Derivation of analytical refraction, propagation and reflection equations for Higher Order Aberrations of wavefronts

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Abstract

Derivation of analytical refraction, propagation and reflection equations for Higher Order Aberrations of wavefronts

From literature the analytical calculation of Lower Order Aberrations (LOA) of a wavefront after refraction, propagation and reflection is well-known, it is for local Power and Astigmatism performed by the Coddington equation for refraction and reflection and the classical vertex correction formula for propagation. However, equivalent analytical equations for Higher Order aberrations (HOA) do not exist. Since HOA play an increasingly important role in many fields of optics, e.g. ophthalmic optics, it is the purpose of this study to extend the analytical Generalized Coddington Equation and the analytical Transfer Equation, which deals with second order aberration, to the case of HOA (e.g. Coma and Spherical Aberration). This is achieved by local power series expansions.

The purpose of this PhD was to extend the analytical Generalized Coddington Equation and the analytical Transfer Equation, which deals with Lower Order Aberrations (power and astigmatism), to the case of Higher Order Aberrations (e.g. Coma and Spherical Aberration).

In summary, with the novel results presented here, it is now possible to calculate analytically the aberrations of an outgoing wavefront directly from the aberrations of the incoming wavefront and the refractive or reflective surface and the aberrations of a propagated wavefront directly from the aberrations of the original wavefront containing both low-order and high-order aberrations.

Keywords: wavefront · Higher Order Aberration · Refraction Coddington Equation · Coma · spherical Aberration Propagation Reflection

Prologue

Aberrations play a decisive role in optics. They describe the deviation from the perfect image. Wavefront aberrations are usually described by a power series expansion or by Zernike polynomials [1,2 ,3]. The wavefront aberrations describe the differences in optical path length between the ideal and the actual wavefront. From literature the calculation of Lower Order Aberrations (LOA) as Power and Astigmatism of a local wavefront after refraction and reflection at a given surface is known. In the case of orthogonal incidence this relation is described by the “Vergence Equation [1,2,3], and in the case of oblique incidence by the “Coddington Equation” [3,4,5,6,7,8,9]. For Higher Order Aberrations (HOA) equivalent analytical equations do not exist.

An imagery will be said to be free from aberrations if every point of an object is imaged perfectly. Aberrations are deviations from this situation. A wavefront based description of these aberrations can either refer to the geometrical shape of the real *wavefronts* in space or by a *wave aberration function* which measures the optical path differences (OPD) between the real wavefronts and the reference sphere along the real occurring rays. 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. It is a very interesting subtopic to consider the aberration function for fixed image point and consequently as a function of the pupil coordinates only [2]. In this case, which is the focus of the present PhD study, the aberration function is often called a *wavefront aberration*.

The awareness of the role of Higher Order Aberrations (HOA) has significantly increased also in optometry and ophthalmology [10,11,12,13,15,16,17,18]. Hitherto for determining HOA, the wavefront in the pupil was calculated by ray-tracing [1,2,3,19,20,21,28,29,30] a precise method when a large number of rays are used. In the field of spectacle optics the use of local wavefronts (determined by their local derivatives) to calculate the Lower Order Aberrations (Power and Astigmatism) is well established [3,4,5,6,7,22,23]. Wavefront tracing is a very fast semi-analytical method because it is only necessary to calculate the chief ray by numerical ray tracing. The coefficients of the wavefront itself, determined by their local derivatives, are calculated analytically.

In terms of rays, the ideal image point serves as a reference point which any ray starting from the object point through the aperture has to hit. In terms of waves, the ideal image point serves as 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.

For calculating the wavefront aberrations of an entire lens, especially of a spectacle lens, it is necessary to propagate the wavefront from the intersection point of the chief ray at the front surface along the chief ray to the intersection point at the rear surface and further to the vertex sphere or the entrance pupil of the eye. Because the refracting plane (plane of incidence) at the front and rear surface are not congruent, it is also necessary to rotate the coefficients of the wavefront. For second order aberrations

(Power and Astigmatism) the propagation and rotation of the coefficients of the wavefront is known and described by the analytical Transfer equation [7,24].

