# Derivation of the refraction equations for higher-order aberrations of local wavefronts at oblique incidence

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From the literature the calculation of power and astigmatism of a local wavefront after refraction at a given surface is known from the vergence and Coddington equations. For higher-order aberrations (HOAs) equivalent analytical equations do not exist. Since HOAs play an increasingly important role in many fields of optics, e.g., ophthalmic optics, it is the purpose of this study to extend the "generalized Coddington equation" to the case of HOA (e.g., coma and spherical aberration). This is done by local power series expansions. In summary, with the results presented here, it is now possible to calculate analytically the local HOA of an outgoing wavefront directly from the aberrations of the incoming wavefront and the refractive surface. © 2010 Optical Society of America

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## 1. INTRODUCTION

Aberrations play a decisive role in optics. In this work, we deal with them in the framework of geometric optics in which the wavelength is neglected ($\lambda \to 0$) with respect to diffraction effects [1,2]. In this case, also the notions of both rays and wavefronts still do exist. A wavefront, in general defined as a surface of constant phase, is in this limit a surface of constant optical path length. A ray is a virtual infinitesimally small bundle of light, the direction of which is defined by the normal of the wavefront.

### A. Rays, Wavefronts, and Aberrations

An imagery will be said to be free of aberrations if every point of an object is imaged perfectly. For a given object point this will be the case if it is imaged to its paraxially conjugate image point. In terms of rays, this image point serves as a reference point that any ray starting from the object point through the aperture has to hit. In terms of waves, the image point serves as the center of a reference sphere, usually through the center of the exit pupil. The point will be imaged without aberrations if the wavefront originating from the object point coincides with this reference sphere.

Aberrations are deviations from this situation. They can be described in either the ray picture or the wave picture, leading to ray or wave aberrations, respectively [3]. The two pictures, i.e., ray and wave aberrations, are equivalent and can be translated into each other.

Throughout this paper, we will refer to wave aberrations. A wavefront-based description of these aberrations can either refer to the geometrical shape of the real *wavefronts* in space (as we will do) or be expressed by a *wave aberration function* which measures the optical path difference (OPD) between the real wavefronts and the reference sphere along the real occurring rays.

### B. Classification of Aberrations

The aberration function can be written as a power series expansion in both the image coordinates and the pupil coordinates or some combinations of these. Depending on symmetry and conventions, this series expansion may have different appearances, but in all cases the respective coefficients are used for classifying the aberrations present. In the case of wave aberrations of rotationally symmetric systems, for example, it is customary to consider *Seidel* (primary) aberrations, *Schwarzschild* (secondary) aberrations, etc. Synonymously, those are sometimes also called fourth-order, sixth-order, etc., aberrations. In terms of ray aberrations, different expressions for the same aberrations would occur, which in that picture are called third-order, fifth-order, etc., aberrations. Therefore, the "order" of an aberration is meaningful only in connection with the underlying aberration scheme.

While the treatment of rotationally symmetric systems is well established in the literature [2,3], there exist rather few publications about non-symmetric systems. Thompson has treated the third-order aberrations [4] and the fifth-order aberrations [5] (in the picture of rays) of misaligned or generally non-symmetric optical systems made of otherwise rotationally symmetric optical surfaces. Quite recently, Thompson *et al.* established a real-ray-based method for calculating these aberrations [6].

It is a very interesting subtopic to consider the aberration function for a single surface for a fixed image point and consequently as a function of the pupil coordinates only [2], but without any restrictions on the symmetries of surfaces or wavefronts. In this case, which is the focus of the present work, the aberration function is often called a *wavefront aberration*. This aberration is often referred to a plane orthogonal to the chief ray instead of the reference sphere, which is, e.g., usual in aberrometry [7]. We will also do so in this work. The above-mentioned series expansion then reduces to an expansion in terms of the pupil coordinates $x$ and $y$ only. The terms in this series give rise to the definition of the order of an aberration as the highest number of added powers of $x$ and $y$ [7,8], as will be introduced in detail in Section 2. It is well accepted that there is no one-to-one correspondence between the order we use and the more general one described above [2]. This situation arises because different orders concerning the image coordinates are summarized within one order of pupil coordinates. Throughout the paper, we will summarize first-order aberrations (tilt) and second-order aberrations (comprising defocus and astigmatism) as *lower-order aberrations* (LOAs) and all aberrations of third order (coma, trefoil), fourth order (e.g., spherical aberration), and higher will be summarized as *higher-order aberrations* (HOAs), as is also done in [7,9].

### C. Scope of the Work

The awareness of the role of HOAs has increased in optometry and ophthalmology [7–13]. HOAs are known to become important for large pupil sizes only and are therefore associated with a wavefront description over the entire pupil. Despite this, it is the aim of this work to establish a description of HOA that is based on local derivatives but that is nevertheless suitable for describing all effects of a large pupil. In Section 2, we show that this description is indeed fully equivalent to the usual approaches that are tailored to describing the entire pupil (e.g., by means of Zernike polynomials). Our local description has the advantage of permitting the derivation of analytical formulas for computing HOA, which represents significant progress in the general understanding and in reduced numerical effort.

Hitherto for determining HOA, the wavefront in the pupil was calculated by ray tracing [14], a precise method when a large number of rays are used but at the same time a very time-consuming iterative numerical method. In the field of spectacle optics, the use of local wavefronts to calculate power and astigmatism is well established [3,15–20]. Wavefront tracing is a very fast semi-analytical method [15,16]. Especially in spectacle lens optics, local features of a wavefront are very important, because the aperture stop is not stationary as in technical optics. Also, magnification and anamorphotic distortion previously have been calculated locally [21–23].

It is known from the literature how to calculate power and astigmatism of a local wavefront after refraction at a given surface. In the case of orthogonal incidence this relation is described by the vergence equation [1,2] and in the case of oblique incidence by the Coddington equation [1,17,18,24].

The purpose of this study is to extend the generalized Coddington equation [3,17–20,24,25] to the case of higher-order aberrations (e.g., coma and spherical aberration), in order to decrease the computational effort with the intrinsic accuracy of an analytical method.

## 2. METHODS AND THEORETICAL BACKGROUND

It turns out to be very practical to establish the treatment of refraction including HOA on the basis of wavefront sagittas in space and not directly with OPD-based aberrations. In the end, we provide a connection between those two pictures (see Appendix B). Refraction equations are a set of relations between the incoming wavefront, the outgoing wavefront, and the refractive surface. Regardless of which two of those three surfaces are given, the relations can always be rearranged in order to determine the third surface as a function of the other two.

### A. Definitions and Notation

#### 1. Coordinate Systems

In order to describe the incoming wavefront, the refractive surface, and the outgoing wavefront, three different local Cartesian coordinate systems $(x,y,z)$, $(\bar{x},\bar{y},\bar{z})$, and $(x',y',z')$, respectively, are used. (see Fig. 1). They are determined by the chief ray corresponding to the fixed image point. The origins of these coordinate systems coincide in the chief ray's intersection point with the refractive surface. The systems possess as common axis $x=x'=\bar{x}$ the normal of the refracting plane, which is the plane containing the normals of the incoming wavefront, the refractive surface, and the outgoing wavefront. Consequently, the $y-z$ plane, the $y'-z'$ plane, and the $\bar{y}-\bar{z}$ plane coincide with each other and with the refracting plane. The $z$ axis points along the incoming chief ray, the $z'$ axis points along the outgoing chief ray, and the $\bar{z}$ axis points along the normal of the refractive surface. The orientations of the $y$ axis, the $y'$ axis, and the $\bar{y}$ axis are such that each system is right-handed.

In this work we use the following notation: scalars are written in plain letters, such as $x$, $y$, $w$ or $S$ for coordinates, wavefront aberrations, or vergences, respectively. Vectors are written as bold lowercase letters, such as $\mathbf{r}$ for position or $\mathbf{n}$ for normal vectors, and matrices are written as bold uppercase letters, such as $\mathbf{R}$ for spatial rotations. Any object (i.e., quantity, space point, or vector) that is specified in the $(x,y,z)$ frame is represented by an unprimed symbol (e.g., $x,\mathbf{r},\mathbf{n},\ldots$), whereas the representation of the same object in the primed frame or in the frame $(\bar{x},\bar{y},\bar{z})$ is given by a prime or a bar on its symbol, respectively. The above definitions imply that the representations of any vector-like quantity $\mathbf{v}$ are connected to each other by the relations

$$\mathbf{v}=\mathbf{R}(\epsilon)\bar{\mathbf{v}}, \qquad \mathbf{v}'=\mathbf{R}(\epsilon')\bar{\mathbf{v}}, \tag{1}$$

where $\mathbf{R}$ stands for spatial rotations about the common $x$ axis, defined by the three-dimensional rotation matrix

$$\mathbf{R}(\epsilon)=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\epsilon & -\sin\epsilon\\ 0 & \sin\epsilon & \cos\epsilon\end{pmatrix}. \tag{2}$$

In order to avoid confusion between primes for coordinate systems and derivatives, we shall denote the derivatives of a function $f(x)$ as $f^{(1)}(x),f^{(2)}(x),f^{(3)}(x),\ldots$ instead of $f'(x),f''(x),f'''(x),\ldots$, respectively. Analogously, we denote the derivatives of a function $f(x,y)$ as $f^{(1,0)}(x,y),f^{(0,1)}(x,y)$,

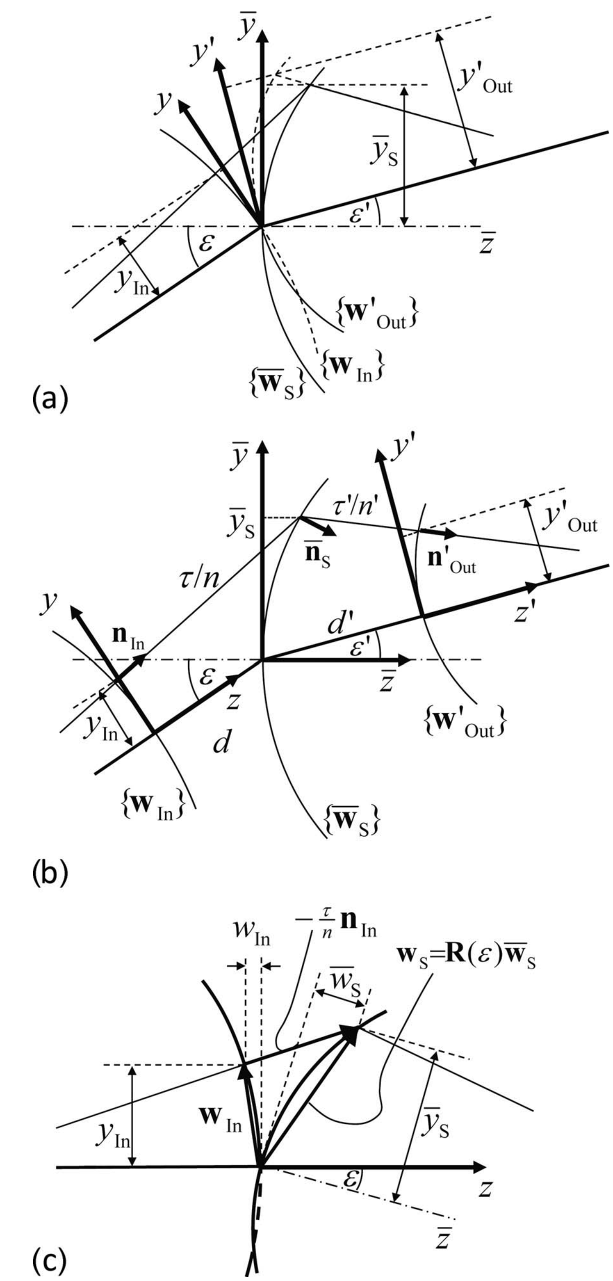


Fig. 1. Local coordinate systems of the refractive surface of the incoming wavefront and the outgoing wavefront. (a) True situation that the origins of all coordinate systems coincide. (b) Fictitious situation of separated origins for a better understanding of the nomenclature. The surface normal vectors along the neighboring ray are also drawn, referred to as $\bar{\mathbf{n}}_{\mathrm{In}}$, $\bar{\mathbf{n}}_{\mathrm{S}}$, $\bar{\mathbf{n}}'_{\mathrm{Out}}$ in their preferred local coordinate systems $(\bar{x},\bar{y},\bar{z})$ coincide. (c) Meaning of the vector sum in Eq. (25).

$f^{(2,0)}(x,y),\ldots$ instead of $\partial/\partial x f(x,y)$, $\partial/\partial y f(x,y)$, $\partial^2/\partial x^2 f(x,y),\ldots$, respectively. Consequently, for functions $f'(x')$ or $\bar{f}(\bar{x})$, the symbolism $f'^{(1)}(x')$ or $\bar{f}^{(1)}(\bar{x})$ refers to $\partial/\partial x' f'(x')$ and $\partial/\partial\bar{x}\bar{f}(\bar{x})$, respectively.

In addition to the coordinate notation, we introduce a lower index notation for labeling whether a quantity belongs to the incoming wavefront, the refractive surface, or the outgoing wavefront. Regardless of which frame is used for mathematical description, the index "In" belongs to the incoming wavefront (e.g., the normal vector is represented as $\mathbf{n}_{\mathrm{In}}$, $\mathbf{n}'_{\mathrm{In}}$, $\bar{\mathbf{n}}_{\mathrm{In}}$ in the three frames, respectively), the index "Out" stands for the outgoing wavefront ($\mathbf{n}_{\mathrm{Out}}$, $\mathbf{n}'_{\mathrm{Out}}$, $\bar{\mathbf{n}}_{\mathrm{Out}}$, respectively), and the index "S" stands for the refractive surface ($\mathbf{n}_{\mathrm{S}}$, $\mathbf{n}'_{\mathrm{S}}$, $\bar{\mathbf{n}}_{\mathrm{S}}$, respectively). Although all representations are used, the preferred frame of each quantity is the one in which the corresponding normal vector in the origin has the components $(0,0,1)^T$, where the index $T$ indicates the transpose. Therefore, the preferred frame is the unprimed one for "In" quantities, the primed one for "Out" quantities, and the frame $(\bar{x},\bar{y},\bar{z})$ for "S" quantities; i.e., the preferred representations for the normal vectors are $\mathbf{n}_{\mathrm{In}}$, $\mathbf{n}'_{\mathrm{Out}}$, and $\bar{\mathbf{n}}_{\mathrm{S}}$, and similarly for all other kinds of vectors.

*2. Description of Wavefronts*

Since the wavefronts and the refractive surface are likewise described by their sagittas, here and in the following the notion "surface" refers to any of the refractive surface, the incoming wavefront, or the outgoing wavefront, unless those are distinguished explicitly.

Any surface sagitta, provided that it is continuous and infinitely often differentiable within the pupil, can be expanded with respect to any complete system of functions spanning the vector space of such functions, which is mathematically denoted by $C^\infty(P)$, where $P\subset\mathbb{R}^2$ is the subset of the pupil plane inside the pupil.

For circular pupils it is common to use the orthogonal complete system of *Zernike circle polynomials* [2,26]. Even for these polynomials there exist different conventions, indexing schemes, and normalizations [1,8]. We use the OSA standard of Zernike polynomials $Z_k^m(\rho,\vartheta)$ of Ref. [8], which describes a surface $w(x,y)$ within a pupil with radius $r_0$ as the expansion

$$w(x,y)=\sum_{k=0}^{\infty}\sum_{m=-k}^{k} c_k^m Z_k^m(\rho,\vartheta), \qquad (m-k)\text{ even}, \tag{3}$$

where $\rho=r/r_0$, $x=r\sin\vartheta$, $y=r\cos\vartheta$, and the $c_k^m$ are the Zernike coefficients. Alternatively, any other complete system can be used for expansion, e.g., the infinite set of monomials of the variables, i.e., 1, $x$, $y$, $x^2$, $xy$, $y^2$, etc., yielding

$$w(x,y)=\sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a_{m,k-m}}{m!(k-m)!}x^m y^{k-m}, \tag{4}$$

which represents the power expansion in a Taylor series [1,2], and the coefficients are simply given by derivatives of the surface:

$$a_{m,k-m}=\left.\frac{\partial^k}{\partial x^m\partial y^{k-m}}w(x,y)\right|_{x=0,y=0}=w^{(m,k-m)}(0,0). \tag{5}$$

As long as the series expansion is infinite, a transformation between any of the representations in Eqs. (3) and (4) is legitimate, well defined, and unique.

In practice, however, an expansion is always truncated at some finite order, justified by the observation that the major part of the light information content is already sufficiently accurately described by the truncated series. Instead of a series we then deal simply with a polynomial. This polynomial can then be considered as a projection of the aberration function onto the vector subspace of $C^{\infty}(P)$ that is spanned by the finite (incomplete) basis system of functions underlying the truncated series. In general, if two different complete systems are truncated arbitrarily to finite basis systems, then the remaining vector subspaces spanned by those two basis systems will not necessarily be identical. If, however, the subspaces happen to be identical, then the projection of any function onto the subspace will be unique, regardless of which basis system has originally been used for representation. For example, if a function is described by a Zernike expansion up to radial order $k=6$ to some accuracy, yielding a sixth-order polynomial in $x$ and $y$, then the same polynomial will be obtained by a Taylor series expansion order up to order $k=6$, and it will represent the function to the same accuracy, because the Zernike basis up to sixth radial order and the monomial basis up to sixth order span the same subspace of $C^{\infty}(P)$.

