchanged. Thus, we have

$$\Delta \hat{x} = \Delta x = \frac{\xi}{\zeta} z, \quad \Delta h = -uz \quad (16)$$

and therefore

$$\Delta \hat{\tau}_x = \frac{1}{H} (nu \Delta x + \frac{n\xi}{\zeta} \Delta h) = 0. \quad (17)$$

Consider now the case of transfer between two curved lens surfaces. At every surface we consider the plane tangent to the surface at its vertex (the polar tangent plane). Obviously, Eqn (17) also holds if instead of  $x$  we consider the quantity  $\hat{x}$  defined as the  $x$ -coordinate of the intersection point of the transferred ray (or its prolongation) with the corresponding polar tangent plane. Thus, the quantities  $\hat{x}$  and  $\hat{y}$  in Eqn (6) must be the polar-tangent-plane coordinates of the given ray.

A similar procedure can be followed in case the object is at infinity. We then have at the first surface of the system (prior to refraction)  $n_1 u_1 = 0$  and, if the medium between object and the first surface is homogeneous,  $\hat{\tau}_{x1} = \hat{\tau}_x$  and  $\hat{\tau}_{y1} = \hat{\tau}_y$ . It follows then from Eqs (6) that

$$\hat{\xi}_1 = -n_1 w_1 \tau_x, \quad \hat{\eta}_1 = -n_1 w_1 \tau_y \quad (18)$$

or, using Eqs (14)

$$\frac{\xi_1}{\zeta_1} = -w_1 \tau_x, \quad \frac{\eta_1}{\zeta_1} = -w_1 \tau_y. \quad (19)$$

Thus, if the object is at infinity, the field coordinates are defined by Eqs (18) or (19) instead of Eqs (2).

Having established the form of the quantities appearing in Eqs (6) we turn to the case of refraction. As a preliminary remark we note that for computational purposes it is more convenient to use the quantity

$$H \hat{\tau}_x = nu \hat{x} + h \hat{\xi} \quad (20)$$

instead of  $\hat{\tau}_x$ . If at the paraxial image plane we write  $H = r_Q n_Q u_Q$ , it follows from Eqs (10) and (11) that

$$\Xi_x = \frac{1}{n_Q u_Q} \sum_{\text{surfaces}} \Delta(H \hat{\tau}_x), \quad (21)$$

a similar relation being valid for  $\Xi_y$ . Equation (21) gives the decomposition of the transverse aberration of an arbitrary ray in contributions from refraction at each surface of the system. Thus, for computing the aberration coefficients, we have to consider the change of Eqn (20) at each surface and determine the coefficients of its power series expansion with respect to  $\sigma_x, \sigma_y, \tau_x, \tau_y$ . Let us therefore first see how  $\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}$  change at refraction at a given surface.

#### 4 Refraction formulae

In the following, we limit our considerations to spherical surfaces. Let  $\rho$  be the surface curvature and  $\delta z$  be the  $z$ -coordinate of the ray-surface intersection point measured from the surface vertex. The normal to the surface is the vector of unit length  $\mathbf{N}$  having the components

$$\mathbf{N} = (N_x, N_y, N_z) = (-\rho x, -\rho y, 1 - \rho \delta z). \quad (22)$$

Given  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{\xi}$ ,  $\hat{\eta}$  prior to refraction, let us determine the expressions of the same quantities after refraction. Considering the transfer of the ray prior to refraction from the polar tangent plane to the intersection point with the surface, we have

$$x = \hat{x} + \frac{\xi}{\zeta} \delta z. \quad (23)$$

It will turn out later during the computer algebra computations that more compact expressions of the aberration coefficients can be obtained if instead of the refractive index  $n$  we use its reciprocal value

$$\nu = n^{-1}. \quad (24)$$

Thus, using Eqs (14) and (24), Eqn (23) reads

$$x = \hat{x} + \nu \hat{\xi} \delta z. \quad (25)$$

Writing a similar relation for the ray after refraction, we obtain by subtraction

$$\hat{x}' = \hat{x} - \delta z (\nu' \hat{\xi}' - \nu \hat{\xi}). \quad (26)$$

We can determine  $\delta z$  from the condition  $N^2 = 1$ . After some elementary calculations, using Eqs (22) and (25), we get

$$\varrho(\hat{x}^2 + \hat{y}^2) + 2\nu\varrho\delta z(\hat{x}\hat{\xi} + \hat{y}\hat{\eta}) + \varrho\nu^2(\hat{\xi}^2 + \hat{\eta}^2)\delta z^2 - 2\delta z + \varrho\delta z^2 = 0. \quad (27)$$