In this context, **the purpose of this PhD was to extend the analytical Generalized Coddington Equation and the analytical Transfer Equation, which deals with second order aberration (power and astigmatism), to the case of Higher Order Aberrations (HOA)** (e.g. Coma and Spherical Aberration). Therefore, it is now possible for the first time to calculate analytically the wavefront Higher Order Aberrations of a spectacle lens or in general of an optical system by wavefront tracing. This new approach has significant advantages with respect to the state of the art methods. First, the analytical nature of the solution yields more detailed insight into the underlying optical process. Second, the dramatic reduction of computational time in comparison to numerical methods opens new possibilities for the solution of practical problems in optics. Although the method is based on local techniques, it yields results which are by no means restricted to small apertures, as it is been shown theoretically as well as in two examples as described in the J. Opt. Soc. Am. A “Derivation of the refraction equations for higher order aberrations of local wavefronts by oblique incidence” by Esser et al [25], in J. Opt. Soc. Am. A “Derivation of the propagation equations for higher order aberrations of local wavefronts” by Esser et al [26] and in Advances in Imaging and Electron Physics “Derivation of the reflection equations for higher order aberrations of local wavefronts by oblique incidence” by Esser et al [27].

The main advantage of the approach is that it is based exclusively on analytical formulas. This saves much computation time compared to numerical iteration routines which would otherwise be necessary for determining the higher order aberrations. The thesis is structured in four principal objectives as described in the proposal and two additional objectives. Every principal objective describes a process, which is necessary to calculate the wavefront Higher Order aberration of a spectacle lens or an entire optical system [see Figure 1]. The principal objective 1 deals with the derivation of the analytical refraction equations, which is the first basic process. This objective is described in chapter 3 “Derivation of the Refraction Equations”. The principal objective 2 deals with the relation between the coefficients of Zernike series polynomials and the coefficients of power series polynomials and is demonstrated in chapter 4.4 “Relation between Zernike series and power series”. The principal objective 3 deals with the rotation of the coordinate system. This is only a support process because the wavefront is not changing; only the coordinate system is rotated. This objective is shown in chapter 4 “Description of a Wavefront in a rotated Coordinate System”. The principal objective 4 deals with the derivation of the analytical propagation equations, which is the second basic process and is described in chapter 5 “Derivation of the Propagation Equations”. The additional principal objective 5 deals with the derivation of the analytical reflection equations and is demonstrated in chapter 6 “Derivation of the Reflection Equations”. The derived equations in the chapters 3, 5 and 6 are based on wavefront (sagittal) aberrations. In Appendix A: Relation between sagitta derivatives and OPD derivatives are equations provided for transforming wavefront (sagitta) aberrations to OPD aberrations. The method, used in this thesis, has also the capability to derive directly the equations for OPD aberrations. This is done exemplarily in the case of propagation in chapter 7 “Propagation of OPD Aberrations”.