By the order of an aberration term we mean the number $k$, in either Eq. (3) or Eq. (4). But we draw attention to the fact that an aberration of a certain order is unique only in connection with a specified basis set. For example, in Eq. (3) the Zernike aberration in the term $Z_4^0=\sqrt{5}(6\rho^4-6\rho^2+1)=\sqrt{5}(6(x^2+y^2)^2/r_0^4-6(x^2+y^2)/r_0^2+1)$ due to $\rho=r/r_0$ with order $k=4$, usually called spherical aberration, also contains quadratic and constant terms, whereas any $k=4$ term in Eq. (4) is a monomial with pure value $k=4$ for added $x$ and $y$ powers. An explicit transformation between the Zernike basis and the monomial basis is provided in Appendix A.

In contrast to the Zernike polynomials, which are tailored to a surface description over a finite pupil size, it seems at first glance that a description of local derivatives might be valid only in an infinitesimal neighborhood of the pupil center. However, the above vector space arguments show that a basis of local derivatives does not suffer for any loss of information over the entire pupil size either, provided that the order of derivatives chosen is sufficiently high.

For later application, we introduce

$$w_{\mathrm{In}}(x,y)=\sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a_{\mathrm{In},m,k-m}}{m!(k-m)!}x^m y^{k-m},$$

$$w'_{\mathrm{Out}}(x',y')=\sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a'_{\mathrm{Out},m,k-m}}{m!(k-m)!}x'^m y'^{k-m}, \tag{6}$$

and

$$\bar{w}_{\mathrm{S}}(\bar{x},\bar{y})=\sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{\bar{a}_{m,k-m}}{m!(k-m)!}\bar{x}^m \bar{y}^{k-m} \tag{7}$$

to describe the incoming wavefront, the outgoing wavefront, and the refractive surface, respectively.

The central mathematical idea for the method given in this work is that the coefficients of the unknown surface—it having been assumed to be describable by a finite polynomial function so that once the coefficients are known the surface is known—may be found by taking derivatives and evaluating them at $(x,y)=(0,0)$, where it is known that the value of a derivative of order $k$ equals the value of coefficient $k$.

### *3. Local Properties of Wavefronts and Surface*

Considering the infinitesimal area around the optical axis or rather around the chief ray leads to Gaussian optics (or paraxial optics). For the aberrations of second order the refraction of a spherical wavefront with orthogonal incidence onto a spherical surface with the surface power $\bar{S}$ (Fig. 2) is described by the vergence equation [1,2]:

$$S'=S+\bar{S}, \tag{8}$$

where

$S=n/s$ is the vergence at the object side;
$S'=n/s'$ is the vergence at the image side;
$\bar{S}=(n'-n)/r$ is the surface power;
$s$ is the vertex distance at the object side (axial distance from the refractive surface to the object point), which is equivalent to the radius of curvature of the incoming wavefront;
$s'$ is the vertex distance at the image side (axial distance from the refractive surface to the image point), which is equivalent to the radius of curvature of the outgoing wavefront;
$r$ is the radius of curvature of the refractive surface (distance from center point of the refractive surface to the refractive surface);
$n$ is the refractive index of the medium at the object side;
$n'$ is the refractive index of the medium at the image side;

In the literature, the notion of vergences is usually extended to three-dimensional (3D) space to describe the sphero-cylindrical power of a surface by the following steps. First, the curvatures $1/s$, $1/s'$, and $1/r$ in Eq. (8) are identified with the second derivatives of the sagittas of the incoming wavefront, the outgoing wavefront, and the surface, respectively. Further, in 3D space the second derivatives $w_{\mathrm{In}}^{(2,0)}=\partial^2 w_{\mathrm{In}}/\partial x^2$, $w_{\mathrm{In}}^{(1,1)}=\partial^2 w_{\mathrm{In}}/\partial x\partial y$, and $w_{\mathrm{In}}^{(0,2)}=\partial^2 w_{\mathrm{In}}/\partial y^2$, are summarized in terms of $2\times 2$ vergence matrices [24,27] in the shape

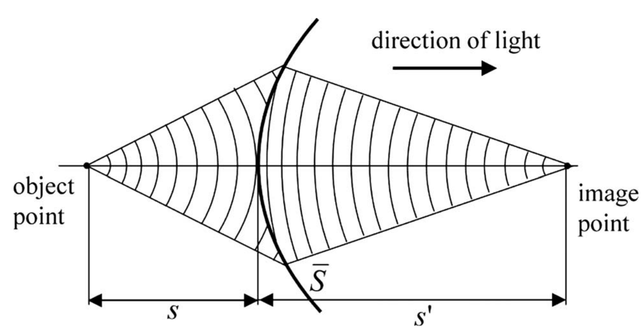


Fig. 2. Orthogonal incidence of a spherical wavefront with vergence $S=n/s$ onto a spherical surface with surface power $\bar{S}$.

$$n\begin{pmatrix} w_{\mathrm{In}}^{(2,0)} & w_{\mathrm{In}}^{(1,1)} \\ w_{\mathrm{In}}^{(1,1)} & w_{\mathrm{In}}^{(2,0)} \end{pmatrix},$$

and similarly for $w'_{\mathrm{Out}}(x',y')$ and $\bar{w}_{\mathrm{S}}(\bar{x},\bar{y})$, for which the prefractors are $n'$ and $(n'-n)$ instead of $n$, and the derivatives are taken with respect to $x',y'$ and $\bar{x},\bar{y}$ instead of $x,y$, respectively.

In addition to the description in terms of vergence matrices, an equivalent description is common in the 3D vector space of power vectors [28–30], which we will apply throughout the paper. For the incoming and the outgoing wavefront, as well as the refractive surface, we introduce the power vectors

$$\mathbf{s} = \begin{pmatrix} S_{xx} \\ S_{xy} \\ S_{yy} \end{pmatrix} = n\begin{pmatrix} w_{\mathrm{In}}^{(2,0)} \\ w_{\mathrm{In}}^{(1,1)} \\ w_{\mathrm{In}}^{(0,2)} \end{pmatrix}, \qquad \mathbf{s}' = \begin{pmatrix} S'_{xx} \\ S'_{xy} \\ S'_{yy} \end{pmatrix} = n'\begin{pmatrix} w'^{(2,0)}_{\mathrm{Out}} \\ w'^{(1,1)}_{\mathrm{Out}} \\ w'^{(0,2)}_{\mathrm{Out}} \end{pmatrix},$$

$$\bar{\mathbf{s}} = \begin{pmatrix} \bar{S}_{xx} \\ \bar{S}_{xy} \\ \bar{S}_{yy} \end{pmatrix} = (n'-n)\begin{pmatrix} \bar{w}_{\mathrm{S}}^{(2,0)} \\ \bar{w}_{\mathrm{S}}^{(1,1)} \\ \bar{w}_{\mathrm{S}}^{(0,2)} \end{pmatrix}. \tag{9}$$

The symbolism $S_{xx}$, $S_{xy}$ etc., is understood merely as component labeling of the vector $\mathbf{s}$. Nevertheless, it will remind the reader of the fact that the value of $S_{xx}$ is proportional to the second derivative $w_{\mathrm{In}}^{(2,0)}$ of the wavefront sagitta. It is well known that the components of Eq. (9) are in ophthalmic terms given by

$$S_{xx} = \left(Sph + \frac{Cyl}{2}\right) - \frac{Cyl}{2}\cos 2\alpha,$$

$$S_{xy} = -\frac{Cyl}{2}\sin 2\alpha,$$

$$S_{yy} = \left(Sph + \frac{Cyl}{2}\right) + \frac{Cyl}{2}\cos 2\alpha, \tag{10}$$

where

*Sph* is the spherical power of the incoming wavefront,
*Cyl* is the cylindrical power of the incoming wavefront,
$\alpha$ is the axis of the cylindrical Power of the incoming wavefront,

and equivalently for $\mathbf{s}'$ and $\bar{\mathbf{s}}$.

One well-established generalization of Eq. (8) relating the components of Eq. (9) to one another is the "Coddington equation." It describes the case of a spherical wavefront hitting a spherical or astigmatic surface under oblique incidence such that one principal curvature direction is lying in the refracting plane [1,17,18,24].

The most general case is characterized by an astigmatic wavefront hitting an astigmatic surface under oblique incidence but such that no special orientation among the refracting plane, the directions of the principal power of the incoming wavefront, and the directions of the principal power of the refractive surface has to be assumed at all. This is the most complex case, described by the generalized Coddington equation (3), (17)–(20), (24), and (25), in compact form written in terms of power vectors,

$$\mathbf{C}'\mathbf{s}' = \mathbf{C}\mathbf{s} + \nu\bar{\mathbf{s}}, \tag{11}$$

where we have introduced the matrices

$$\mathbf{C}' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon' & 0 \\ 0 & 0 & \cos^2\epsilon' \end{pmatrix}, \qquad \mathbf{C} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\epsilon & 0 \\ 0 & 0 & \cos^2\epsilon \end{pmatrix} \tag{12}$$

and the factor

$$\nu = \frac{n'\cos\epsilon' - n\cos\epsilon}{n'-n}. \tag{13}$$

Analogously to the definition of the power vectors for aberrations of order $k=2$, we define for aberrations of higher order $k \geqslant 2$ similar vectors $\mathbf{e}_k$, $\mathbf{e}'_k$, $\bar{\mathbf{e}}_k$ of dimension $k+1$ by

$$\mathbf{e}_k = \begin{pmatrix} E_{x\ldots xx} \\ E_{x\ldots xy} \\ \vdots \\ E_{y\ldots yy} \end{pmatrix} := n\begin{pmatrix} w_{\mathrm{In}}^{(k,0)} \\ w_{\mathrm{In}}^{(k-1,1)} \\ \vdots \\ w_{\mathrm{In}}^{(0,k)} \end{pmatrix},$$

$$\mathbf{e}'_k = \begin{pmatrix} E'_{x\ldots xx} \\ E'_{x\ldots xy} \\ \vdots \\ E'_{y\ldots yy} \end{pmatrix} := n'\begin{pmatrix} w'^{(k,0)}_{\mathrm{Out}} \\ w'^{(k-1,1)}_{\mathrm{Out}} \\ \vdots \\ w'^{(0,k)}_{\mathrm{Out}} \end{pmatrix},$$

$$\bar{\mathbf{e}}_k = \begin{pmatrix} \bar{E}_{x\ldots xx} \\ \bar{E}_{x\ldots xy} \\ \vdots \\ \bar{E}_{y\ldots yy} \end{pmatrix} := (n'-n)\begin{pmatrix} \bar{w}_{\mathrm{S}}^{(k,0)} \\ \bar{w}_{\mathrm{S}}^{(k-1,1)} \\ \vdots \\ \bar{w}_{\mathrm{S}}^{(0,k)} \end{pmatrix}, \tag{14}$$

such that in particular $\mathbf{e}_2=\mathbf{s}$, $\mathbf{e}'_2=\mathbf{s}'$, and $\bar{\mathbf{e}}_2=\bar{\mathbf{s}}$. We use the vectors $\mathbf{e}_k$, $\mathbf{e}'_k$, $\bar{\mathbf{e}}_k$ merely as a device for a compact notation to be used later. Although they form a vector space (which follows directly from the linearity of the derivative), we do not make explicit use of this fact.

Finally, Eq. (12) can also be extended to all $k \geqslant 2$ by the definition

$$\mathbf{C}'_k = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \cos\epsilon' & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cos^k\epsilon' \end{pmatrix},$$

$$\mathbf{C}_k = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \cos\epsilon & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cos^k\epsilon \end{pmatrix}. \tag{15}$$

### B. Mathematical Approach in the Two-Dimensional Case

*1. Coordinates in the Two-Dimensional Case*

To give insight into the method with smallest possible effort, we first treat in detail a fictitious two-dimensional (2D) problem in which the third space dimension does not exist. Later we will transfer the corresponding approach to the 3D case, the case of interest, but for the moment we will drop the $x$ degree of freedom and consider the three coordinate frames $(y,z)$, $(y',z')$, and $(\bar{y},\bar{z})$ spanning one common plane. Instead of a refractive surface in space there is now only a curve $(\bar{y},w(\bar{y}))^T$ in that plane, and similarly the wavefronts are described by curves in that plane (which, for simplicity, will still be called 'surface'). All rays and normal vectors then lie in that plane, too. We summarize this situation with the term "2D." If one likes to, one can imagine the problem to be posed as a 3D one with the symmetry of translational invariance in the $x$ direction, but this is by no means necessary since it is inherent in the mathematics of the two-component system that any ray deflection in a direction other than that in the given plane cannot occur.

The 2D version of the rotation matrix takes the form

$$\mathbf{R}(\epsilon) = \begin{pmatrix} \cos\epsilon & -\sin\epsilon \\ \sin\epsilon & \cos\epsilon \end{pmatrix}. \tag{16}$$

*2. Description of Wavefronts in the 2D Case*

The surfaces themselves are each described by power series expansions specified in the corresponding preferred frame. Any point on the incoming wavefront is given by the vector

$$\mathbf{w}_{\mathrm{In}}(y) = \begin{pmatrix} y \\ w_{\mathrm{In}}(y) \end{pmatrix}, \tag{17}$$

where in the 2D case $w_{\mathrm{In}}(y)$ is the curve defined by

$$w_{\mathrm{In}}(y) = \sum_{k=0}^{\infty} \frac{a_{\mathrm{In},k}}{k!} y^k, \tag{18}$$

which corresponds to Eq. (6) in the 3D case. Equivalently, we represent the outgoing wavefront and the refractive surface in their preferred frames by the vectors

$$\mathbf{w}'_{\mathrm{Out}}(y') = \begin{pmatrix} y' \\ w'_{\mathrm{Out}}(y') \end{pmatrix}, \qquad \bar{\mathbf{w}}_{\mathrm{S}}(\bar{y}) = \begin{pmatrix} \bar{y} \\ \bar{w}_{\mathrm{S}}(\bar{y}) \end{pmatrix}, \tag{19}$$

where

$$w'_{\mathrm{Out}}(y') = \sum_{k=0}^{\infty} \frac{a'_{\mathrm{Out},k}}{k!} y'^k, \qquad \bar{w}_{\mathrm{S}}(\bar{y}) = \sum_{k=0}^{\infty} \frac{\bar{a}_{\mathrm{S},k}}{k!} \bar{y}^k. \tag{20}$$

As in Eq. (5), again the normalization factor $k!$ is chosen such that the coefficients $a_{\mathrm{In},k}$ are given by the derivatives of the wavefront at $y=0$

$$a_{\mathrm{In},k} = \left. \frac{\partial^k}{\partial y^k} w_{\mathrm{In}}(y) \right|_{y=0} = w_{\mathrm{In}}^{(k)}(0). \tag{21}$$

In the 2D case the vector $\mathbf{e}_k$ in Eq. (14) reduces to a scalar, $E_k = n w_{\mathrm{In}}^{(k)} = n a_{\mathrm{In},k}$; e.g., for second- and third-order aberrations, we have $E_2 = n w_{\mathrm{In}}^{(2)} = n a_2$, $E_3 = n w_{\mathrm{In}}^{(3)} = n a_3$, etc. A similar reasoning applies for the vectors $\mathbf{e}'_k$, $\bar{\mathbf{e}}_k$ and yields the local aberrations $E'_k$, $\bar{E}_k$, connected to the coefficients $a'_{\mathrm{Out},k}$, $\bar{a}_{\mathrm{S},k}$ by multiplication by the refractive index $n'$ for the outgoing wavefront and by the factor $n'-n$ for the refractive surface, respectively.

It is important to note that each surface has zero slope at its coordinate origin because by construction the $z$ axis points along the normal of its corresponding surface. Furthermore, since all surfaces are evaluated at the intersection point, each of them has zero offset, too. In terms of series coefficients, this means that all the prism and offset coefficients vanish, i.e., $a_{\mathrm{In},k}=0$, $a'_{\mathrm{Out},k}=0$, $\bar{a}_{\mathrm{S},k}=0$ for $k<2$.