If we define

$$\alpha = \hat{x}^2 + \hat{y}^2, \quad \beta = \nu(\hat{x}\hat{\xi} + \hat{y}\hat{\eta}), \quad \gamma = \nu^2(\hat{\xi}^2 + \hat{\eta}^2) + 1, \quad (28)$$

the quadratic equation (27) can be written as

$$\varrho\gamma\delta z^2 + 2(\beta\varrho - 1)\delta z + \varrho\alpha = 0. \quad (29)$$

Since  $\delta z$  has to vanish for  $\alpha = \beta = 0$ , we find

$$\delta z = \frac{1 - \beta\varrho - \sqrt{(1 - \beta\varrho)^2 - \varrho^2\alpha\gamma}}{\varrho\gamma}. \quad (30)$$

For determining the expression for  $\hat{\xi}'$  we start from the expression for the optical ray vector  $\epsilon' = (\xi', \eta', \zeta')$  after refraction ([Bo], [SG]),

$$\epsilon' = \epsilon + N(\sqrt{n'^2 - n^2 + (\epsilon N)^2} - \epsilon N). \quad (31)$$

By using the abbreviation

$$J = \frac{1}{\zeta}(\sqrt{\nu'^{-2} - \nu^{-2} + (\epsilon N)^2} - \epsilon N) \quad (32)$$

the first and third component of Eqn (31) can be written

$$\xi' = \xi + N_x J \zeta, \quad \zeta' = \zeta + N_z J \zeta. \quad (33)$$



Thus, we have

$$\hat{\xi}' = \frac{n'\xi'}{\zeta'} = \frac{1}{\nu'} \frac{\xi + N_z J \zeta}{\zeta + N_z J \zeta} = \frac{1}{\nu'} \frac{\nu \hat{\xi} + N_z J}{1 + N_z J} \quad (34)$$

or

$$\hat{\xi}' = \frac{1}{\nu'} = \frac{\nu \hat{\xi} - \rho(\hat{x} + \nu \hat{\xi} \delta z) J}{1 + (1 - \rho \delta z) J}. \quad (35)$$

In order to compute Eqn (32), consider first the quantity

$$\theta = \frac{\epsilon \mathbf{N}}{\zeta} = N_x \frac{\xi}{\zeta} + N_y \frac{\eta}{\zeta} + N_z = -\rho \nu ((\hat{x} + \nu \hat{\xi} \delta z) \hat{\xi} + (\hat{y} + \nu \hat{\eta} \delta z) \hat{\eta}) + 1 - \rho \delta z, \quad (36)$$

which finally reads

$$\theta = 1 - \rho \beta - \rho \gamma \delta z. \quad (37)$$

Eqn (32) can now be written

$$J = \sqrt{(\nu'^{-2} - \nu^{-2}) \zeta^{-2} + \theta^2 - \theta}. \quad (38)$$

Since it follows from Eqs (15) and (28) that

$$\frac{1}{\nu^2 \zeta^2} = \frac{\xi^2}{\zeta^2} + \frac{\eta^2}{\zeta^2} + 1 = \gamma. \quad (39)$$

Eqn (38) finally becomes

$$J = \sqrt{\gamma \left( \frac{\nu^2}{\nu'^2} - 1 \right) + \theta^2 - \theta}. \quad (40)$$

To summarize the above results:  $\hat{x}'$  and  $\hat{\xi}'$  are obtained by substituting Eqs (28), (30), (37) and (40) into Eqs (26) and (35). Similar equations to Eqs (26) and (35) can be written down for  $\hat{y}'$  and  $\hat{\eta}'$  by replacing  $x$  by  $y$  and  $\xi$  by  $\eta$ .

Finally, consider the refraction at a surface of the paraxially traced marginal and chief rays. Obviously, the ray heights at the surface  $h$  and  $m$  do not change at refraction. If  $i$  and  $j$  are the incidence angles of the marginal and chief rays, then the quantities

$$f = ni, \quad g = nj \quad (41)$$

are paraxial refraction invariants. As is well known (see e.g. [Ho] or [Bo]), the paraxial marginal and chief ray slopes before and after refraction are related to the invariants (41) by

$$n' h \rho - n' u' = n' i' = ni = n h \rho - nu, \quad n' m \rho - n' w' = n' j' = nj = n m \rho - nw. \quad (42)$$

Later on we will see that the (intrinsic) aberration coefficients can be expressed in terms of marginal and chief ray data. In fact, various equivalent expressions can be obtained, by expressing some of the quantities appearing in Eqs (42) through others. The choice we will make is to express ray slopes prior and after refraction through the invariants (41). Thus, we have

$$nu = \frac{h \rho}{\nu} - f, \quad nw = \frac{m \rho}{\nu} - g. \quad (43)$$

## 5 Aberration coefficients

As shown at the end of §3, in order to determine the aberration coefficients we have to compute the power series expansion with respect to  $\sigma_x, \sigma_y, \tau_x, \tau_y$  of the change at a surface of the quantity  $H\hat{\tau}_x$  given by Eqn (20). Let us first determine the precise form of this expansion from the property of rotational symmetry of the system.