*3. Normal Vectors and Their Derivatives*

The normal vector $\mathbf{n}_w(y)$ of any surface $w(y)$ (i.e., curve in the 2D case) is given by $\mathbf{n}_w(y) = (-w^{(1)}(y),1)^T/\sqrt{1+w^{(1)}(y)^2}$, where $w^{(1)} = \partial w/\partial y$. In principle, we are interested in derivatives of $\mathbf{n}_w(y)$ with respect to $y$. Observing, however, that $\mathbf{n}_w(y)$ depends on $y$ only via the slope $w^{(1)}(y)$, it is very practical to concentrate on this dependence $\mathbf{n}_w(w^{(1)})$ first and to deal with the inner dependence $w^{(1)}(y)$ later. To do this, we set $v \equiv w^{(1)}$ and to introduce the function

$$\mathbf{n}(v) := \frac{1}{\sqrt{1+v^2}} \begin{pmatrix} -v \\ 1 \end{pmatrix}. \tag{22}$$

Since at the intersection point all slopes vanish, only the behavior of that function $\mathbf{n}(v)$ for vanishing argument $v=0$ is of interest. It is now straightforward to provide the first few derivatives $\mathbf{n}^{(1)}(0) \equiv \partial/\partial v\, \mathbf{n}(v)|_{v=0}$, $\mathbf{n}^{(2)}(0) \equiv \partial^2/\partial v^2 \mathbf{n}(v)|_{v=0}$, etc.:

$$\mathbf{n}(0) := \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \mathbf{n}^{(1)}(0) := \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \qquad \mathbf{n}^{(2)}(0) := \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$

$$\mathbf{n}^{(3)}(0) := \begin{pmatrix} 3 \\ 0 \end{pmatrix}, \qquad \mathbf{n}^{(4)}(0) := \begin{pmatrix} 0 \\ 9 \end{pmatrix}, \text{ etc.} \tag{23}$$

In application to the functions of interest, $\mathbf{n}_{\mathrm{In}}(y) = \mathbf{n}(w_{\mathrm{In}}^{(1)}(y))$, $\mathbf{n}'_{\mathrm{Out}}(y') = \mathbf{n}(w_{\mathrm{Out}}'^{(1)}(y'))$, $\bar{\mathbf{n}}_{\mathrm{S}}(\bar{y}) = \mathbf{n}(\bar{w}_{\mathrm{S}}^{(1)}(\bar{y}))$, this means that $\mathbf{n}_{\mathrm{In}}(0) = (0,1)^T$, $\mathbf{n}'_{\mathrm{Out}}(0) = (0,1)^T$, $\bar{\mathbf{n}}_{\mathrm{S}}(0) = (0,1)^T$, where each equation is valid in its local coordinate system. Further, the first derivatives are given by

$$\frac{\partial}{\partial y}\mathbf{n}_{\mathrm{In}}(y)\bigg|_{y=0} \equiv \mathbf{n}_{\mathrm{In}}^{(1)}(0) = \mathbf{n}^{(1)}(0)w_{\mathrm{In}}^{(2)}(0) = \begin{pmatrix}-1\\0\end{pmatrix}w_{\mathrm{In}}^{(2)}(0),$$

$$\frac{\partial}{\partial y'}\mathbf{n}'_{\mathrm{Out}}(y')\bigg|_{y'=0} \equiv \mathbf{n}'^{(1)}_{\mathrm{Out}}(0) = \mathbf{n}^{(1)}(0)w'^{(2)}_{\mathrm{Out}}(0) = \begin{pmatrix}-1\\0\end{pmatrix}w'^{(2)}_{\mathrm{Out}}(0),$$

$$\frac{\partial}{\partial \bar{y}}\bar{\mathbf{n}}_{\mathrm{S}}(\bar{y})\bigg|_{\bar{y}=0} \equiv \bar{\mathbf{n}}_{\mathrm{S}}^{(1)}(0) = \mathbf{n}^{(1)}(0)\bar{w}_{\mathrm{S}}^{(2)}(0) = \begin{pmatrix}-1\\0\end{pmatrix}\bar{w}_{\mathrm{S}}^{(2)}(0), \tag{24}$$

and similarly for the higher derivatives.

*4. Ansatz for Determining the Refraction Equations*

Once the local aberrations of two of the surfaces are given, their corresponding $a_k$ coefficients are directly determined, too, and equivalently the surface derivatives. It is our aim to calculate the third surface in the sense that its derivatives and thus its $a_k$ coefficients [see Eqs. (18)–(21)] are determined for all orders $2 \leq k \leq k_0$ for the order $k_0$ of interest, and to assign values to its corresponding local aberrations.

Our starting point is the following situation. While the chief ray and the coordinate systems are fixed, a neighboring ray scans the incoming wavefront $\{\mathbf{w}_{\mathrm{In}}\}$ and hits it at an intercept $y_{\mathrm{In}} \neq 0$, then hits the refractive surface $\{\bar{\mathbf{w}}_{\mathrm{S}}\}$, and finally propagates to the outgoing wavefront $\{\mathbf{w}'_{\mathrm{Out}}\}$, where the brackets $\{.\}$ denote the entity of vectors described by Eqs. (17) and (19) [see Figs. 1(a) and 1(b)]. Except for the limiting case $y_{\mathrm{In}} \to 0$, the three points in space, $\mathbf{w}_{\mathrm{In}}$, $\mathbf{w}'_{\mathrm{Out}}$, $\bar{\mathbf{w}}_{\mathrm{S}}$, in general do not coincide. As shown in Fig. 1, and consistently with our notation, we denote as $y_{\mathrm{In}}$ the projection of the neighboring ray's intersection with $\{\mathbf{w}_{\mathrm{In}}\}$ onto the $y$ axis. Analogously, the projection of the intersection with $\{\mathbf{w}'_{\mathrm{Out}}\}$ onto the $y'$ axis is denoted as $y'_{\mathrm{Out}}$, and the projection of the intersection with $\{\bar{\mathbf{w}}_{\mathrm{S}}\}$ onto the $\bar{y}$ axis is called $\bar{y}_{\mathrm{S}}$.

The mutual position of the points and surfaces is shown in Fig. 1(a). Although both wavefronts in general penetrate the refractive surface, the definition of the intersection coordinates as projections will be meaningful if we formally allow all parts of the rays and wavefronts to be extended into both half-spaces [indicated as dashed curves in Fig. 1(a)].

It might appear helpful for the reader to imagine for a short instant that the incoming wavefront is evaluated at a distance $d>0$ before the refraction and that the outgoing wavefront is evaluated at a distance $d'>0$ after the refraction, measured along the chief ray. In this fictitious situation of separated intersections even along the chief ray (and therefore also separated origins of the coordinate frames) it is much easier to identify the various coordinates, as shown in Fig. 1(b). The true situation $d=d'=0$, which is relevant throughout the paper, is shown in Fig. 1(a). While in Figs. 1(a) and 1(b) all quantities are drawn in their preferred frames, Fig. 1(c) shows the quantities concerning the incoming wavefront and the refractive surface in the common frame $(y,z)$. The vector $\mathbf{w}_{\mathrm{In}} = \mathbf{w}_{\mathrm{In}}(y_{\mathrm{In}})$ [see Eq. (17)] points to the neighboring ray's intersection point with the incoming wavefront, and the wavefront's OPD referred to the refractive surface along the ray is denoted by $\tau$, and correspondingly the vector from the wavefront to the surface is $-\tau/n\mathbf{n}_{\mathrm{In}}$. Hence, the vector to the point on the surface itself, $\mathbf{w}_{\mathrm{S}}$, must be equal to the vector sum $\mathbf{w}_{\mathrm{S}} = \mathbf{w}_{\mathrm{In}} - \tau/n\mathbf{n}_{\mathrm{In}}$. Transforming $\mathbf{w}_{\mathrm{S}}$ to its preferred frame by $\mathbf{w}_{\mathrm{S}} = \mathbf{R}(\epsilon)\bar{\mathbf{w}}_{\mathrm{S}}$ [see Eqs. (1) and (16)] yields the first of the fundamental equations in Eq. (25).

Analogously we have $\mathbf{w}'_{\mathrm{Out}} - \tau'/n'\mathbf{n}'_{\mathrm{Out}} = \mathbf{w}'_{\mathrm{S}}$ for the outgoing wavefront in the frame $(y',z')$, yielding the second equation in Eq. (25). A condition for the outgoing wavefront to be the surface of constant OPD is that $\tau = \tau'$ for all neighboring rays. Inserting this condition, we establish as starting point of our computations the fundamental equations

$$\begin{pmatrix} y_{\mathrm{In}} \\ w_{\mathrm{In}}(y_{\mathrm{In}}) \end{pmatrix} - \frac{\tau}{n}\mathbf{n}_{\mathrm{In}} = \mathbf{R}(\epsilon)\begin{pmatrix} \bar{y}_{\mathrm{S}} \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix},$$

$$\begin{pmatrix} y'_{\mathrm{Out}} \\ w'_{\mathrm{Out}}(y'_{\mathrm{Out}}) \end{pmatrix} - \frac{\tau}{n'}\mathbf{n}'_{\mathrm{Out}} = \mathbf{R}(\epsilon')\begin{pmatrix} \bar{y}_{\mathrm{S}} \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix}. \tag{25}$$

From Eq. (25), it is now possible to derive the desired relations order by order. For this purpose, it turns out to be practical to consider formally both wavefronts as given and to ask for the refractive surface $\bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}})$ as the unknown function. Although only the surface is of interest, in Eq. (25) additionally the four quantities $\tau, y_{\mathrm{In}}, y'_{\mathrm{Out}}, \bar{y}_{\mathrm{S}}$ are also unknown. However, they are not independent of each other: if any one of them is given, the other three can no longer be chosen independently. We use $\bar{y}_{\mathrm{S}}$ as the independent variable and consider the three other unknowns $\tau, y_{\mathrm{In}}, y'_{\mathrm{Out}}$ as functions of it.

We arrive at the conclusion that Eq. (25) represents a nonlinear system of four algebraic equations for the four unknown functions $\bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}), y_{\mathrm{In}}(\bar{y}_{\mathrm{S}}), y'_{\mathrm{Out}}(\bar{y}_{\mathrm{S}}), \tau(\bar{y}_{\mathrm{S}})$. Even if we are interested in a solution only for the function $\bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}})$, we cannot obtain it without simultaneously solving the equations for all four unknowns order by order. Introducing the vector of unknown functions as

$$\mathbf{p}(\bar{y}_{\mathrm{S}}) = \begin{pmatrix} y_{\mathrm{In}}(\bar{y}_{\mathrm{S}}) \\ y'_{\mathrm{Out}}(\bar{y}_{\mathrm{S}}) \\ \tau(\bar{y}_{\mathrm{S}}) \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix} \tag{26}$$

and observing that the initial condition $\mathbf{p}(0) = \mathbf{0}$ has to be fulfilled, it is now straightforward to compute all the derivatives of Eq. (25) up to some order, which yields relations between the curvatures, third derivatives, etc., of the wavefronts and the refractive surface. Rewriting these relations in terms of series coefficients $a_{\mathrm{In},k}$, $a'_{\mathrm{Out},k}$, $\bar{a}_{\mathrm{S},k}$ and solving them for the desired coefficients $\bar{a}_{\mathrm{S},k}$ yields the desired result.

Before solving Eq. (25), we distinguish whether the independent variable $\bar{y}_{\mathrm{S}}$ enters into Eq. (25) explicitly, as in the first component of the vector $(\bar{y}_{\mathrm{S}}, \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}))^T$, or implicitly via one of the components of Eq. (26). To this end, we define the function $(\mathbb{R}^4 \times \mathbb{R}) \mapsto \mathbb{R}^4 : (\mathbf{p}, \bar{y}_{\mathrm{S}}) \mapsto \mathbf{f}$ by

$$\mathbf{f}(\mathbf{p},\bar{y}_S) = \begin{pmatrix} y_{In} - \frac{\tau}{n} n_y(w_{In}^{(1)}(y_{In})) - (\bar{y}_S \cos \epsilon - \bar{w}_S \sin \epsilon) \\ w_{In}(y_{In}) - \frac{\tau}{n} n_z(w_{In}^{(1)}(y_{In})) - (\bar{y}_S \sin \epsilon + \bar{w}_S \cos \epsilon) \\ y'_{Out} - \frac{\tau}{n} n_y(w'^{(1)}_{Out}(y'_{Out})) - (\bar{y}_S \cos \epsilon' - \bar{w}_S \sin \epsilon') \\ w'_{Out}(y'_{Out}) - \frac{\tau}{n} n_z(w'^{(1)}_{Out}(y'_{Out})) - (\bar{y}_S \sin \epsilon' + \bar{w}_S \cos \epsilon') \end{pmatrix}, \tag{27}$$

where $(p_1,p_2,p_3,p_4)=(y_{In},y'_{Out},\tau,\bar{w}_S)$ are the components of $\mathbf{p}$. Now setting $\mathbf{p}=\mathbf{p}(\bar{y}_S)$, Eq. (27) allows us to rewrite the fundamental system of Eq. (25) in a more compact way as

$$\mathbf{f}(\mathbf{p}(\bar{y}_S),\bar{y}_S) = \mathbf{0}, \tag{28}$$

as can be verified explicitly by componentwise comparison with Eq. (25).

The key ingredient of our method is that the relations between the derivatives of wavefronts and surfaces can be obtained by the first, second, etc., total derivative of Eq. (28) with respect to $\bar{y}_S$, evaluated in the origin. The advantage of the form of Eq. (28) using Eq. (27) is that the various terms can be tracked in a fairly compact manner.

The total derivative of $\mathbf{f}(\mathbf{p}(\bar{y}_S),\bar{y}_S)$ in Eq. (28) is obtained by applying the principles from the theory of implicit functions. Hence, the total derivative is given by the partial derivatives of $\mathbf{f}$ with respect to the components $p_i$ of $\mathbf{p}$, times the derivatives of $p_i(\bar{y}_S)$, plus the partial derivative of $\mathbf{f}$ with respect to the explicit dependence on $\bar{y}_S$. This transforms the system of algebraic equations in Eq. (25) to the system of differential equations

$$\sum_{j=1}^{4} \frac{\partial f_i}{\partial p_j} p_j^{(1)}(\bar{y}_S) + \frac{\partial f_i}{\partial \bar{y}_S} = 0, \qquad i = 1, \ldots, 4, \tag{29}$$

where the matrix with elements $A_{ij} := \partial f_i / \partial p_j$ is the Jacobian matrix $\mathbf{A}$ of $\mathbf{f}$ with respect to its vector argument $\mathbf{p}$, evaluated for $\mathbf{p}=\mathbf{p}(\bar{y}_S)$. The Jacobian $\mathbf{A}$ reads

$$\mathbf{A} := \begin{pmatrix} \frac{\partial f_1}{\partial y_{In}} & \frac{\partial f_1}{\partial y'_{Out}} & \frac{\partial f_1}{\partial \tau} & \frac{\partial f_1}{\partial \bar{w}_S} \\ \frac{\partial f_2}{\partial y_{In}} & \frac{\partial f_2}{\partial y'_{Out}} & \frac{\partial f_2}{\partial \tau} & \frac{\partial f_2}{\partial \bar{w}_S} \\ \frac{\partial f_3}{\partial y_{In}} & \frac{\partial f_3}{\partial y'_{Out}} & \frac{\partial f_3}{\partial \tau} & \frac{\partial f_3}{\partial \bar{w}_S} \\ \frac{\partial f_4}{\partial y_{In}} & \frac{\partial f_4}{\partial y'_{Out}} & \frac{\partial f_4}{\partial \tau} & \frac{\partial f_4}{\partial \bar{w}_S} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\tau}{n} n_{In,y}^{(1)} w_{In}^{(2)} & 0 & \frac{1}{n} n_{In,y} & \sigma \\ w_{In}^{(1)} - \frac{\tau}{n} n_{In,z}^{(1)} w_{In}^{(2)} & 0 & \frac{1}{n} n_{In,z} & -\chi \\ 0 & 1 - \frac{\tau}{n'} n'^{(1)}_{Out,y} w'^{(2)}_{Out} & \frac{1}{n'} n'_{Out,y} & \sigma' \\ 0 & w'^{(1)}_{Out} - \frac{\tau}{n'} n'^{(1)}_{Out,z} w'^{(2)}_{Out} & \frac{1}{n'} n'_{Out,z} & -\chi' \end{pmatrix}. \tag{30}$$

In Eq. (30), the occurring expressions are understood as $w_{In}^{(1)} \equiv w_{In}^{(1)}(y_{In})$, $w_{In}^{(2)} \equiv w_{In}^{(2)}(y_{In})$, $n_{In,y} \equiv n_{In,y}(w_{In}^{(1)}(y_{In}))$, $n_{In,y}^{(1)} \equiv n_{In,y}^{(1)}(w_{In}^{(1)}(y_{In}))$, etc., and analogously for the "Out" quantities; additionally, $y_{In}, y'_{Out}, \tau, \bar{w}_S$ are themselves functions of $\bar{y}_S$.

The derivative vector $\partial f_i / \partial \bar{y}_S$ in Eq. (29) is summarized as

$$\mathbf{b} := -\frac{\partial \mathbf{f}}{\partial \bar{y}_S} = \begin{pmatrix} \chi \\ \sigma \\ \chi' \\ \sigma' \end{pmatrix}, \tag{31}$$

where for convenience we have introduced $\sigma = \sin \epsilon$, $\chi = \cos \epsilon$, and similarly for $\epsilon'$.

Both $\mathbf{A}$ and $\mathbf{b}$ are deduced from $\mathbf{f}(\mathbf{p}(\bar{y}_S),\bar{y}_S)$ and must in general themselves have the same kind of dependence, i.e., $\mathbf{A}(\mathbf{p}(\bar{y}_S),\bar{y}_S)$ and $\mathbf{b}(\mathbf{p}(\bar{y}_S),\bar{y}_S)$. However, due to the special property of $\mathbf{f}$ of being linear in $\bar{y}_S$, $\mathbf{b}$ is constant. Additionally, $\mathbf{A}$ has no explicit dependence on $\bar{y}_S$ besides the implicit dependence via $\mathbf{p}(\bar{y}_S)$. Hence we write $\mathbf{b}$ without argument and $\mathbf{A}=\mathbf{A}(\mathbf{p}(\bar{y}_S))$, and Eq. (29) can be written in the form

$$\mathbf{A}(\mathbf{p}(\bar{y}_S))\mathbf{p}^{(1)}(\bar{y}_S) = \mathbf{b}. \tag{32}$$

### *5. Solving Techniques for the Fundamental Equation*

Equation (32) is the derivative of the fundamental equation in Eq. (28), and therefore it is itself a fundamental equation. But, in addition, it allows a stepwise solution for the derivatives $\mathbf{p}^{(k)}(\bar{y}_S=0)$ for increasing order $k$. Formally, Eq. (32) can be solved for $\mathbf{p}^{(1)}(\bar{y}_S)$ by

$$\mathbf{p}^{(1)}(\bar{y}_S) = \mathbf{A}(\mathbf{p}(\bar{y}_S))^{-1}\mathbf{b}. \tag{33}$$

Equation (33) holds as a function of $\bar{y}_S$, but of course for arbitrary $\bar{y}_S$ both sides of Eq. (33) are unknown. However, evaluating Eq. (33) for $\bar{y}_S=0$ exploits that then the right-hand side (rhs) is known because $\mathbf{p}(0)=\mathbf{0}$ is known! In the same manner, Eq. (33) serves as starting point for a recursion scheme by repeated total derivative and evaluation for $\bar{y}_S=0$. Remembering that $\mathbf{b}$ is constant, we obtain

$$\mathbf{p}^{(1)}(0) = \mathbf{A}^{-1}\mathbf{b},$$

$$\mathbf{p}^{(2)}(0) = (\mathbf{A}^{-1})^{(1)}\mathbf{b},$$

$$\ldots$$

$$\mathbf{p}^{(k)}(0) = (\mathbf{A}^{-1})^{(k-1)}\mathbf{b},$$

$$\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}, \tag{34}$$

where

$$(\mathbf{A}^{-1})^{(1)} = \left.\frac{d}{d\bar{y}_S}\mathbf{A}(\mathbf{p}(\bar{y}_S))^{-1}\right|_{\bar{y}_S=0}, \ldots,$$

$$(\mathbf{A}^{-1})^{(k-1)} = \left.\frac{d^{k-1}}{d\bar{y}_S^{k-1}}\mathbf{A}(\mathbf{p}(\bar{y}_S))^{-1}\right|_{\bar{y}_S=0}$$

are total derivatives of the function $\mathbf{A}(\mathbf{p}(\bar{y}_S))^{-1}$. The reason that Eq. (34) really does provide solutions for $\mathbf{p}^{(1)} \times(0), \mathbf{p}^{(2)}(0), \ldots \mathbf{p}^{(k)}(0)$ is that in any row of Eq. (34) the entries on the rhs are all known, assuming that the equations above are already solved. Although on the rhs there occur implicit derivatives $\mathbf{p}^{(1)}(0), \mathbf{p}^{(2)}(0), \ldots$, as well, they are always of an order less than on the left-hand side (lhs). For example, the second row in Eq. (34) reads in explicit form,

$$\mathbf{p}^{(2)}(0) = \left.\sum_{i=1}^{4}\left(\frac{\partial}{\partial p_i}\mathbf{A}(\mathbf{p})^{-1}\right)p_i^{(1)}\right|_{\bar{y}_S=0} \cdot \mathbf{b},$$

where $\bar{y}_S=0$ implies $\mathbf{p}=\mathbf{0}$ and where on the rhs the highest occurring derivative of $\mathbf{p}$ is $\mathbf{p}^{(1)}(0)$, which is already known as a result of the first row in Eq. (34). Generally, the highest derivative of $\mathbf{p}$ occurring in $((d^{k-1}/d\bar{y}_S^{k-1})\mathbf{A}(\mathbf{p}(\bar{y}_S))^{-1})|_{\bar{y}_S=0}$ is $\mathbf{p}^{(k-1)}(0)$, which is already known at the stage when $\mathbf{p}^{(k)}(0)$ is to be computed by Eq. (34).

Although looking attractive and formally simple, applying Eq. (34) in practice still requires some algebra. One part of the effort arises because it is the inverse of $\mathbf{A}$ which has to be differentiated with respect to $\mathbf{p}$. The other part of the effort is due to the large number of terms, since the higher derivatives will involve more and more cross derivatives like $\partial^2/\partial p_i \partial p_j$. It is straightforward to execute both tasks by a computer algebra package, but they are nevertheless lengthy and not the best way to gain more insight.

While cross-derivatives are inevitable, there exists an alternative recursion scheme for which it is sufficient to differentiate the matrix $\mathbf{A}$ itself instead of its inverse $\mathbf{A}^{-1}$, which means an enormous reduction of complexity! For this purpose, we start the recursion scheme from Eq. (32) instead of Eq. (33). The first $(k-1)$ total derivatives of Eq. (32) are

$$\mathbf{A}\mathbf{p}^{(1)}(0) = \mathbf{b}, \quad \text{(a)}$$

$$\mathbf{A}^{(1)}\mathbf{p}^{(1)}(0) + \mathbf{A}\mathbf{p}^{(2)}(0) = \mathbf{0}, \quad \text{(b)}$$

$$\mathbf{A}^{(2)}\mathbf{p}^{(1)}(0) + 2\mathbf{A}^{(1)}\mathbf{p}^{(2)}(0) + \mathbf{A}\mathbf{p}^{(3)}(0) = \mathbf{0}, \quad \text{(c)}$$

$$\ldots$$

$$\sum_{j=1}^{k}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0) = \mathbf{0}, \qquad k \geqslant 2 \quad \text{(d)}, \tag{35}$$

where

$$\mathbf{A} = \mathbf{A}(\mathbf{p}(0)) = \mathbf{A}(\mathbf{0}),$$

$$\mathbf{A}^{(1)} = \left.\frac{d}{d\bar{y}_S}\mathbf{A}(\mathbf{p}(\bar{y}_S))\right|_{\bar{y}_S=0}, \ldots,$$

$$\mathbf{A}^{(k-j)} = \left.\frac{d^{k-j}}{d\bar{y}_S^{k-j}}\mathbf{A}(\mathbf{p}(\bar{y}_S))\right|_{\bar{y}_S=0}$$

are are total derivatives of the function $\mathbf{A}(\mathbf{p}(\bar{y}_S))$. For the last line of Eq. (35) we have applied the formula for the $p$th derivative of a product,

$$(fg)^{(p)} = \sum_{j=0}^{p}\binom{p}{j}f^{(p-j)}g^{(j)}.$$

Equation (35) represents a recursion scheme where in each equation containing $\mathbf{p}^{(1)}(0), \mathbf{p}^{(2)}(0), \ldots \mathbf{p}^{(k)}(0)$, only $\mathbf{p}^{(k)}(0)$ (in the last term for $j=k$) is unknown provided that all previous equations for $\mathbf{p}^{(1)}(0), \mathbf{p}^{(2)}(0), \ldots, \mathbf{p}^{(k-1)}(0)$ are already solved. A formal solution for $\mathbf{p}^{(k)}(0)$, expressed in terms of its predecessors, is

$$\mathbf{p}^{(1)}(0) = \mathbf{A}^{-1}\mathbf{b}, \qquad k = 1,$$

$$\mathbf{p}^{(k)}(0) = -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), \qquad k \geqslant 2. \tag{36}$$

Although quite different in appearance at first glance, Eq. (36) yields exactly the same solutions as Eq. (34).

### *6. Solutions for the General Refraction Equations*

In the result for $\mathbf{p}^{(1)}(0)$, the first rows of both Eqs. (34) and (36) involve $\mathbf{A}(\mathbf{0})^{-1}$. To obtain $\mathbf{A}(\mathbf{0})^{-1}$, we evaluate Eq. (30) for $\mathbf{p}=\mathbf{0}$ and apply Eqs. (23), yielding

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1 & 0 & 0 & \sigma \\ 0 & 0 & -1/n & -\chi \\ 0 & 1 & 0 & \sigma' \\ 0 & 0 & -1/n' & -\chi' \end{pmatrix} \Rightarrow$$

$$\mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} 1 & -n\sigma/\eta & 0 & n'\sigma/\eta \\ 0 & -n\sigma'/\eta & 1 & n'\sigma'/\eta \\ 0 & -nn'\chi'/\eta & 0 & nn'\chi/\eta \\ 0 & n/\eta & 0 & -n'/\eta \end{pmatrix}$$

$$\text{with } \eta = n'\chi' - n\chi. \tag{37}$$

The last component of $\mathbf{p}^{(1)}(0)$, which is the refractive surface slope, is obtained as $\bar{w}_{\mathrm{S}}^{(1)}(0) = -(n'\sigma' - n\sigma)/\eta$. This is formally correct since we have not yet made any assumption about the angles $\epsilon$, $\epsilon'$. If, however, we claim that $\bar{w}_{\mathrm{S}}^{(1)}(0)=0$, we will obtain the refraction law $n'\sigma' - n\sigma \equiv n'\sin\epsilon' - n\sin\epsilon = 0$. Exploiting this in all further calculations, the final result for $\mathbf{p}^{(1)}(0)$ is

$$\mathbf{p}^{(1)}(0) = \begin{pmatrix} \chi \\ \chi' \\ -n\sigma \\ 0 \end{pmatrix}. \tag{38}$$

For the orders $k \geqslant 2$ we apply Eqs. (36). The derivatives $\mathbf{A}^{(1)} = (d/d\bar{y}_{\mathrm{S}})\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))|_{\bar{y}_{\mathrm{S}}=0}$, etc., are directly obtained by total derivative of Eq. (30) with respect to $\bar{y}_{\mathrm{S}}$, evaluating for $\bar{y}_{\mathrm{S}}=0$ and again applying Eqs. (23). For the orders $k \geqslant 2$ only the results $\bar{w}_{\mathrm{S}}^{(k)}(0)$ for the refractive surface are of interest; therefore we directly provide those results. The resulting second-order law is [omitting the argument (0)]

$$\eta \cdot \bar{w}_{\mathrm{S}}^{(2)} = \chi'^2 n' w_{\mathrm{Out}}'^{(2)} - \chi^2 n w_{\mathrm{In}}^{(2)}, \tag{39}$$

which is well known as the Coddington equation and turns out to be a special case of our results. The resulting higher-order laws can be written in a similar fashion:

$$\eta \cdot \bar{w}_{\mathrm{S}}^{(3)} = \chi'^3 n' w_{\mathrm{Out}}'^{(3)} - \chi^3 n w_{\mathrm{In}}^{(3)} + R_3,$$

$$\eta \cdot \bar{w}_{\mathrm{S}}^{(4)} = \chi'^4 n' w_{\mathrm{Out}}'^{(4)} - \chi^4 n w_{\mathrm{In}}^{(4)} + R_4,$$

$$\cdots$$

$$\eta \cdot \bar{w}_{\mathrm{S}}^{(k)} = \chi'^k n' w_{\mathrm{Out}}'^{(k)} - \chi^k n w_{\mathrm{In}}^{(k)} + R_k, \tag{40}$$

with the remainder terms $R_k$, which are given for orders $k=3,4$ explicitly as

$$R_3 = -\frac{3n\sigma\chi\chi'}{\eta}(n w_{\mathrm{Out}}'^{(2)} - n' w_{\mathrm{In}}^{(2)})(\chi' w_{\mathrm{Out}}'^{(2)} - \chi w_{\mathrm{In}}^{(2)}), \tag{41}$$

$$\begin{aligned} R_4 = {} & (\alpha w_{\mathrm{Out}}'^{(2)} + \beta w_{\mathrm{In}}^{(2)}) w_{\mathrm{Out}}'^{(3)} + (\beta' w_{\mathrm{Out}}'^{(2)} + \alpha' w_{\mathrm{In}}^{(2)}) w_{\mathrm{In}}^{(3)} \\ & + \gamma' (w_{\mathrm{Out}}'^{(2)})^3 + \delta' (w_{\mathrm{Out}}'^{(2)})^2 w_{\mathrm{In}}^{(2)} + \delta w_{\mathrm{Out}}'^{(2)} (w_{\mathrm{In}}^{(2)})^2 \\ & + \gamma (w_{\mathrm{In}}^{(2)})^3, \end{aligned} \tag{42}$$

with

$$\alpha = \frac{2n\sigma\chi'^3}{\eta}(n'\chi' - 6n\chi), \qquad \beta = \frac{2n\sigma\chi\chi'^2}{\eta}(2n'\chi' + 3n\chi),$$

$$\gamma = \frac{3n\chi^2}{\eta^2}(2n'\chi^2\chi'\eta - \sigma^2(n^2\chi^2 + 4n'^2\chi'^2)),$$

$$\begin{aligned} \delta = {} & \frac{3n'\chi}{n\eta^2}((2n'\chi' + n\chi)(n^2\chi^2 + 2nn'\chi\chi' + 2n'^2\chi'^2)\sigma'^2 \\ & - 2\eta(n\chi\chi')^2), \end{aligned} \tag{43}$$

and $\alpha'$, $\beta'$, $\gamma'$, $\delta'$ are obtained from $-\alpha, -\beta, -\gamma, -\delta$, respectively, by interchanging $n \leftrightarrow n'$, $\chi \leftrightarrow \chi'$, $\sigma \leftrightarrow \sigma'$, $\eta \leftrightarrow -\eta$. Results for even higher orders $k=5,6$ are provided in[31].

Equation (40) holds likewise for the derivatives and for the coefficients $a_{\mathrm{In},k}$, $a'_{\mathrm{Out},k}$, $\bar{a}_{\mathrm{S},k}$ due to Eqs. (18)–(21). In terms of local aberrations, Eq. (40) reads (after replacing $\chi$, $\chi'$ by the cosines)

$$\nu \cdot \bar{E}_k = E'_k \cos^k \epsilon' - E_k \cos^k \epsilon + R_k, \tag{44}$$

where in $R_k$ all wavefront derivatives are expressed in terms of local aberrations.

### 7. Generalization of the Coddington Equation

Although application of Eq. (34) or Eq. (36) provides a solution for $w_{\mathrm{S}}^{(k)}(0)$ up to arbitrary order $k$, it is very instructive to analyze the solutions more closely for one special case. We observe that the expressions in Eqs. (41) and (42) for $R_3$ (or $R_4$) will vanish if we set $w_{\mathrm{In}}^{(j)}=0$ and $w_{\mathrm{Out}}'^{(j)}=0$ for all lower orders $j<k$ (for $k=3$ or $k=4$, respectively). This leads to the assumption that the following statement is generally true: if aberrations only for one single given order $k$ are present while for all lower orders $j<k$ we have $w_{\mathrm{In}}^{(j)}=0$ and $w_{\mathrm{Out}}'^{(j)}=0$, then $R_k=0$, which means for fixed order $k$ that Eq. (40) will be valid for vanishing remainder term. This assumption can in fact be shown to hold generally.

For this purpose, we start from the recursion scheme in Eq. (36) and show that only the term containing $\mathbf{p}^{(1)}$ can contribute to the sum if all aberrations vanish for order less than $k$. To do so, it is necessary to exploit two basic properties of the derivatives $\mathbf{A}^{(m)} = (d^m/d\bar{y}_{\mathrm{S}}^m)\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))|_{\bar{y}_{\mathrm{S}}=0}$ of the matrix $\mathbf{A}$ for the orders $1 \leqslant m \leqslant k-1$. As can be shown by elementwise differentiation of the matrix $\mathbf{A}$, the highest wavefront derivatives present in $\mathbf{A}^{(m)}(\mathbf{p}(\bar{y}_{\mathrm{S}}))$ [see Eq. (30)] occur in the terms proportional to $\tau$, and those are proportional to either $w_{\mathrm{In}}^{(m+2)}$ or $w_{\mathrm{Out}}'^{(m+2)}$. Evaluating $\mathbf{A}^{(m)}(\mathbf{p}(\bar{y}_{\mathrm{S}}))$ at the position $\bar{y}_{\mathrm{S}}=0$ implies $\tau=0$, such that $\mathbf{A}^{(m)}$ cannot contain any higher wavefront derivatives than $w_{\mathrm{In}}^{(m+1)}$ or $w_{\mathrm{Out}}'^{(m+1)}$. It follows that

(i) The highest possible wavefront derivatives present in $\mathbf{A}^{(m)}$ are $w_{\mathrm{In}}^{(m+1)}$ or $w_{\mathrm{Out}}'^{(m+1)}$.

(ii) If all wavefront derivatives even up to order $(m+1)$ vanish, then $\mathbf{A}^{(m)}$ itself will vanish. This is in contrast to $\mathbf{A}$ itself, which contains constants and therefore will be finite even if all wavefront derivatives vanish.