Note that each of the pairs  $(\hat{x}, \hat{y}), (\hat{\xi}, \hat{\eta}), (\hat{\Xi}_x, \hat{X}i_y), (\sigma_x, \sigma_y), (\tau_x, \tau_y), (\hat{\sigma}_x, \hat{\sigma}_y), (\hat{\tau}_x, \hat{\tau}_y)$  can be regarded as a two-component vector. This means that all vectors transform in the same way under rotation about the symmetry axis of the system. Therefore, the total order in  $\sigma_x, \sigma_y, \tau_x, \tau_y$  for any term of the expansion of  $H\Delta\hat{\tau}_x$  is always odd. We denote the sum of all terms of order  $2k+1$  in  $\sigma_x, \sigma_y, \tau_x, \tau_y$  by  $B_{2k+1,x}$  and the corresponding sum for  $H\Delta\hat{\tau}_y$  by  $B_{2k+1,y}$ . Because  $\hat{\tau}_x$  and  $\hat{\tau}_y$  reduce in the paraxial approximation to  $\tau_x$  and  $\tau_y$ , which by definition do not change, the linear terms of the expansions vanish, i.e.

$$B_{1,x}(\sigma_x, \sigma_y, \tau_x, \tau_y) = B_{1,y}(\sigma_x, \sigma_y, \tau_x, \tau_y) = 0. \quad (44)$$

Thus, the lowest order non-vanishing terms are the third-order terms and we have

$$H\Delta\hat{\tau}_l = B_{3,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) + \dots + B_{2k+1,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) + \dots, \quad l \in \{x, y\}. \quad (45)$$

Note also that the quantities

$$\sigma^2 = \sigma_x^2 + \sigma_y^2, \quad \sigma\tau = \sigma_x\tau_x + \sigma_y\tau_y, \quad \tau^2 = \tau_x^2 + \tau_y^2 \quad (46)$$

remain unchanged under rotation about the symmetry axis. Consequently, we must have

$$B_{2k+1,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) = \quad (47)$$

$$\sum_{j=0}^k \sum_{i=0}^{k-j} (b_{\tau\sigma, k-i-j, j, i} \sigma_l + b_{\tau\tau, k-i-j, j, i} \tau_l) (\sigma^2)^{k-i-j} (\sigma\tau)^j (\tau^2)^i, \quad k = 1, 2, \dots; \quad l \in \{x, y\}.$$

The coefficients  $b_{\tau\sigma}$  and  $b_{\tau\tau}$  describe the contributions of the given surface to the total aberrations of the system. The technique for deriving their analytic expressions will be given in the next section.

If the coefficients  $b_{\tau\sigma}$  and  $b_{\tau\tau}$  are determined for each surface of the system, it follows from Eqn (21) that the components of the transverse aberration vector can be written as

$$\Xi_l = \frac{1}{n_Q u_Q} (A_{3,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) + \dots + A_{2k+1,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) + \dots), \quad l \in \{x, y\}, \quad (48)$$

where

$$A_{2k+1,l}(\sigma_x, \sigma_y, \tau_x, \tau_y) = \quad (49)$$

$$\sum_{j=0}^k \sum_{i=0}^{k-j} (a_{\tau\sigma, k-i-j, j, i} \sigma_l + a_{\tau\tau, k-i-j, j, i} \tau_l) (\sigma^2)^{k-i-j} (\sigma\tau)^j (\tau^2)^i, \quad k = 1, 2, \dots; \quad l \in \{x, y\}.$$

In Eqn (49)  $a_{\tau\sigma}$  and  $a_{\tau\tau}$  are the total aberration coefficients of the system. They are obtained by summing up all individual surface contributions

$$a_{\tau m, i, j, k} = \sum_{\text{surfaces}} b_{\tau m, i, j, k}, \quad m \in \{\sigma, \tau\}. \quad (50)$$

It turns out that for each value of  $k$ , the number of coefficients  $b_{\tau m}$  appearing in Eqn (47) is in fact larger than the number of coefficients resulting from Hamilton's theory. However, retaining this excess of coefficients simplifies considerably the derivation of analytic expressions for them. For a discussion of the relationships between coefficients we refer the reader to [Bu].