Analyzing the terms in Eq. (36), we notice that the occurring derivatives of the matrix $\mathbf{A}$ are

$\mathbf{A}^{(k-1)},\mathbf{A}^{(k-2)},\ldots,\mathbf{A}^{(2)},\mathbf{A}^{(1)}$ for $j=1,2,\ldots,(k-1)$, respectively. It follows from property (i) that the highest occurring wavefront derivatives in these terms are $k,(k-1),\ldots,3,2$, respectively. Now, if all wavefront derivatives up to order $(k-1)$ vanish, it will follow from property (ii) that all the matrix derivatives $\mathbf{A}^{(k-2)},\ldots,\mathbf{A}^{(2)},\mathbf{A}^{(1)}$ must vanish, leaving only $\mathbf{A}^{(k-1)}$. Therefore all terms in Eq. (36) vanish, excluding only the contribution for $j=1$. We directly conclude that

$$\mathbf{p}^{(k)} = -\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{p}^{(1)} = -(\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{A}^{-1})\cdot\mathbf{b} \quad k \geq 2. \tag{45}$$

To evaluate $\mathbf{A}^{(k-1)}$ we set $k-1=:m$, and it is straightforward to show by induction that if all aberrations vanish for order less than or equal to $m$, then

$$\mathbf{A}^{(m)} = \begin{pmatrix} -m\chi^{m-1}\sigma w_{\mathrm{In}}^{(m+1)} & 0 & \dfrac{\chi^m}{n} w_{\mathrm{In}}^{(m+1)} & 0 \\ \chi^m w_{\mathrm{In}}^{(m+1)} & 0 & 0 & 0 \\ 0 & -m\chi'^{m-1}\sigma' w_{\mathrm{Out}}'^{(m+1)} & \dfrac{\chi'^m}{n'} w_{\mathrm{In}}^{(m+1)} & 0 \\ 0 & \chi'^m w_{\mathrm{In}}^{(m+1)} & 0 & 0 \end{pmatrix} \tag{46}$$

where $y_{\mathrm{In}}^{(1)}$, $y_{\mathrm{Out}}'^{(1)}$, and $\tau^{(1)}$ have been replaced by their solutions $\chi$, $\chi'$, and $ns$, respectively, wherever they occur [see Eq. (38)]. Inserting $\mathbf{A}^{(m)}(0)$ for $m=k-1$ and $\mathbf{A}(0)^{-1}$ from Eq. (37) into Eq. (45) yields directly that

$$\eta\cdot\bar{s}^{(k)}(0) = \chi'^k n' w_{\mathrm{Out}}'^{(k)}(0) - \chi^k n w_{\mathrm{In}}^{(k)}(0) \tag{47}$$

for all orders $k \geq 2$.

The resulting refraction equation in the situation of Eq. (47) in terms of local aberrations reads

$$\nu\cdot\bar{E}_k = E'_k \cos^k \epsilon' - E_k \cos^k \epsilon, \tag{48}$$

which is indeed Eq. (44) for $R_k=0$.

### C. Mathematical Approach in the 3D Case

#### 1. Wavefronts and Normal Vectors

Although more lengthy to demonstrate than the 2D case, conceptually the 3D case can be treated analogously to the 2D case. Therefore, we will report only the most important differences. Analogously to Eq. (17), the incoming wavefront is now represented by the 3D vector

$$\mathbf{w}_{\mathrm{In}}(x,y) = \begin{pmatrix} x \\ y \\ w_{\mathrm{In}}(x,y) \end{pmatrix}, \tag{49}$$

where $w_{\mathrm{In}}(x,y)$ is given by Eq. (6), and the relation between the coefficients and the derivatives is now given by a relation like Eq. (5). The connection between coefficients and local aberrations is now given by $\mathbf{e}_2=(S_{xx},S_{xy},S_{yy})^T = n(a_{\mathrm{In},2,0},a_{\mathrm{In},1,1},a_{\mathrm{In},0,2})^T$, $\mathbf{e}_3=(E_{xxx},E_{xxy},E_{xyy},E_{yyy})^T = n(a_{\mathrm{In},3,0},a_{\mathrm{In},2,1},a_{\mathrm{In},1,2},a_{\mathrm{In},0,3})^T$, etc. [see Eq. (14) for $\mathbf{e}_k$]. The outgoing wavefront and the refractive surface are treated similarly.

To treat the normal vectors, we introduce the functions analogous to Eq. (22) as

$$\mathbf{n}(u,v) := \frac{1}{\sqrt{1+u^2+v^2}}\begin{pmatrix} -u \\ -v \\ 1 \end{pmatrix}, \tag{50}$$

such that the normal vector to a surface $\mathbf{w}(x,y) := (x,y,w(x,y))^T$ is given by

$$\frac{\mathbf{w}^{(1,0)}\times\mathbf{w}^{(0,1)}}{|\mathbf{w}^{(1,0)}\times\mathbf{w}^{(0,1)}|} = \frac{1}{\sqrt{1+w^{(1,0)^2}+w^{(0,1)^2}}}\begin{pmatrix} -w^{(1,0)} \\ -w^{(0,1)} \\ 1 \end{pmatrix} = \mathbf{n}(w^{(1,0)},w^{(0,1)}) = \mathbf{n}(\nabla w).$$

In the intersection point, we now have $\mathbf{n}_{\mathrm{In}}(0,0) = (0,0,1)^T$, $\mathbf{n}'_{\mathrm{Out}}(0,0)=(0,0,1)^T$, $\bar{\mathbf{n}}_{\mathrm{S}}(0,0)=(0,0,1)^T$, and the derivatives corresponding to Eq. (23) can directly be obtained from Eq. (50).

#### 2. Ansatz for Determining the Refraction Equations

The starting point for establishing the relations between the wavefronts and the refractive surface is now given by equations analogous to Eq. (25), with the only difference that $x$ and $y$ components are simultaneously present and that the original 3D rotation matrix from Eq. (2) has to be used.

The vector of unknown functions is now given by

$$\mathbf{p}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) = \begin{pmatrix} x_{\mathrm{In}}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \\ y_{\mathrm{In}}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \\ x'_{\mathrm{Out}}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \\ y'_{\mathrm{Out}}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \\ \tau(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \\ \bar{s}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) \end{pmatrix}, \tag{51}$$

and the 3D analog to Eq. (25) now leads to

$$\mathbf{f}(\mathbf{p}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}),\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) = \mathbf{0}, \tag{52}$$

where $\mathbf{f}$ is the 3D analog to Eq. (27).

One important difference from the 2D case is that there are two arguments with respect to which derivatives have to be taken. This implies that the dimension of the linear problems to solve grows with increasing order: while there are only 6 different unknown functions, the first-order problem possesses already 12 unknown first-order derivatives, then there are 18 second-order derivatives, etc.

Another implication of the existence of two independent variables is that from the very beginning there are two different first-order equations,

$$\mathbf{A}(\mathbf{p}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}))\mathbf{p}^{(1,0)}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) = \mathbf{b}_x,$$

$$\mathbf{A}(\mathbf{p}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}))\mathbf{p}^{(0,1)}(\bar{x}_{\mathrm{S}},\bar{y}_{\mathrm{S}}) = \mathbf{b}_y, \tag{53}$$

where the different inhomogeneities are given as column vectors:

$$\mathbf{b}_x = -\frac{\partial \mathbf{f}}{\partial \bar{x}_S} = (1 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)^T,$$

$$\mathbf{b}_y = -\frac{\partial \mathbf{f}}{\partial \bar{y}_S} = (0 \quad \chi \quad \sigma \quad 0 \quad \chi' \quad \sigma')^T. \tag{54}$$

The structure of $\mathbf{b}_x$ arises because there is no respective tilt in this coordinate direction between the wavefronts and the refractive surface.

The Jacobian matrix $\mathbf{A}(\mathbf{p}(\bar{x}_S,\bar{y}_S))$ with elements $A_{ij} \coloneqq \partial f_i/\partial p_j$ is the same for both equations and is analogous to Eq. (30) but now of size $6 \times 6$. It is practical to provide it in block structure notation,

$$\mathbf{A}(\mathbf{p}(\bar{x}_S,\bar{y}_S)) = \left(\begin{matrix} \mathbf{A}_{\text{In}} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}'_{\text{Out}} \end{matrix} \middle| \begin{matrix} \mathbf{A}_\tau & \bar{\mathbf{A}}_S \end{matrix}\right), \tag{55}$$

where $\mathbf{0}$ is a $3 \times 2$ block with entry zero,

$$\mathbf{A}_{\text{In}} = \begin{pmatrix} 1 - \frac{\tau}{n}(n_{\text{In},x}^{(0,1)} w_{\text{In}}^{(1,1)} + n_{\text{In},x}^{(1,0)} w_{\text{In}}^{(2,0)}) & -\frac{\tau}{n}(n_{\text{In},z}^{(0,1)} w_{\text{In}}^{(0,2)} + n_{\text{In},z}^{(1,0)} w_{\text{In}}^{(1,1)}) \\ -\frac{\tau}{n}(n_{\text{In},y}^{(0,1)} w_{\text{In}}^{(1,1)} + n_{\text{In},y}^{(1,0)} w_{\text{In}}^{(2,0)}) & 1 - \frac{\tau}{n}(n_{\text{In},y}^{(0,1)} w_{\text{In}}^{(0,2)} + n_{\text{In},y}^{(1,0)} w_{\text{In}}^{(1,1)}) \\ w_{\text{In}}^{(1,0)} - \frac{\tau}{n}(n_{\text{In},z}^{(0,1)} w_{\text{In}}^{(1,1)} + n_{\text{In},z}^{(1,0)} w_{\text{In}}^{(2,0)}) & w_{\text{In}}^{(0,1)} - \frac{\tau}{n}(n_{\text{In},z}^{(0,1)} w_{\text{In}}^{(0,2)} + n_{\text{In},z}^{(1,0)} w_{\text{In}}^{(1,1)}) \end{pmatrix}, \tag{56}$$

and a similar block expression for $\mathbf{A}'_{\text{Out}}$. The other two blocks are given as column vectors:

$$\mathbf{A}_\tau = \begin{pmatrix} n_{\text{In},x}/n \\ n_{\text{In},y}/n \\ n_{\text{In},z}/n \\ n'_{\text{Out},x}/n' \\ n'_{\text{Out},y}/n' \\ n'_{\text{Out},z}/n' \end{pmatrix}, \qquad \bar{\mathbf{A}}_S = \begin{pmatrix} 0 \\ \sigma \\ -\chi \\ 0 \\ \sigma' \\ -\chi' \end{pmatrix}. \tag{57}$$

*3. Solutions for the General Refraction Equations*

The direct solutions analogous to Eq. (34) are now given by

$$\mathbf{p}^{(1,0)}(0,0) = \mathbf{A}^{-1}\mathbf{b}_x,$$

$$\mathbf{p}^{(0,1)}(0,0) = \mathbf{A}^{-1}\mathbf{b}_y,$$

$$\mathbf{p}^{(2,0)}(0,0) = (\mathbf{A}^{-1})^{(1,0)}|\mathbf{b}_x,$$

$$\mathbf{p}^{(1,1)}(0,0) = (\mathbf{A}^{-1})^{(0,1)}\mathbf{b}_x = (\mathbf{A}^{-1})^{(1,0)}|\mathbf{b}_y,$$

$$\mathbf{p}^{(0,2)}(0,0) = (\mathbf{A}^{-1})^{(0,1)}\mathbf{b}_y,$$

$$\ldots$$

$$\mathbf{p}^{(k_x,k_y)}(0,0) = \begin{cases} (\mathbf{A}^{-1})^{(k_x-1,0)}\mathbf{b}_x, & k_x \neq 0, k_y = 0, \\ (\mathbf{A}^{-1})^{(k_x-1,k_y)}\mathbf{b}_x = (\mathbf{A}^{-1})^{(k_x,k_y-1)}\mathbf{b}_y, & k_x \neq 0, k_y \neq 0, \\ (\mathbf{A}^{-1})^{(0,k_y-1)}\mathbf{b}_y, & k_x = 0, k_y \neq 0, \end{cases} \tag{58}$$

where

$$\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0,0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}, \quad \text{and}$$

$$(\mathbf{A}^{-1})^{(1,0)} = \left.\frac{d}{d\bar{x}_S}\mathbf{A}(\mathbf{p}(\bar{x}_S,\bar{y}_S))^{-1}\right|_{\bar{x}_S=0,\bar{y}_S=0},$$

$$(\mathbf{A}^{-1})^{(k_x,k_y)} = \left.\frac{d^{k_x}}{d\bar{x}_S^{k_x}}\frac{d^{k_y}}{d\bar{x}_S^{k_y}}\mathbf{A}(\mathbf{p}(\bar{x}_S,\bar{y}_S))^{-1}\right|_{\bar{x}_S=0,\bar{y}_S=0},$$

etc. The fact that there are two starting equations (53) reflects itself in the existence of two formally different solutions for the mixed derivatives, e.g., $\mathbf{p}^{(1,1)}$. However, since both starting equations originate from one common function $\mathbf{f}$ in Eq. (52), for each $\mathbf{p}^{(k_x,k_y)}$ the two solutions must essentially be identical, as can also be verified, e.g., for $\mathbf{p}^{(1,1)}$ directly by some algebra.

In analogy to Eqs. (37) and (38) for the 2D case, we provide here the explicit results,

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \sigma \\ 0 & 0 & 0 & 0 & -1/n & -\chi \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \sigma' \\ 0 & 0 & 0 & 0 & -1/n' & -\chi' \end{pmatrix} \Rightarrow$$

$$\mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -n\sigma/\eta & 0 & 0 & n'\sigma/\eta \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -n\sigma'/\eta & 0 & 1 & n'\sigma'/\eta \\ 0 & 0 & -nn'\chi'/\eta & 0 & 0 & nn'\chi/\eta \\ 0 & 0 & n/\eta & 0 & 0 & -n'/\eta \end{pmatrix}, \tag{59}$$

and, after application of Eqs. (54) and (58) the solutions

$$\mathbf{p}^{(1,0)}(0,0)=\begin{pmatrix}1\\0\\1\\0\\0\\0\end{pmatrix},\qquad \mathbf{p}^{(0,1)}(0,0)=\begin{pmatrix}0\\ \chi\\0\\ \chi'\\ -n\sigma\\0\end{pmatrix}. \tag{60}$$

The general result for the refraction equation can be written in this way:

$$\eta\bar{w}_{\mathrm{S}}^{(k_x,k_y)}=\chi'^{k_y}n'w'^{(k_x,k_y)}_{\mathrm{Out}}-\chi^{k_y}nw^{(k_x,k_y)}_{\mathrm{In}}+R_{k_x,k_y}. \tag{61}$$

It is interesting to note that only $k_y$ but not $k_x$ occurs in the exponents of the cosines. This is a consequence of the fact that the refraction takes place in the $y-z$ plane, whereas in the $x$ direction no tilting cosines occur at all. Summarizing all components of Eq. (61) for a fixed value of $k=k_x+k_y$ and applying Eqs. (5), (15), and (14) yields the refraction equation in terms of local aberrations,

$$\nu\cdot\bar{\mathbf{e}}_k=\mathbf{C}'_k\mathbf{e}'_k-\mathbf{C}_k\mathbf{e}_k+\mathbf{r}_k, \tag{62}$$

where $\mathbf{r}_k$ is a vector collecting the remainder terms $R_{k_x,k_y}$ in Eq. (61) analogously to $R_k$ in Eq. (44). Equation (62) is the general refraction equation for aberrations of any order in the 3D case.

### 4. Generalization of the Coddington Equation

Although Eq. (58) represents the full solution, we provide here a more detailed result for $\mathbf{p}^{(k_x,k_y)}(0,0)$ in the case of vanishing wavefront derivatives $w_{\mathrm{In}}^{(j_x,j_y)}$, $w'^{(j_x,j_y)}_{\mathrm{Out}}$ for all lower orders, i.e., for $j_x+j_y<k_x+k_y$. This works analogously to the treatment of Eqs. (35)–(47), with the only difference that the notation requires more effort.

Analogously to Eq. (36) we obtain the result that

$$\mathbf{p}^{(k_x,0)}(0,0)=-\mathbf{A}^{-1}\sum_{j_x=1}^{k_x-1}\binom{k_x-1}{j_x-1}\mathbf{A}^{(k_x-j_x,0)}\mathbf{p}^{(j_x,0)},\qquad k_x\geqslant 2,\quad k_y=0, \tag{63a}$$

$$\mathbf{p}^{(k_x,k_y)}(0,0)=-\mathbf{A}^{-1}\sum_{\substack{j_x\geqslant1,j_y\geqslant0\\ j_x+j_y<k_x+k_y}}\binom{k_x-1}{j_x-1}\binom{k_y}{j_y}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)} \tag{63b}$$

$$=-\mathbf{A}^{-1}\sum_{\substack{j_x\geqslant0,j_y\geqslant1\\ j_x+j_y<k_x+k_y}}\binom{k_x}{j_x}\binom{k_y-1}{j_y-1}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)},\qquad k_x\neq 0,\quad k_y\neq 0, \tag{63c}$$

$$\mathbf{p}^{(0,k_y)}(0,0)=-\mathbf{A}^{-1}\sum_{j_y=1}^{k_y-1}\binom{k_y-1}{j_y-1}\mathbf{A}^{(0,k_y-j_y)}\mathbf{p}^{(0,j_y)},\qquad k_x=0,\quad k_y\geqslant 2, \tag{63d}$$

where again for $\mathbf{p}^{(k_x,k_y)}$ two formally different solutions occur that are essentially identical. We recognize that Eq. (63a) is a special case of Eq. (63b) for $k_y=0$, $j_y=0$, and similarly Eq. (63d) is a special case of Eq. (63c) for $k_x=0$, $j_x=0$. By means of a reasoning similar to that in the 2D case, it is found that if all lower-order aberrations for $j_x+j_y<k_x+k_y$ vanish, then Eqs. (63) will reduce to the lowest term, yielding

$$\mathbf{p}^{(k_x,0)}(0,0)=-\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,0)}\mathbf{p}^{(1,0)},\qquad k_x\geqslant 2,\quad k_y=0, \tag{64a}$$

$$\mathbf{p}^{(k_x,k_y)}(0,0)=-\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,k_y)}\mathbf{p}^{(1,0)}=-\mathbf{A}^{-1}\mathbf{A}^{(k_x,k_y-1)}\mathbf{p}^{(0,1)},\qquad k_x\neq 0,\quad k_y\neq 0, \tag{64b}$$

$$\mathbf{p}^{(0,k_y)}(0,0)=-\mathbf{A}^{-1}\mathbf{A}^{(0,k_y-1)}\mathbf{p}^{(0,1)},\qquad k_x=0,\quad k_y\geqslant 2. \tag{64c}$$

To finally evaluate Eqs. (63), we need the partial derivatives of the matrix $\mathbf{A}$ under the assumption that all lower-order aberrations for $j_x+j_y<k_x+k_y$ vanish, which are given as

$$\mathbf{A}^{(m_x,m_y)}=\left(\begin{array}{cc|cc}\mathbf{A}_{\mathrm{In}}^{(m_x,m_y)} & \mathbf{0} & \mathbf{A}_{\tau}^{(m_x,m_y)} & \bar{\mathbf{A}}_{\mathrm{S}}^{(m_x,m_y)}\\ \mathbf{0} & \mathbf{A}'^{(m_x,m_y)}_{\mathrm{Out}} & & \end{array}\right) \tag{65}$$

with the block

$$\mathbf{A}_{\mathrm{In}}^{(m_x,m_y)}=\begin{pmatrix}-m_y\chi^{m_y-1}\sigma w_{\mathrm{In}}^{(m_x+2,m_y-1)} & -m_y\chi^{m_y-1}\sigma w_{\mathrm{In}}^{(m_x+1,m_y)}\\ -m_y\chi^{m_y-1}\sigma w_{\mathrm{In}}^{(m_x+1,m_y)} & -m_y\chi^{m_y-1}\sigma w_{\mathrm{In}}^{(m_x,m_y+1)}\\ \chi^{m_y}w_{\mathrm{In}}^{(m_x+1,m_y)} & \chi^{m_y}w_{\mathrm{In}}^{(m_x,m_y+1)}\end{pmatrix} \tag{66}$$

and a similar expression for the block $\mathbf{A}'^{(m_x,m_y)}_{\mathrm{Out}}$. The other two blocks are given as column vectors,

$$\mathbf{A}_{\tau}=\begin{pmatrix}\chi^{m_y}w_{\mathrm{In}}^{(m_x+1,m_y)}/n\\ \chi^{m_y}w_{\mathrm{In}}^{(m_x,m_y+1)}/n\\0\\ \chi'^{m_y}w'^{(m_x+1,m_y)}_{\mathrm{Out}}/n'\\ \chi'^{m_y}w'^{(m_x,m_y+1)}_{\mathrm{Out}}/n'\\0\end{pmatrix},\qquad \bar{\mathbf{A}}_{\mathrm{S}}=\mathbf{0}, \tag{67}$$

where $x_{\mathrm{In}}^{(1,0)}$, $x_{\mathrm{In}}^{(0,1)}$, $y_{\mathrm{In}}^{(1,0)}$, $y_{\mathrm{In}}^{(0,1)}$, etc., have been replaced by their solutions according to Eq. (60). Inserting $\mathbf{A}^{(m_x,m_y)}$ from Eqs. (65)–(67) and $\mathbf{A}(\mathbf{0})^{-1}$ from Eq. (59) into Eqs. (64) yields one common relation for $\bar{w}_{\mathrm{S}}^{(k_x,k_y)}$ for the various subcases in Eqs. (64) [omitting the argument (0,0)]:

$$\eta\bar{w}_{\mathrm{S}}^{(k_x,k_y)}=\chi'^{k_y}n'w'^{(k_x,k_y)}_{\mathrm{Out}}-\chi^{k_y}nw_{\mathrm{In}}^{(k_x,k_y)} \tag{68}$$

for all orders $k\geqslant 2$.

Equation (68) can be summarized similarly to Eq. (61) to a vector equation in the very appealing form

$$\nu\bar{\mathbf{e}}_k = \mathbf{C}'_k \mathbf{e}'_k - \mathbf{C}_k \mathbf{e}_k, \tag{69}$$

which is Eq. (62) for $\mathbf{r}_k = \mathbf{0}$. Equation (69), an interesting result of the present paper, is the refraction equation for aberrations of fixed order $k \geqslant 2$ under the assumption that all aberrations with order lower than $k$ vanish.

## 3. RESULTS AND DISCUSSION

One standard situation in optics is that a given wavefront hits a given refractive surface and that the outgoing wavefront is the unknown quantity. Therefore, we provide in the following the derived refraction equations, solved for the outgoing wavefront's aberration.

### A. 2D Case

Equation (48) describes the special case that for given order $k$ the aberrations of the incoming and the outgoing wavefront for all orders less than $k$ are zero ($E_j = 0$; $E'_j = 0$ for $j < k$). For calculation of the aberrations of the outgoing wavefront, Eq. (48) can be transformed to

$$E'_k \cos^k \epsilon' = E_k \cos^k \epsilon + \nu \cdot \bar{E}_k. \tag{70}$$

We could generally show this statement to hold for all orders $k \geqslant 2$ including as a special case for $k=2$ the well-known Coddington and vergence equations. Therefore Eq. (70) represents an interesting result of the present paper.

Also Eq. (44) for the general case can be transformed in such a way that $E'_k$ of the outgoing wavefront is the unknown quantity to be determined:

$$E'_k \cos^k \epsilon' = E_k \cos^k \epsilon + \nu \cdot \bar{E}_k - R_k. \tag{71}$$

Equation (71) is the general refraction equation for aberrations of any order in the 2D case. In $R_k$ only aberrations $E_j, E'_j$ of order $j < k$ occur. These aberrations can be determined by successively solving of Eq. (71) for lower orders.

For example, assume that the aberrations $E'_k$ of the outgoing wavefront up to order $k=3$ ($E'_2 \equiv S', E'_3$) are the unknown quantities and that the aberrations $E_k$ of the incoming wavefront and $\bar{E}_k$ of the refractive surface are given. In a first step the aberrations of order $k=2$ are calculated using Eq. (71), which is in this case identical to the well-known Coddington equation:

$$S' \cos^2 \epsilon' = S \cos^2 \epsilon + \frac{n' \cos \epsilon' - n \cos \epsilon}{n' - n} \cdot \bar{S}. \tag{72}$$

In a second step the aberrations of order $k=3$ are calculated using Eq. (71) and the results of Eq. (72),

$$E'_3 \cos^3 \epsilon' = E_3 \cos^3 \epsilon + \frac{n' \cos \epsilon' - n \cos \epsilon}{n' - n} \cdot \bar{E}_3 - R_3, \tag{73}$$

with

$$R_3 = -\frac{3n \sin \epsilon \cos \epsilon \cos \epsilon'}{n' \cos \epsilon' - n \cos \epsilon}\left(\frac{n}{n'}S' - \frac{n'}{n}S\right) \times \left(\frac{\cos \epsilon'}{n'}S' - \frac{\cos \epsilon}{n}S\right).$$

### B. 3D Case

Equivalently to the 2D case, transforming Eq. (69) leads to $\mathbf{C}'_k \mathbf{e}'_k = \mathbf{C}_k \mathbf{e}_k + \nu \bar{\mathbf{e}}_k$ for the case that $\mathbf{e}_j = \mathbf{0}; \mathbf{e}'_j = \mathbf{0}$ for $j < k$, a statement that we could generally show to hold for all orders $k \geqslant 2$, including the special case of the Coddington equation.

In the general case, Eq. (62) can as well be transformed in such a way that the unknown aberration vector $\mathbf{e}'_k$ of the outgoing wavefront is determined by the incoming wavefront and the refractive surface,

$$\mathbf{C}'_k \mathbf{e}'_k = \mathbf{C}_k \mathbf{e}_k + \nu \cdot \bar{\mathbf{e}}_k - \mathbf{r}_k, \tag{74}$$

where in $\mathbf{r}_k$, only aberrations of order $j < k$ occur. Therefore, $\mathbf{r}_k$ can be determined by successively solving Eq. (74) for lower orders. Equation (74) is the general refraction equation for aberrations of any order in the 3D case.

## 4. EXAMPLES AND APPLICATIONS

### A. Aspherical Surface Correction up to Sixth Order

One important application of the derived equations is that they allow us to determine a refractive surface, which not only has a defined power $\bar{S}$ but also generates an outgoing wavefront that shows no deviation from an ideal sphere up to the order $k=6$.

Because of the analytical nature of the equations it is not necessary to use an iterative numerical method. The task is to determine a rotationally symmetric aspherical surface $\bar{S}$, which images an axial object point with the distance $s$ to the refractive surface to an axial image point with the distance $s'$ to the refractive surface (Fig. 2).

The object-side vergence and the image-side vergence are given by $S = n/s$ and $S' = n'/s'$, respectively, expressed in terms of the reciprocals of the object and image distances. Treating the rotationally symmetric problem as a 2D problem in the $y$–$z$ plane, a sphere with radius $r$ is exactly described by

$$f(y) = r(1 - \sqrt{1 - y^2/r^2}), \tag{75}$$

whose series expansion up to the order $k=6$ is

$$f(y) = \frac{1}{2r}y^2 + \frac{1}{8r^3}y^4 + \frac{1}{16r^5}y^6 + \dots. \tag{76}$$

Applying Eq. (76) once on $f(y) = w_{\mathrm{In}}(y)$, $r = s$ and again on $f(y') = w'_{\mathrm{Out}}(y')$, $r = s'$ (including in both cases the sign of $s$ or $s'$) allows us to identify the wavefronts' coefficients in the sense of Eqs. (18)–(21):

$$a_{\mathrm{In},2} = \frac{1}{s} = \frac{S}{n}, \qquad a_{\mathrm{In},4} = 3\frac{1}{s^3} = 3\left(\frac{S}{n}\right)^3,$$

$$a_{\mathrm{In},6} = 45\frac{1}{s^5} = 45\left(\frac{S}{n}\right)^5,$$

$$a'_{\mathrm{Out},2}=\frac{1}{s'}=\frac{S'}{n'},\qquad a'_{\mathrm{Out},4}=3\frac{1}{s'^3}=3\left(\frac{S'}{n'}\right)^3,$$

$$a'_{\mathrm{Out},6}=45\frac{1}{s'^5}=45\left(\frac{S'}{n'}\right)^5. \tag{77}$$

The solution for the desired refractive surface, described by the series

$$\bar{s}(y)=\frac{\bar{a}_{\mathrm{S},2}}{2}y^2+\frac{\bar{a}_{\mathrm{S},4}}{24}y^4+\frac{\bar{a}_{\mathrm{S},6}}{720}y^6+\ldots \tag{78}$$

as in Eq. (20), will be found up to the order $k=6$ if we provide expressions for the three coefficients $\bar{a}_{\mathrm{S},2}$, $\bar{a}_{\mathrm{S},4}$, and $\bar{a}_{\mathrm{S},6}$ (the odd coefficients for $k=3,5,7,\ldots$ are not present because of the rotational symmetry of the problem).

Since the local aberrations of higher order have no influence on the local aberrations of lower order, the coefficient of second-order $\bar{a}_{\mathrm{S},2}$ can be directly determined by Eq. (39). In the present case of orthogonal incidence we exploit that $\sigma=\sigma'=0$, $\chi=\chi'=1$, and $\eta=n'-n$ such that Eq. (39) reads as $(n'-n)\bar{a}_{S,2}=n'a'_{\mathrm{Out},2}-na_{\mathrm{In},2}$ [equivalent to the vergence equation $\bar{S}=S'-S$ in Eq. (8)], yielding

$$\bar{a}_{\mathrm{S},2}=\frac{S'-S}{n'-n}. \tag{79}$$

To find $\bar{a}_{\mathrm{S},4}$, we have to apply Eqs. (40)–(43). Due to the orthogonal incidence, Eq. (43) simplifies to

$$\alpha=0,\qquad \beta=0,\qquad \gamma=\frac{6nn'}{n'-n},\qquad \delta=-\frac{6nn'}{n'-n}, \tag{80}$$

and consequently Eq. (42) simplifies to

$$R_4=\frac{6nn'}{n'-n}(w'^{(2)}_{\mathrm{Out}}-w^{(2)}_{\mathrm{In}})^2(w'^{(2)}_{\mathrm{Out}}+w^{(2)}_{\mathrm{In}}). \tag{81}$$

Inserting Eq. (81) into Eq. (40) and replacing $w^{(2)}_{\mathrm{In}}, w'^{(2)}_{\mathrm{Out}}$ by the coefficients in Eq. (77) yields

$$\begin{aligned}\bar{a}_{\mathrm{S},4}=\bar{w}^{(4)}_{\mathrm{S}}&=\frac{1}{n'-n}(n'w'^{(4)}_{\mathrm{Out}}-nw^{(4)}_{\mathrm{In}}+R_4)=\frac{1}{n'-n}\Bigg(n'a'_{\mathrm{Out},4}\\&\quad-na_{\mathrm{In},4}+\frac{6nn'}{n'-n}(a'_{\mathrm{Out},2}-a_{\mathrm{In},2})^2(a'_{\mathrm{Out},2}+a_{\mathrm{In},2})\Bigg)\\&=\frac{3}{(n'-n)^2}\Bigg(\frac{(n'+n)S^3}{n^2}-\frac{2S^2S'}{n}-\frac{2SS'^2}{n'}\\&\quad+\frac{(n'+n)S'^3}{n'^2}\Bigg).\end{aligned} \tag{82}$$

Similarly, we find that

$$\begin{aligned}\bar{a}_{\mathrm{S},6}=\bar{w}^{(6)}_{\mathrm{S}}=\frac{45}{(n'-n)^3}\Bigg(&-\frac{(n'+n)^2S^5}{n^4}+\frac{3(n'+n)S^4S'}{n^3}\\&-\frac{(n'-3n)S^3S'^2}{n^2n'}+\frac{(n'+n)S'^4}{n'^4}-\frac{3(n'+n)S'S'^4}{n'^3}\\&+\frac{(n-3n')S^2S'^3}{nn'^2}\Bigg).\end{aligned} \tag{83}$$

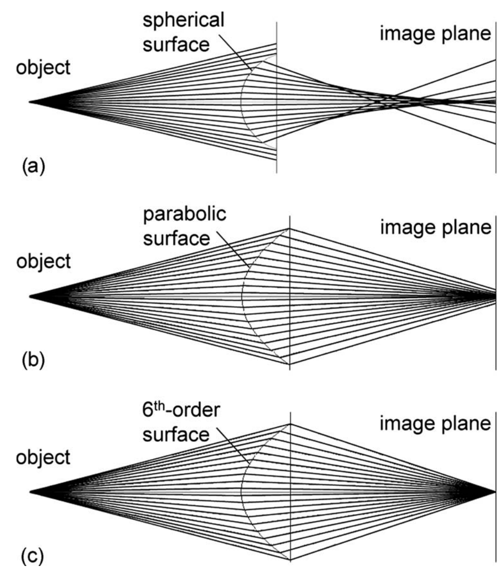


Fig. 3. Ray-tracing plots for example A generated by ZEMAX. (a) Spherical surface with radius $r=1/\bar{a}_{\mathrm{S},2}$. (b) Parabolic surface with local curvature $\bar{a}_{\mathrm{S},2}$. (c) Strongly reduced aberrations due to aspherical surface of sixth order with coefficients $\bar{a}_{\mathrm{S},2}$, $\bar{a}_{\mathrm{S},4}$, and $\bar{a}_{\mathrm{S},6}$. The vertical lines in the middle of the drawings are construction lines of ZEMAX and have no relevance in our context.

Equations (82) and (83) complete the required solution [31]; i.e., the coefficients $\bar{a}_{\mathrm{S},2}$, $\bar{a}_{\mathrm{S},4}$, and $\bar{a}_{\mathrm{S},6}$ of the aspherical refractive surface are determined such that an object point with the vergence $S$ is imaged to a point with the vergence $S'$ without aberrations with order less or equal to $k=6$.