Let us now see how the quasi-invariants (12) and (13) can be expressed at a given surface in terms of the aberration coefficients.

As suggested by Eqs (7),  $\hat{\sigma}_x$  and  $\hat{\sigma}_y$  can be obtained at an arbitrary surface by adding to the aberration-free values  $\sigma_x$  and  $\sigma_y$  at the stop plane  $\mathcal{S}$  the changes due to all surfaces between the stop and the considered surface. However, we must distinguish between surfaces situated before and after the stop. We adopt the convention that  $\Delta$  always denotes the change at refraction of a given quantity for a ray propagating from the object plane to the image plane. Therefore, if the considered surface is situated before the stop, the contributions to  $\Delta\hat{\sigma}_l$  from the surfaces situated in between must be added with changed sign. Otherwise, the contributions will be added as usual. This special summation convention will be denoted by

$$\hat{\sigma}_l = \sigma_l \pm \sum_{-S+} \Delta\hat{\sigma}_l. \quad (51)$$

Similarly, by considering the surfaces between the object plane  $\mathcal{P}$  and the given surface, we have

$$\hat{\eta}_l = \eta_l + \sum_{P+} \Delta\hat{\eta}_l. \quad (52)$$

Since all surfaces are situated after the object plane, in Eqn (52) the surface contributions are always added with unchanged sign. For  $H\Delta\hat{\sigma}_l$  ( $l = x, y$ ), power series expansions similar to Eqs (45) and (47) can be written. Let  $b_{\sigma\sigma}$  and  $b_{\sigma\tau}$  be the coefficients appearing in the expansions of  $H\Delta\hat{\sigma}_l$  (These coefficients describe pupil aberrations). If for  $m = \tau, \sigma$  we define

$$s_{\sigma m, i, j, k} = \pm \frac{1}{H} \sum_{-S+} b_{\sigma m, i, j, k} \quad (53)$$

and

$$s_{\tau m, i, j, k} = \frac{1}{H} \sum_{P+} b_{\tau m, i, j, k}, \quad (54)$$

Eqs (51) and (52) can be written as

$$\hat{\sigma}_l = \sigma_l + S_{\sigma\sigma}\sigma_l + S_{\sigma\tau}\tau_l, \quad \hat{\eta}_l = \eta_l + S_{\tau\sigma}\sigma_l + S_{\tau\tau}\tau_l, \quad (55)$$

where we have used the abbreviations

$$S_{mn} = \sum_{k=1}^{\infty} \sum_{j=0}^k \sum_{i=0}^{k-j} s_{mn,k-i-j,i} (\sigma^2)^{k-j-i} (\sigma\tau)^j (\tau^2)^i, \quad m, n \in \{\sigma, \tau\}. \quad (56)$$

Thus, the relationships between the quasi-invariants at a given surface and the surface contributions to the aberration coefficients are given by Eqs (53)-(56).

## 6 Intrinsic and extrinsic surface contributions

In this section an algorithm for the symbolic computation of the surface contributions  $b_{\tau\sigma}$  and  $b_{\tau\tau}$  to the aberration coefficients of the system  $a_{\tau\sigma}$  and  $a_{\tau\tau}$  will be described.

As can be seen from Eqs (45) and (47), for determining the coefficients  $b_{\tau\sigma}$  and  $b_{\tau\tau}$ , it suffices to consider the quantity  $H\Delta\hat{\tau}_x$ . It follows from Eqs (20) and (43) that

$$H\Delta\hat{\tau}_x = h\rho\left(\frac{\hat{x}'}{\nu'} - \frac{\hat{x}}{\nu}\right) - f(\hat{x}' - \hat{x}) + h(\hat{\xi}' - \hat{\xi}). \quad (57)$$

By substituting in Eqn (57) the refraction formulae developed in §4,  $H\Delta\hat{\tau}_x$  will be expressed in terms of  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{\xi}$ ,  $\hat{\eta}$ . Consider then the power series expansion of  $H\Delta\hat{\tau}_x$  with respect to  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{\xi}$ ,  $\hat{\eta}$ . Because of the rotational symmetry we have

$$H\Delta\hat{\tau}_x = T_{1,x}(\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}) + T_{3,x}(\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}) + \dots + T_{2k+1,x}(\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}) + \dots \quad (58)$$

where  $T_{2k+1,x}$  denotes the sum of all terms of total order  $2k+1$  in  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{\xi}$ ,  $\hat{\eta}$ .