The results of Eqs. (79), (82), and (83) can be illustrated by a numerical example in which the refractive index of the first medium is $n=1$, that of the second medium is $n'=1.5168$, and the object and image distance are given by $s=-50.0$ mm and $s'=60.0$ mm, respectively. Equations (79), (82), and (83) then yield $\bar{a}_{\mathrm{S},2}=0.0876161\ \mathrm{mm}^{-1}$, $\bar{a}_{\mathrm{S},4}=-0.00006550\ \mathrm{mm}^{-3}$, $\bar{a}_{\mathrm{S},6}=0.00002147\ \mathrm{mm}^{-5}$. By means of a ray-tracing approach using the optical design package ZEMAX, we have generated layout plots showing rays corresponding to these values. As a comparison, we have first traced rays through a spherical surface with radius $r=1/\bar{a}_{\mathrm{S},2}=11.4134$ mm [see Fig. 3(a)]. Paraxially the imaging is perfect, but the peripheral rays introduce large errors. Next, we have considered a parabolic surface with the same paraxial curvature $\bar{a}_{\mathrm{S},2}$ [see Fig. 3(b)], but now we have chosen a stop with semi-diameter $r_{\mathrm{stop}}=16.0$ mm, which is considerably larger than the surface radius in Fig. 3(a). Again, the peripheral rays introduce large errors.

Although such a system has a very low $f$-number, it is now possible to reduce these errors dramatically by choosing a sixth-order asphere based on the locally determined values $\bar{a}_{\mathrm{S},2}$, $\bar{a}_{\mathrm{S},4}$, and $\bar{a}_{\mathrm{S},6}$. Figure 3(c) shows that the errors are reduced to a level that is no longer visible on the scale of the plot.

### B. A Spherical Incoming Wavefront Hits a Spherical Refractive Surface at Oblique Incidence

In this example we use the derived equations to determine the aberrations of the outgoing wavefront up to order $k=6$ and compare them with the results calculated with ZEMAX. Given are the spherical incoming wavefront with a vergence $S=10D$ and a spherical refractive surface with power $\bar{S}=20D$. The refractive index of the first medium is $n=1$, that of the second medium is $n'=1.5168$, and the angle of incidence is $\epsilon=40°$. Therefore, the vergence vector of the incoming wavefront and the power vector of the refractive surface have the appearances $\mathbf{s}^T=(S,0,S)$ and $\bar{\mathbf{s}}^T=(\bar{S},0,\bar{S})$, respectively.

The aberrations of second order of the outgoing wavefront are determined by Eq. (11) $\mathbf{C}'\mathbf{s}'=\mathbf{C}\mathbf{s}+\nu\bar{\mathbf{s}}$, yielding a vergence vector of the form $\mathbf{s}'^T=(S'_{xx},0,S'_{yy})$. Numerical values for $S'_{xx},S'_{yy}$ are given in Table 1.

The third-order error vectors $\mathbf{e}_3$ and $\bar{\mathbf{e}}_3$ are $\mathbf{0}$, because the incoming wavefront and the refractive surface are spherical. Then Eq. (74) simplifies to $\mathbf{C}'_3\mathbf{e}'_3=-\mathbf{r}_3$ (the vector $\mathbf{r}_3$ is shown in Appendix C as a function of the given vergence $S$ and the quantities $S'_{xx},S'_{yy}$ determined before). Numerical values for $\mathbf{e}'_3$ are given in Table 1.

The error vectors of fourth order of the spherical incoming wavefront and refractive surface have the appearances $\mathbf{e}_4{}^T=(3S^3,0,S^3,0,3S^3)$ and $\bar{\mathbf{e}}_4{}^T=(3\bar{S}^3,0,\bar{S}^3,0,3\bar{S}^3)$, respectively. Using Eq. (74) leads to the resulting error vector of fourth order whose values are again given in Table 1. The fifth- and sixth-order aberrations for the local wavefront aberrations are also numerically provided in Table 1.

**Table 1. Local Aberrations of the Outgoing Wavefront in Example B[a]**

| order | wavefront aberration (sagitta) | | wave aberration (OPD) | |
|---|---|---|---|---|
| | symbol | *value* × 1000 | symbol | *value* × 1000 |
| $k=2$ | $S'_{xx}$ | 8.226176 $mm^{-1}$ | $S'^{OPD}_{xx}$ | 8.226176 $mm^{-1}$ |
| | $S'_{xy}$ | 0 | $S'^{OPD}_{xy}$ | 0 |
| | $S'_{yy}$ | 17.221464 $mm^{-1}$ | $S'^{OPD}_{yy}$ | 17.221464 $mm^{-1}$ |
| $k=3$ | $E'_{xxx}$ | 0 | $E'^{OPD}_{xxx}$ | 0 |
| | $E'_{xxy}$ | 0.681892 $mm^{-2}$ | $E'^{OPD}_{xxy}$ | 0.681892 $mm^{-2}$ |
| | $E'_{xyy}$ | 0 | $E'^{OPD}_{xyy}$ | 0 |
| | $E'_{yyy}$ | 2.076540 $mm^{-2}$ | $E'^{OPD}_{yyy}$ | 2.076540 $mm^{-2}$ |
| $k=4$ | $E'_{xxxx}$ | 0.155799 $mm^{-3}$ | $E'^{OPD}_{xxxx}$ | 0.154347 $mm^{-3}$ |
| | $E'_{xxxy}$ | 0 | $E'^{OPD}_{xxxy}$ | 0 |
| | $E'_{xxyy}$ | 0.054537 $mm^{-3}$ | $E'^{OPD}_{xxyy}$ | 0.052970 $mm^{-3}$ |
| | $E'_{xyyy}$ | 0 | $E'^{OPD}_{xyyy}$ | 0 |
| | $E'_{yyyy}$ | 0.148661 $mm^{-3}$ | $E'^{OPD}_{yyyy}$ | 0.135341 $mm^{-3}$ |
| $k=5$ | $E'_{xxxxx}$ | 0 | $E'^{OPD}_{xxxxx}$ | 0 |
| | $E'_{xxxxy}$ | 0.000713 $mm^{-4}$ | $E'^{OPD}_{xxxxy}$ | 0.000010 $mm^{-4}$ |
| | $E'_{xxxyy}$ | 0 | $E'^{OPD}_{xxxyy}$ | 0 |
| | $E'_{xxyyy}$ | −0.000946 $mm^{-4}$ | $E'^{OPD}_{xxyyy}$ | −0.002170 $mm^{-4}$ |
| | $E'_{xyyyy}$ | 0 | $E'^{OPD}_{xyyyy}$ | 0 |
| | $E'_{yyyyy}$ | −0.013123 $mm^{-4}$ | $E'^{OPD}_{yyyyy}$ | −0.023830 $mm^{-4}$ |
| $k=6$ | $E'_{xxxxxx}$ | 0.000339 $mm^{-5}$ | $E'^{OPD}_{xxxxxx}$ | −0.000078 $mm^{-5}$ |
| | $E'_{xxxxxy}$ | 0 | $E'^{OPD}_{xxxxxy}$ | 0 |
| | $E'_{xxxxyy}$ | −0.000294 $mm^{-5}$ | $E'^{OPD}_{xxxxyy}$ | −0.000563 $mm^{-5}$ |
| | $E'_{xxxyyy}$ | 0 | $E'^{OPD}_{xxxyyy}$ | 0 |
| | $E'_{xxyyyy}$ | −0.000663 $mm^{-5}$ | $E'^{OPD}_{xxyyyy}$ | −0.001228 $mm^{-5}$ |
| | $E'_{xyyyyy}$ | 0 | $E'^{OPD}_{xyyyyy}$ | 0 |
| | $E'_{yyyyyy}$ | −0.004746 $mm^{-5}$ | $E'^{OPD}_{yyyyyy}$ | −0.009508 $mm^{-5}$ |

[a]Left column, values based on the wavefront sagitta; right column, OPD-based values.

As mentioned at the beginning of this paper, our whole treatment is based on the description of aberrations by their wavefront sagitta. For completeness, it is important also to provide aberration results in the OPD picture. In Appendix B, we provide relations between sagitta derivatives and OPD derivatives. Analogously to Eq. (14), we define OPD-based vectors of aberrations for the wavefronts by

$$\mathbf{e}_k^{\mathrm{OPD}}=\begin{pmatrix}E^{\mathrm{OPD}}_{x\ldots xx}\\E^{\mathrm{OPD}}_{x\ldots xy}\\\vdots\\E^{\mathrm{OPD}}_{y\ldots yy}\end{pmatrix}=\begin{pmatrix}\tau_{\mathrm{In}}^{(k,0)}\\\tau_{\mathrm{In}}^{(k-1,1)}\\\vdots\\\tau_{\mathrm{In}}^{(0,k)}\end{pmatrix},$$

$$\mathbf{e}_k'^{\mathrm{OPD}}=\begin{pmatrix}E'^{\mathrm{OPD}}_{x\ldots xx}\\E'^{\mathrm{OPD}}_{x\ldots xy}\\\vdots\\E'^{\mathrm{OPD}}_{y\ldots yy}\end{pmatrix}=\begin{pmatrix}\tau_{\mathrm{Out}}'^{(k,0)}\\\tau_{\mathrm{Out}}'^{(k-1,1)}\\\vdots\\\tau_{\mathrm{Out}}'^{(0,k)}\end{pmatrix}, \quad (84)$$

where $\tau_{\mathrm{In}}^{(k_x,k_y)},\tau_{\mathrm{Out}}'^{(k_x,k_y)}$ are in this context OPD derivatives of the incoming and the outgoing wavefront that play the role of the generically used symbol $\tau_w^{(k_x,k_y)}$ in Appendix B. The values of the aberrations $\mathbf{e}_k'^{\mathrm{OPD}}$ are listed in Table 1, too, together with their counterparts $\mathbf{e}'_k$. In accordance with Appendix B, $\mathbf{e}_k'^{\mathrm{OPD}}$ is equal to $\mathbf{e}'_k$ up to the order $k=3$. For $k=4$, the values of $\mathbf{e}_k'^{\mathrm{OPD}}$ and $\mathbf{e}'_k$ are slightly different, and for $k\geqslant 5$ the deviations between the two pictures are considerable. We remark that this is the reason that it was necessary to treat the relations between the different coordinates simultaneously with the wavefront derivatives from the very beginning [see Eqs. (26) and (51)]. This confirms that the vector of six unknowns in Eq. (51) does not introduce additional complexity to the problem, but it is rather the only consistent way to treat carefully the inherent complexity such that numbers like those in Table 1 are meaningful.

Apart from yielding exact values for the local derivatives, our method will also be suitable for computing Zernike coefficients over a full pupil size if local aberrations up to sufficiently high order are involved, as argued in Section 2. In Table 2, we provide the Zernike coefficients up to order $k=6$ for our example, assuming a pupil with semi-diameter $r_0=3.0$ mm. The coefficients have been computed using Eqs. (A2) and (A3) for the order $k=6$.

For comparison, we have also calculated the solution of the same problem with a ray-tracing approach using ZEMAX (see Fig. 4) followed by a Zernike analysis. Those values are provided in Table 2 as a reference. The agreement between the two results is obvious. We would like to stress again that our local aberration values are obtained by an analytical method and therefore by definition are

**Table 2. Zernike Coefficients of the Outgoing Wavefront in Example B[a]**

| order | Symbol (OSA standard) | Zernike coefficients (our method) value/μm | Zernike coefficients (ZEMAX) value/μm |
|---|---|---|---|
| $k=2$ | $c_2^{-2}$ | 0 | $-2.4\times10^{-8}$ |
| | $c_2^{0}$ | 16.672042 | 16.672048 |
| | $c_2^{2}$ | −8.251706 | −8.251718 |
| $k=3$ | $c_3^{-3}$ | −0.008734 | −0.008746 |
| | $c_3^{-1}$ | 1.092135 | 1.092042 |
| | $c_3^{1}$ | 0 | $-2.9\times10^{-8}$ |
| | $c_3^{3}$ | 0 | $-5.8\times10^{-9}$ |
| $k=4$ | $c_4^{-4}$ | 0 | $-2.4\times10^{-8}$ |
| | $c_4^{-2}$ | 0 | $-1.8\times10^{-8}$ |
| | $c_4^{0}$ | 0.036792 | 0.036794 |
| | $c_4^{2}$ | 0.003041 | 0.003034 |
| | $c_4^{4}$ | −0.003785 | −0.003780 |
| $k=5$ | $c_5^{-5}$ | −0.000060 | −0.000052 |
| | $c_5^{-3}$ | 0.000723 | 0.000719 |
| | $c_5^{-1}$ | −0.001026 | −0.001058 |
| | $c_5^{1}$ | 0 | $1.2\times10^{-8}$ |
| | $c_5^{3}$ | 0 | $1.2\times10^{-8}$ |
| | $c_5^{5}$ | 0 | $1.8\times10^{-8}$ |
| $k=6$ | $c_6^{-6}$ | 0 | $-1.2\times10^{-8}$ |
| | $c_6^{-4}$ | 0 | 0.000000 |
| | $c_6^{-2}$ | 0 | $1.2\times10^{-8}$ |
| | $c_6^{0}$ | 0.000089 | 0.000089 |
| | $c_6^{2}$ | 0.000085 | 0.000083 |
| | $c_6^{4}$ | 0.000005 | 0.000004 |
| | $c_6^{6}$ | −0.000005 | −0.000005 |

[a]Left column, values based on our method; right column, values based on ray-tracing (ZEMAX).

exact. The transformation of our local coefficients to Zernike coefficients, on the other hand, yields only a (however, very good) approximation for their numerical values based on the assumption that the truncated subspaces of order $k=6$ describe the aberrations sufficiently well. But still, within this approximation, the results are analytical, such that a Zernike coefficient obtained as zero is exactly zero, whereas a ray-tracing value is always numerical in nature, resulting in small deviations from zero (Table 2).

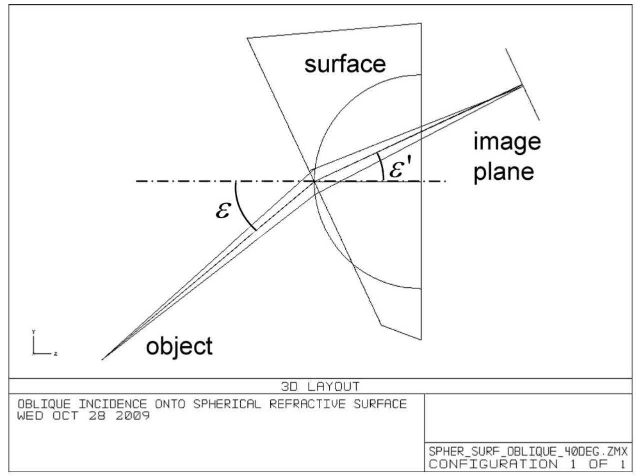


Fig. 4. Ray-tracing plot for example B generated by ZEMAX. A spherical wavefront is refracted by a spherical surface under oblique incidence, giving rise to coma in the outgoing wavefront. The box drawn around the refractive object consists of construction lines of ZEMAX and has no relevance in our context.

## 5. SUMMARY

In the present work we have developed a general method for generating refraction equations for local wavefront aberrations of any order under arbitrarily oblique incidence conditions. These results include as a special case the well-known scalar vergence equation as well as the Coddington equation (order $k=2$) but extend these refraction equations to aberrations of any arbitrary higher order $k>2$.

The refraction equations are relations between an incoming wavefront, a refractive surface, and an outgoing wavefront. In detail, we have defined local aberrations of those three surfaces in terms of local power series coefficients, which describe the surfaces in local coordinate systems aligned with the chief rays or the surface normal. The general refraction equations are established as a sequence of analytical relations between these series coefficients. We have been able to show that to each given order $k\geqslant 2$ it is possible to assign one equation taken from that sequence whose leading-order terms represent a straightforward generalization of the Coddington equation to the order $k$ and which in general contains some additional terms whose order is always less than $k$. A direct consequence is that if aberrations of only one single order $k$ are present, then the generalization of the Coddington equation will be exact for that order $k$; it reads $E'_k \cos^k \epsilon' = E_k \cos^k \epsilon + \nu\cdot\bar{E}_k$ for the 2D problem, and the vector-valued version of it reads $\mathbf{C'}_k\mathbf{e'}_k=\mathbf{C}_k\mathbf{e}_k+\nu\bar{\mathbf{e}}_k$ in the 3D case.

For convenience, we have distinguished between the 2D and the 3D problem in deriving the refraction equations. While the part representing the generalization of the Coddington equation can in either dimension be expressed symbolically as a function of the order $k$, the additional terms of order less than $k$ must be derived in a recursive process for increasing orders $k=2,3,4,\ldots$. We have provided this procedure generally, and for the orders $k=3,4$ we have provided explicit formulas for the resulting terms in the 2D case. As an application of the refraction equations, it is possible to determine an unknown surface among the refractive surface and the two wavefronts up to an order $k$, provided that the two other surfaces are given up to the same order $k$. The standard situation is that an incoming wavefront and a refractive surface are given and that the outgoing wavefront is to be determined, as we have illustrated by an example. However, the reverse problem can likewise be treated. As we have shown explicitly in an example, if the incoming and the outgoing wavefront are both given without deviation from an ideal sphere up to the order $k=6$, our equations directly allow determination of the refractive surface necessary for this imagery.

The main advantage of our approach is that it is based exclusively on analytical formulas. This saves much computation time compared with numerical iteration routines that would otherwise be necessary for determining the higher-order aberrations.