Let us first show that  $T_{1,x} = 0$ . Consider the linear approximation for the refraction formulae of §4. Keeping only the lowest order terms, the equations (23), (14), (15), (28), (37) and (40) become

$$\hat{x}' = \hat{x} = x, \quad \hat{\xi} = \xi, \quad \zeta = n, \quad \gamma = 1, \quad \theta = 1, \quad J = \frac{n}{n'} - 1. \quad (59)$$

In the linear approximation, the first of Eqs (33) then reads

$$\xi' = \xi - \rho x \Delta n. \quad (60)$$

Consequently, Eqn (57) becomes

$$T_{1,x}(\hat{x}, \hat{y}, \hat{\xi}, \hat{\eta}) = h\rho x \Delta n + h(\xi' - \xi) = 0. \quad (61)$$

Thus, the lowest order non-vanishing term in Eqn (58) is the third order term  $T_{3,x}$ .

By means of Eqs (6) and (55)-(56),  $\hat{x}$ ,  $\hat{y}$ ,  $\hat{\xi}$ ,  $\hat{\eta}$  can be expressed through  $\sigma_x$ ,  $\sigma_y$ ,  $\tau_x$ ,  $\tau_y$ . Let us examine for a given value of  $k$ , the structure of  $T_{2k+1,x}$  if the latter quantity is expressed through  $\sigma_x$ ,  $\sigma_y$ ,  $\tau_x$ ,  $\tau_y$ . Consider first the terms of lowest total order in  $\sigma_x$ ,  $\sigma_y$ ,  $\tau_x$ ,  $\tau_y$ . These terms are of order  $2k+1$  and are obtained by keeping in Eqs (55) only the lowest order contributions

$$\hat{\sigma}_l = \sigma_l, \quad \hat{\tau}_l = \tau_l, \quad l \in \{x, y\}. \quad (62)$$



Compare now Eqs (58) and (67) with Eqs (45) and (47). We obtain the fundamental relationship

$$\sum_{k=1}^{\infty} \sum_{j=0}^k \sum_{i=0}^{k-j} (b_{\tau\sigma, k-i-j, j, i} \sigma_l + b_{\tau\tau, k-i-j, j, i} \tau_l) (\sigma^2)^{k-i-j} (\sigma\tau)^j (\tau^2)^i = \quad (69)$$

$$\sum_{k=1}^{\infty} \sum_{j=0}^k \sum_{i=0}^{k-j} (c_{\tau\sigma, k-i-j, j, i} \hat{\sigma}_l + c_{\tau\tau, k-i-j, j, i} \hat{\tau}_l) (\hat{\sigma}^2)^{k-i-j} (\hat{\sigma}\hat{\tau})^j (\hat{\tau}^2)^i.$$

Thus, the coefficients  $b_{\tau\sigma}$  and  $b_{\tau\tau}$  can be obtained by substituting Eqs (55)-(56) into the right-hand side of Eqn (69) and equating the coefficients of equal powers of aperture and field coordinates on both sides. In order to obtain the right-hand side of Eqn (69) in terms of  $\sigma_x$ ,  $\tau_x$ ,  $\sigma^2$ ,  $\sigma\tau$ ,  $\tau^2$ , instead of Eqs (68) we substitute the following relations resulting from Eqs (55)

$$\hat{\sigma}^2 = (1+S_{\sigma\sigma})^2 \sigma^2 + 2S_{\sigma\tau}(1+S_{\sigma\sigma})\sigma\tau + S_{\sigma\tau}^2 \tau^2, \quad \hat{\tau}^2 = S_{\tau\sigma}^2 \sigma^2 + 2S_{\tau\sigma}(1+S_{\tau\tau})\sigma\tau + (1+S_{\tau\tau})^2 \tau^2 \quad (70)$$

$$\hat{\sigma}\hat{\tau} = S_{\tau\sigma}(1+S_{\sigma\sigma})\sigma^2 + (S_{\sigma\tau}S_{\tau\sigma} + (1+S_{\sigma\sigma})(1+S_{\tau\tau}))\sigma\tau + S_{\sigma\tau}(1+S_{\tau\tau})\tau^2.$$

The coefficients

$$b_{\tau m, k-i-j, j, i}, \quad j = 0..k; \quad i = 0..k-j; \quad m \in \{\sigma, \tau\}$$

are, for  $k = 1$ , the third-order (or primary) contributions of the given surface to the total aberrations, for  $k = 2$ , the fifth-order (or secondary) contributions, for  $k = 3$ , the seventh-order (or tertiary) contributions, etc. Let us examine, for a given value of  $k$ , which terms in Eqn (58) produce contributions to the coefficients  $b_{\tau\sigma}$  and  $b_{\tau\tau}$ .

Consider first the case  $k = 1$ . Since  $T_{1,x} = 0$ , contributions result only from the term  $T_{3,x}$ . Therefore, for the third order coefficients we have

$$b_{\tau m, 1-i-j, j, i} = c_{\tau m, 1-i-j, j, i}. \quad (71)$$

Consider now the coefficients of order five and higher, i.e.  $k > 1$ . At a particular surface in the system, the term  $T_{2k+1,x}$  contributes to the coefficient  $b_{\tau m, k-i-j, j, i}$  with the term  $c_{\tau m, k-i-j, j, i}$  which is expressed in terms of marginal and chief ray data at that surface. Therefore, the coefficients  $c_{\tau\sigma}$  and  $c_{\tau\tau}$  are called **intrinsic surface contributions**.

However, contributions result also from the terms  $T_{2k'+1,x}$  with  $k' < k$ . As can be seen from Eqs (67) and (53)-(56), these terms are products of lower-order intrinsic contributions  $c_{\tau m, k'-i-j, j, i}$  with coefficients  $s_{\sigma\sigma}$ ,  $s_{\sigma\tau}$ ,  $s_{\tau\sigma}$ ,  $s_{\tau\tau}$ . Since according to Eqs (53)-(54) the latter coefficients are sums of surface contributions coming from **other surfaces**, the contributions resulting from the terms  $T_{2k'+1,x}$  are called **extrinsic surface contributions**. Denoting their sum for all  $k' < k$  by  $d_{\tau m}$ , we obtain

$$d_{\tau m, k-i-j, j, i} = b_{\tau m, k-i-j, j, i} - c_{\tau m, k-i-j, j, i}, \quad m \in \{\sigma, \tau\}. \quad (72)$$

Seidel aberrations	corresponding coefficients
spherical aberration	$-2c_{\tau\sigma,1,0,0}$
coma	$-c_{\tau\sigma,0,1,0} = -2c_{\tau\tau,1,0,0}$
astigmatism	$-c_{\tau\tau,0,1,0}$
Petzval curvature	$c_{\tau\tau,0,1,0} - 2c_{\tau\sigma,0,0,1}$
distortion	$-2c_{\tau\tau,0,0,1}$

Table 1: The third-order Seidel aberrations and their coefficients

## 7 Results

The above algorithm for the derivation of aberration coefficients can be easily translated into any major computer algebra language. As an example, two Mathematica programs generating analytic expressions for the intrinsic and extrinsic surface contributions are given in Appendices A and B together with the corresponding results up to the fifth order.

With these programs, all seventh-order coefficients have also been obtained. The computations have been performed on a Silicon Graphics Challenge L computer with two 150 MHz R4400 MIPS processors and 128 MB internal memory. However, these computations are feasible on smaller computers as well.

In the case of the intrinsic surface contributions, it turns out that for spherical surfaces we have a relation between the  $c_{\tau\sigma}$  and  $c_{\tau\tau}$  coefficients of the form

$$c_{\tau\tau,k-i-j,j,i} = \frac{g}{f} c_{\tau\sigma,k-i-j,j,i} \quad (73)$$

which is valid for all orders. Thus, only the  $c_{\tau\sigma}$  coefficients are printed out in Appendix A. (In the output, the indices  $\sigma$  and  $\tau$  have been replaced by  $s$  and  $t$ . The surface curvature  $g$  and the reciprocal of the refractive index  $v'$  are denoted by  $e$  and  $vv$ .)

The familiar expressions of the Seidel aberration coefficients ([Bo], [We]) can be easily derived from the third-order coefficients given in Appendix A. Using Eqs (42) and (73) it follows after some elementary algebra that we have the correspondence as shown in the table below. As can be seen in the case of coma, not all six coefficients  $c_{\tau\sigma}$  and  $c_{\tau\tau}$  are independent. This excess of coefficients has been already noted in §5.