With the method developed in this work, it is now possible to calculate the local higher-order aberrations of the outgoing wavefront directly in an analytical way from the aberrations of the incoming wavefront and the refractive surface. Although our method is based on local techniques, it yields results that are by no means restricted to small apertures, as we have shown theoretically as well as in two examples.

## APPENDIX A

The Zernike coefficients corresponding to a wavefront $w(x,y)$ are given by the integral

$$c_k^m = \frac{1}{\pi r_0^2}\int\int_{\text{pupil}} Z_k^m\left(\frac{x}{r_0},\frac{y}{r_0}\right) w(x,y)dxdy, \quad \text{(A1)}$$

where $r_0$ is the pupil size. If the wavefront is given as a series as in Eqs. (6) and (7), then the integral in Eq. (A1) will be itself a series, i.e., a linear combination of coefficients $a_{m,k-m}$. Summarizing up to given order $k$ the coefficients $c_k^m$ and $a_{m,k-m}$ as vectors, a transition matrix $\mathbf{T}(k)$ between the Zernike subspace and the Taylor series subspace of order $k$ can be defined by

$$\begin{pmatrix} c_0^0 \\ c_1^{-1} \\ c_1^1 \\ c_2^{-2} \\ c_2^0 \\ c_2^2 \\ c_3^{-3} \\ c_3^{-1} \\ \vdots \\ c_k^k \end{pmatrix} = \mathbf{T}(k)\begin{pmatrix} E \\ r_0E_x \\ r_0E_y \\ r_0^2E_{xx} \\ r_0^2E_{xy} \\ r_0^2E_{yy} \\ r_0^3E_{xxx} \\ r_0^3E_{xxy} \\ \vdots \\ r_0^kE_{yy\ldots y} \end{pmatrix} = n\mathbf{T}(k)\begin{pmatrix} a_{00} \\ r_0a_{10} \\ r_0a_{01} \\ r_0^2a_{20} \\ r_0^2a_{11} \\ r_0^2a_{02} \\ r_0^3a_{30} \\ r_0^3a_{21} \\ \vdots \\ r_0^ka_{0k} \end{pmatrix}. \quad \text{(A2)}$$

If representations of such a matrix are given in a form similar to that in the literature [2,32,33], the prefactors of the underlying power series in the literature will not be the same in detail as in our case. Therefore we provide an explicit expression for $\mathbf{T}^{-1}$ here for order $k=3$, given by

$$\mathbf{T}^{-1}(3) = \begin{pmatrix} 1 & 0 & 0 & 0 & -\sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & -4\sqrt{2} & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & -4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 4\sqrt{3} & -2\sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4\sqrt{3} & 2\sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -12\sqrt{2} & 36\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12\sqrt{2} & -12\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 12\sqrt{2} & 12\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36\sqrt{2} & 12\sqrt{2} \end{pmatrix}. \quad \text{(A3)}$$

## APPENDIX B

If a wavefront is given by its sagitta, then the OPD between the wavefront and a reference plane being tangential to the wavefront can determined from it, and vice versa. In particular, there exists a unique relation between the aberration coefficients in terms of the wavefront (by our definition the sagitta derivatives) and the aberration coefficients in terms of the aberration function (to be defined as the OPD derivatives). For simplicity, we establish this relation first in the 2D case. Formally, the situation can be imagined to be described by Fig. 1(c) for the special case that the refractive surface is a plane and the incidence is orthogonal. Applying to any wavefront in this context, we generically call the wavefront sagitta $w(y)$ instead of $w_{\text{In}}(y_{\text{In}})$, the coordinate in the tangential plane is $\bar{y}_{\text{t}}$ instead of $\bar{y}_{\text{S}}$, and the wavefront's OPD is $\tau_w(\bar{y}_{\text{t}})$ instead of $\tau(\bar{y}_{\text{S}})$ (see Fig. 5). The first equation of Eqs. (25) then takes the form

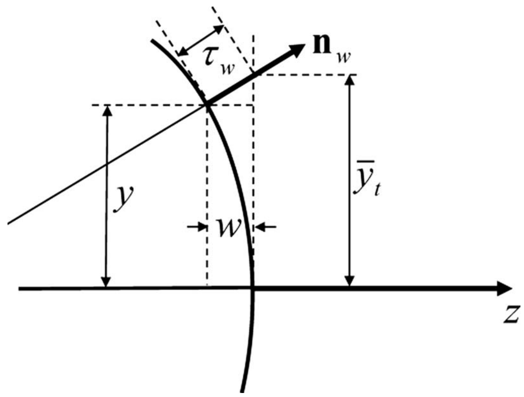


Fig. 5. Relationship between the sagitta $w(y)$ of a wavefront and its OPD given by the function $\tau_w(\bar{y})$.

$$\begin{pmatrix} y \\ w(y) \end{pmatrix} - \frac{\tau_w}{n}\mathbf{n}_w = \begin{pmatrix} \bar{y}_{\mathrm{t}} \\ 0 \end{pmatrix}. \tag{B1}$$

Our question is now posed such that $\tau_w(\bar{y}_{\mathrm{t}})$ is the unknown function of interest while $w(y)$ is given. In this case it is most practical to use $y$ as the independent variable, such that the functions $\bar{y}_{\mathrm{t}}(y)$ and consequently $\tau_w(\bar{y}_{\mathrm{t}}(y))$ enter into Eq. (B1). Inserting $\mathbf{n}_w(y) = (-w^{(1)}(y),1)^T/\sqrt{1+w^{(1)}(y)^2}$ [see Eq. (22)], the second row of Eq. (B1) can be solved for $\tau_w(\bar{y}_{\mathrm{t}}(y))$, yielding

$$\tau_w(\bar{y}_{\mathrm{t}}(y)) = nw(y)\sqrt{1+w^{(1)}(y)^2}. \tag{B2}$$

Then inserting Eq. (B2) into the first row of Eq. (B1) leads to

$$\bar{y}_{\mathrm{t}}(y) = y + w(y)w^{(1)}(y). \tag{B3}$$

To obtain a relationship between the derivatives $\tau_w^{(k)}(\bar{y}_{\mathrm{t}}) \equiv \partial^k \tau_w / \partial \bar{y}_{\mathrm{t}}^k$ and the derivatives $w^{(k)}(y)$, we insert Eq. (B3) into the argument of $\tau_w$ in Eq. (B2), yielding

$$\tau_w(y + w(y)w^{(1)}(y)) = nw(y)\sqrt{1+w^{(1)}(y)^2}. \tag{B4}$$

As is generally the key ingredient in this paper, we now take the subsequent derivatives of Eq. (B4) and evaluate at the position $y=0$. Making use of $w(0)=0$, $w^{(1)}(0)=0$, this leads to

$$\begin{gathered} \tau_w(0) = 0, \\ \tau_w^{(1)}(0) = 0, \\ \tau_w^{(2)}(0) = nw^{(2)}(0), \\ 3w^{(2)}(0)^2\tau_w^{(1)}(0) + \tau_w^{(3)}(0) = nw^{(3)}(0), \\ 10w^{(2)}(0)w^{(3)}(0)\tau_w^{(1)}(0) + 12w^{(2)}(0)^2\tau_w^{(2)}(0) + \tau_w^{(4)}(0) \\ = n(6w^{(2)}(0)^3 + w^{(4)}(0)), \\ \ldots, \end{gathered} \tag{B5}$$

which represents a system for determination of $\tau_w(0)$, $\tau_w^{(1)}(0), \tau_w^{(2)}(0), \tau_w^{(3)}(0), \ldots$. Inserting the result for $\tau_w^{(1)}(0)$ into the successive equations in Eq. (B5), then inserting the result for $\tau_w^{(2)}(0)$, and so on, yields the result [omitting the argument (0)]

$$\begin{gathered} \tau_w = 0, \\ \tau_w^{(1)} = 0, \\ \tau_w^{(2)} = nw^{(2)}, \\ \tau_w^{(3)} = nw^{(3)}, \\ \tau_w^{(4)} = n(w^{(4)} - 6w^{(2)^3}), \\ \tau_w^{(5)} = n(w^{(5)} - 40w^{(2)^2}w^{(3)}), \\ \ldots. \end{gathered} \tag{B6}$$

Equation (B6) shows that up to order $k=3$ the OPD measure of aberrations is, apart from the prefactor $n$, equal to the sagitta measure, but for orders $k \geqslant 4$, there occur more and more transformation terms.

In the 3D case the procedure is analogous, and the result reads

$$\begin{gathered} \tau_w = 0, \\ \begin{pmatrix} \tau_w^{(1,0)} \\ \tau_w^{(0,2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \\ \begin{pmatrix} \tau_w^{(2,0)} \\ \tau_w^{(1,1)} \\ \tau_w^{(0,2)} \end{pmatrix} = n\begin{pmatrix} w^{(2,0)} \\ w^{(1,1)} \\ w^{(0,2)} \end{pmatrix}, \\ \begin{pmatrix} \tau_w^{(3,0)} \\ \tau_w^{(2,1)} \\ \tau_w^{(1,2)} \\ \tau_w^{(0,3)} \end{pmatrix} = n\begin{pmatrix} w^{(3,0)} \\ w^{(2,1)} \\ w^{(1,2)} \\ w^{(0,3)} \end{pmatrix}, \\ \begin{pmatrix} \tau_w^{(4,0)} \\ \tau_w^{(3,1)} \\ \tau_w^{(2,2)} \\ \tau_w^{(1,3)} \\ \tau_w^{(0,4)} \end{pmatrix} = n\left(\begin{pmatrix} w^{(4,0)} \\ w^{(3,1)} \\ w^{(2,2)} \\ w^{(1,3)} \\ w^{(0,4)} \end{pmatrix} - \begin{pmatrix} 6w^{(2,0)}(w^{(1,1)^2} + w^{(2,0)^2}) \\ 3w^{(1,1)}(w^{(1,1)^2} + w^{(2,0)}(w^{(0,2)} + 2w^{(2,0)})) \\ (w^{(0,2)} + w^{(2,0)})(5w^{(1,1)^2} + w^{(0,2)}w^{(2,0)}) \\ 3w^{(1,1)}(w^{(1,1)^2} + w^{(0,2)}(2w^{(0,2)} + w^{(2,0)})) \\ 6w^{(0,2)}(w^{(1,1)^2} + w^{(0,2)^2}) \end{pmatrix}\right), \\ \ldots. \end{gathered} \tag{B7}$$

## APPENDIX C

The vector $\mathbf{r}_3$ is given by

$$\mathbf{r}_3 = \begin{pmatrix} 0 \\ -\dfrac{\sin \epsilon(n \cos \epsilon S'_{xx}(n^2 S'_{xx} - n'^2 S) + n' \cos \epsilon'(n' S^2 - n^2(S'^2_{xx} + SS'_{yy} - S'_{xx}S'_{yy})))}{nn'^2(n' \cos \epsilon' - n \cos \epsilon)} \\ 0 \\ -\dfrac{3 \cos \epsilon \cos \epsilon' \sin \epsilon(n' \cos \epsilon S - n \cos \epsilon' S'_{yy})(n'^2 S - n^2 S'_{yy})}{nn'^2(n' \cos \epsilon' - n \cos \epsilon)} \end{pmatrix}. \quad (C1)$$

## REFERENCES


1. M. Born and E. Wolf, “Foundations of geometrical optics, geometrical theory of optical imaging and geometrical theory of optical aberrations,” in *Principles of Optics* (Pergamon, 1980), pp. 109–232.
2. V. N. Mahajan, “Gaussian optics, optical aberrations and calculation of primary aberrations,” in V. Mahajan *Optical Imaging and Aberrations Part I: Ray Geometrical Optics* (SPIE, 1998), pp. 91–361.
3. R. Shannon, “Geometrical optics,” in *The Art and Science of Optical Design* (Cambridge Univ. Press, 1997), pp. 25–105.
4. K. P. Thompson, “Description of the third-order optical aberrations of near-circular pupil optical systems without symmetry,” J. Opt. Soc. Am. A **22**, 1389–1401 (2005).
5. K. P. Thompson, “Multinodal fifth-order optical aberrations of optical systems without rotational symmetry: spherical aberration,” J. Opt. Soc. Am. A **26**, 1090–1100 (2009).
6. K. P. Thompson, T. Schmid, O. Cakmakci, and J. P. Rolland, “Real-ray-based method for locating individual surface aberration field centers in imaging optical systems without rotational symmetry,” J. Opt. Soc. Am. A **26**, 1503–1517 (2009).
7. R. Krueger, R. Applegate, and S. MacRae, *Wavefront Customized Visual Correction* (Slack, 2004).
8. J. Porter, H. Quener, J. Lin, K. Thorn, and A. Awwal, *Adaptive Optics for Vision Science* (Wiley, 2006).
9. J. Porter, A. Guirao, I. Cox, and D. Williams, “Monochromatic aberrations of the human eye in a large population,” J. Opt. Soc. Am. A **18**, 1793–1803 (2001).
10. R. Applegate, “Glenn Fry Award Lecture 2002: Wavefront sensing, ideal corrections, and visual Performance,” Optom. Vision Sci. **81**, 137–177 (2004).
11. R. Blendowske, “Wieso funktionieren Gleitsichtgläser? Über Aberrationen in der Progressionszone,” Deutsche Optikerzeitung **2**, 60–64 (2007).
12. R. Blendowske, “Brillengläser und die Korrektion der Abbildungsfehler höherer Ordnung,” Deutsche Optikerzeitung **6**, 18–25 (2007).
13. W. Wesemann, “Korrektion der Aberrationen höherer Ordnung des Auges mit Brillengläsern—Möglichkeiten und Probleme,” Deutsche Optikerzeitung **9**, 44–49 (2007).
14. Rodenstock, “Spectacle lens with small higher order aberrations,” U.S. patent 7,063,421 B2, June 20, 2006.
15. Rodenstock, “Method for computing a progressive spectacle lens and methods for manufacturing a spectacle lens of this kind,” U.S. patent 6,832,834 B2, December 21, 2004.
16. Rodenstock, “Method for calculating an individual progressive lens,” U.S. patent application 2007/0132945 A1, June 14, 2007.
17. J. Landgrave and J. Moya-Cessa, “Generalized Coddington equations in ophthalmic lens design,” J. Opt. Soc. Am. A **13**, 1637–1644 (1996).
18. D. Burkhard and D. Shealy, “Simplified formula for the illuminance in an optical system,” Appl. Opt. **20**, 897–909 (1981).
19. O. Stavroudis, “Surfaces,” in O. Stavroudis, *The Optics of Rays, Wavefronts, and Caustics* (Academic, 1972), pp. 136–160.
20. W. Becken, A. Seidemann, H. Altheimer, G. Esser, and D. Uttenweiler, “Spectacle lenses in sports: optimization of the imaging properties based on physiological aspects,” Z. Med. Phys. **17**, 56–66 (2007).
21. E. Acosta and R. Blendowske, “Paraxial optics of astigmatic systems: relations between the wavefront and the ray picture approaches,” Optom. Vision Sci. **84**, 72–78 (2007).
22. W. Becken, H. Altheimer, G. Esser, W. Mueller, and D. Uttenweiler, “Wavefront method for computing the magnification matrix of optical systems: near objects in the paraxial case,” Optom. Vision Sci. **85**, 581–592 (2008).
23. W. Becken, H. Altheimer, G. Esser, W. Mueller, and D. Uttenweiler, “Wavefront method for computing the magnification matrix of optical systems: near objects in the general case of strongly oblique incidence,” Optom. Vision Sci. **85**, 593–604 (2008).
24. C. Campbell, “Generalized Coddington equations found via an operator method,” J. Opt. Soc. Am. A **23**, 1691–1698 (2006).
25. M. A. Golub, “Analogy between generalized Coddington equations and thin optical element approximation,” J. Opt. Soc. Am. A **26**, 1235–1239 (2009).
26. R. Dorsch, W. Haimerl, and G. Esser, “Accurate computation of mean power and astigmatism by means of Zernike polynomials,” J. Opt. Soc. Am. A **15**, 1686–1688 (1998).
27. E. Acosta and R. Blendowske, “Paraxial propagation of astigmatic wavefronts in optical systems by an augmented stepalong method for vergences,” Optom. Vision Sci. **82**, 923–932 (2005).
28. W. Harris, “Dioptric power: its nature and its representation in three- and four-dimensional space,” Optom. Vision Sci. **74**, 349–366 (1997).
29. W. Harris, “Power vectors versus power matrices, and the mathematical nature of dioptric power,” Optom. Vision Sci. **84**, 1060–1063 (2007).
30. L. Thibos, W. Wheeler, and D. Horner, “Power vectors: an application of Fourier analysis to the description and statistical analysis of refractive error,” Optom. Vision Sci. **74**, 367–375 (1997).
31. G. Esser, *Derivation of the Imaging Equations for the Calculation of the Higher Order Aberrations of a Local Wavefront after Refraction* (Hieronymus, 2008).
32. R. K. Tyson, “Conversion of Zernike aberration coefficients to Seidel and higher-order power-series aberration coefficients,” Opt. Lett. **7**, 262–264 (1982).
33. K. Dillon, “Bilinear wavefront transformation,” J. Opt. Soc. Am. A **26**, 1839–1846 (2009).