Because of the complexity of the expressions for the fifth-order coefficients, a comparison with the literature has been made only for spherical aberration. The expressions for the intrinsic and extrinsic fifth-order spherical aberration  $c_{\tau\sigma,2,0,0}$  and  $d_{\tau\sigma,2,0,0}$  turned out to be equivalent to those given in [St]. The main limitation in determining analytic expressions for aberration coefficients of order seven and higher comes from the rapid growth with each additional order of the size of the extrinsic contributions. Already at the seventh order the latter expressions are of considerable length and have therefore not

hdeltattx=h\*e\*(xx/vv-x/v)-f(xx-x)+h(pp-p); (\*Eq. 59\*)

(\* x2=x^2+y^2 \*)  
(\* xp=x\*p+y\*q \*)  
(\* p2=p^2+q^2 \*)

vxp=v\*xp; (\*Eq. 29\*)

vp1=v^2\*p2+1; (\*Eq. 30\*)

z=(1-vxp\*e-Sqrt[(1-vxp\*e)^2-e^2\*x2\*vp1])/(e\*vp1); (\*Eq. 32\*)

tet=1-vxp\*e-vp1\*e\*z; (\*Eq. 39\*)

capj=Sqrt[((v/vv)^2-1)\*vp1+tet^2]-tet; (\*Eq. 42\*)

pp=1/vv\*(v\*p-e\*(x+v\*p\*z)\*capj)/(1+(1-e\*z)\*capj); (\*Eq. 37\*)

xx=x-(vv\*pp-v\*p)\*z; (\*Eq. 26\*)

(\* 2 \*)

ser[u\_, i\_] := Collect[Factor[  
Expand[(PowerExpand[Normal[Series[u/.att1, {o, 0, i}]]]/.att2)]  
], o];

att1={x->o\*xo, y->o\*yo, p->o\*po, q->o\*qo, x2->o^2\*x2o, xp->o^2\*xpo, p2->o^2\*p2o};

att2={xo->x, yo->y, po->p, qo->q, x2o->x2, xpo->xp, p2o->p2};

sermax=ser[hdeltattx, 2\*kmax+1]; (\*Eq. 60\*)

tk[k\_] := Expand[Coefficient[sermax, o, 2\*k+1]]

(\* 3 \*)

nw=-(g-m\*e/v); (\*Eq. 45\*)

nu=-(f-h\*e/v);

repl={

x->m\*tx+h\*sx, (\*Eq. 3\*)

p->-nw\*tx-nu\*sx,

(\* s2=sx^2+sy^2 \*)

(\* st=sx\*tx+sy\*ty \*)

(\* t2=tx^2+ty^2 \*)

x2->m^2\*t2+2\*m\*h\*st+h^2\*s2, (\*Eq. 67\*)

xp->-(nw\*m\*t2+(nw\*h+nu\*m)\*st+nu\*h\*s2),

p2->nw^2\*t2+2\*nu\*nw\*st+nu^2\*s2

};

Do[



$$\begin{aligned}
 & (2 e^2 g h m + e^2 f m^2 - 3 e g h v - 6 e f g m v + \\
 & \quad 3 f g v^2 + e g h v v + 2 e f g m v v - 3 f g^2 v v) / 2 \\
 2 \quad c[ts101] = & (f (-v + v v)
 \end{aligned}$$

$$\begin{aligned}
 & (2 e^3 g h m + e^3 f h m^2 - 2 e^2 g h v - \\
 & \quad 10 e^2 f g h m v + 6 e f g h^2 v + 6 e f^2 g h m v - \\
 & \quad 3 f^2 g h v + 2 e f g h m v v - 2 e f^2 h m v v + \\
 & \quad 3 e f g h v v v + 2 e f^2 g h m v v v + e f^3 m v v v - \\
 & \quad 3 f^2 g h v v v - 3 e f g h^2 v v - 4 e f^2 g h m v v + \\
 & \quad e f^3 m v v + 3 f^2 g h v v v + 3 f g h^2 v v) / 4 \\
 2 \quad c[ts011] = & (f (-v + v v)
 \end{aligned}$$

$$\begin{aligned}
 & (3 e^3 g h m - 8 e^2 g h m v - 5 e f g h m v + \\
 & \quad e f^2 m v + 3 e g h^2 v + 9 e f g h m v - \\
 & \quad 3 f g h v + 2 e g h m v v - e f g h m v v - \\
 & \quad e f^2 m v v + e g h v v v + 4 e f g h m v v v + \\
 & \quad e f g m v v v - 3 f g h v v v - 2 e g h^2 v v - \\
 & \quad 5 e f g h m v v + e f^2 g m v v + 3 f g h v v v + \\
 & \quad 3 \quad 3
 \end{aligned}$$

```

ttx=repl[tx+sx*caps[t,s]+tx*caps[t,t]];

ss2=repl[
                                (*Eq.72*)
s2*(1 + 2*caps[s,s] + caps[s,s]^2) + t2*caps[s,t]^2
+ st*(2*caps[s,t] + 2*caps[s,s]*caps[s,t]);
sstt=repl[
s2*(caps[t,s] + caps[t,s]*caps[s,s]) + st*(1 + caps[t,t] + caps[s,s]
+ caps[t,t]*caps[s,s] + caps[t,s]*caps[s,t])
+ t2*(caps[s,t] + caps[t,t]*caps[s,t]);
tt2=repl[
s2*caps[t,s]^2 + st*(2*caps[t,s] + 2*caps[t,s]*caps[t,t])
+ t2*(1 + 2*caps[t,t] + caps[t,t]^2)];

total=Sum[
                                (*rhs of Eq.71*)
(ssx*c[t,s,k-i-j,j,i]+ttx*c[t,t,k-i-j,j,i])*ss2^(k-i-j)*sstt^j*tt2^i
,{k,1,kmax-1},{j,0,k},{i,0,k-j}];

intrinsic=repl[Sum[
                                (* intrinsic part to be subtracted *)
(sx*c[t,s,k-i-j,j,i]+tx*c[t,t,k-i-j,j,i])*s2^(k-i-j)*st^j*t2^i
,{k,1,kmax-1},{j,0,k},{i,0,k-j}]];

sermax=Collect[Expand[total-intrinsic],o];

(* 2 *)

Do[
dk[k]=Coefficient[sermax,o,2*k+1]
,{k,1,kmax}]

Do[(
                                (*lhs of Eq.71*)
d[t,s,k-i-j,j,i]=Factor[Coefficient[dk[k],sx*s2^(k-i-j)*st^j*t2^i]];
d[t,t,k-i-j,j,i]=Factor[Coefficient[dk[k],tx*s2^(k-i-j)*st^j*t2^i]]
),{k,1,kmax},{i,0,k},{j,0,k-i}]

(* Print *)

Do[(
Print[k," d[ts",k-i-j,j,i,"] = ",d[t,s,k-i-j,j,i]];
Print[k," d[tt",k-i-j,j,i,"] = ",d[t,t,k-i-j,j,i]]
),{k,1,kmax},{i,0,k},{j,0,k-i}]

```

## B.2 The output for $k_{max} = 2$

```

2
{Power}

```

$$\begin{aligned}
& 2 c[t, t, 0, 0, 1] s[t, s, 1, 0, 0] + \\
& c[t, t, 1, 0, 0] s[t, t, 0, 1, 0] + \\
& 2 c[t, t, 0, 1, 0] s[t, t, 1, 0, 0] \\
2 \quad d[ts020] = & 2 c[t, s, 0, 1, 0] s[s, s, 0, 1, 0] + \\
& 2 c[t, s, 1, 0, 0] s[s, t, 0, 1, 0] + \\
& 2 c[t, s, 0, 0, 1] s[t, s, 0, 1, 0] + \\
& c[t, t, 0, 1, 0] s[t, s, 0, 1, 0] + \\
& c[t, s, 0, 1, 0] s[t, t, 0, 1, 0] \\
2 \quad d[tt020] = & c[t, t, 0, 1, 0] s[s, s, 0, 1, 0] + \\
& c[t, s, 0, 1, 0] s[s, t, 0, 1, 0] + \\
& 2 c[t, t, 1, 0, 0] s[s, t, 0, 1, 0] + \\
& 2 c[t, t, 0, 0, 1] s[t, s, 0, 1, 0] + \\
& 2 c[t, t, 0, 1, 0] s[t, t, 0, 1, 0] \\
2 \quad d[ts101] = & 3 c[t, s, 1, 0, 0] s[s, s, 0, 0, 1] + \\
& c[t, s, 0, 0, 1] s[s, s, 1, 0, 0] + \\
& c[t, s, 0, 1, 0] s[s, t, 1, 0, 0] + \\
& c[t, s, 0, 1, 0] s[t, s, 0, 0, 1] + \\
& c[t, t, 1, 0, 0] s[t, s, 0, 0, 1] + \\
& c[t, t, 0, 0, 1] s[t, s, 1, 0, 0] + \\
& 2 c[t, s, 0, 0, 1] s[t, t, 1, 0, 0] \\
2 \quad d[tt101] = & 2 c[t, t, 1, 0, 0] s[s, s, 0, 0, 1] + \\
& c[t, s, 1, 0, 0] s[s, t, 0, 0, 1] + \\
& c[t, s, 0, 0, 1] s[s, t, 1, 0, 0] + \\
& c[t, t, 0, 1, 0] s[s, t, 1, 0, 0] + \\
& c[t, t, 0, 1, 0] s[t, s, 0, 0, 1] +
\end{aligned}$$

3 c[t, t, 0, 0, 1] s[t, t, 0, 0, 1]