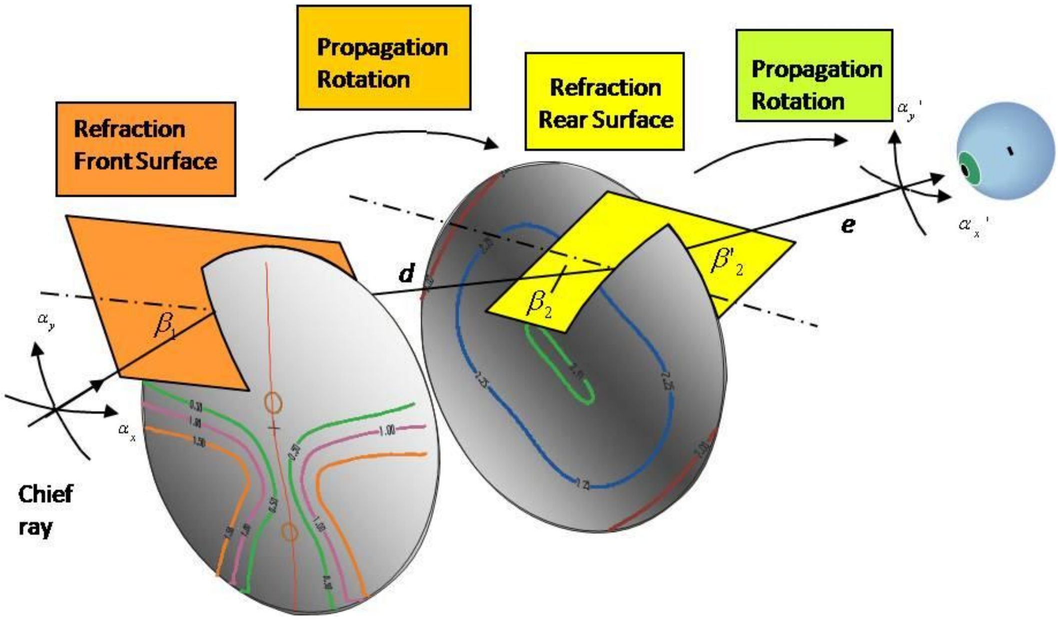

Figure 1: Calculating the wavefront aberrations of a spectacle lens for one viewing direction for given chief (or principle) ray. This calculation process includes the refraction at the front surface (in this example a progressive surface), then the propagation from the front to the rear surface and the description of the wavefront in a rotated cordinate system, because regarding the asymmetrie of the refractive surfaces do the reflecting planes not conciide. The next step is the refraction at the rear surface and then the propgation to the entrance pupil of the eye and desribing the wavefront in the coordinate system of the eye.

Acknowledgments

At this point I would like to thank all who have contributed to finish this thesis successfully. The author wishes to express his gratitude to his supervisors, Prof. Dr. Josep Arasa, Universitat Politècnica de Catalunya, and Prof. Dr. Peter Baumbach, Aalen University, for their professional and excellent support and guidance. Special thanks to Prof. Dr. Montserrat Arjona and Prof. Núria Tomás, Universitat Politècnica de Catalunya, who were abundantly helpful. I wish to thank Prof. Dr. Anna Nagl, Aalen University, for her support and help, especially getting this thesis started. Many thanks to Rodenstock, especially Dr. Werner Müller and Priv. Doz. Dr. Dietmar Uttenweiler, Rodenstock GmbH, for his continuing help and support. I owe my deepest gratitude to Dr. Wolfgang Becken, Rodenstock GmbH, in particular for his extremely competent support, deep and fruitful discussions and detailed feedback. Finally, I would like to thank Heike Hädrich, my wife, for her encouragement and assistance.

Table of contents

List of abbreviations and symbols

LOA: Lower Order Aberrations

HOA: Higher Order Aberrations

OPD: Optical Path Difference

PSF: Point-Spread-Function

RMS: Root-Mean-Square

LASIK: Laser-in-situ-Keratomileusis

$\bar{x},\bar{y},\bar{z}$: Local coordinate system of the refractive or reflective surface

x,y,z : Local coordinate system of the incoming wavefront or global coordinates system in the case of propagation

x',y',z' : Local coordinate system of the outgoing or reflected wavefront

$\mathbf{R}$: Spatial rotations matrix about the common x axis

$f^{(1)}(x)$, $f^{(2)}(x)$, $f^{(3)}(x)$, … $f^{(1,0)}(x,y)$, $f^{(0,1)}(x,y)$, $f^{(2,0)}(x,y)$,

Derivatives of the function $f(x)$ and $f(x,y)$

n : Refractive index of the medium in front of the refractive or reflective surface

n' : Refractive index of the medium behind the refractive surface

ε : Angle of incidence, angle between the incoming ray and the surface normal

ε' : Emergent angle, angle between the emerging ray and the surface normal

$\mathbf{n}_{\mathrm{In}}$: Directional vector of the incoming ray resp. normal of the incoming wavefront in the coordinate system of the incoming wavefront

$\mathbf{n'}_{\mathrm{Out}}$: Directional vector of the emerging ray resp. normal of the outgoing or reflected wavefront in the coordinate system of the outgoing wavefront

$\bar{\mathbf{n}}_{\mathrm{S}}$: Normal of the refractive or reflective surface in the coordinate system of the surface

$w(x,y)$: Wavefront

s : Vertex distance at the object side (Axial distance from the refractive or reflective surface to the object point), which is equivalent to the radius of curvature of the incoming wavefront

s' : Vertex distance at the image side (Axial distance from the refractive or reflective surface to the image point), which is equivalent to the radius of curvature of the outgoing or reflected wavefront

r : Radius of curvature of the refractive or reflective surface (distance from the surface to the center point of the surface)

S : Vergence at the object side

S' :	Vergence at the image side
$\bar{S}$:	Surface Power
$S_x, S'_x, \bar{S}_x$:	Equivalent the vergences in the plane perpendicular to the refracting plane
$S_y, S'_y, \bar{S}_y$:	Vergences in the refracting plane
$\mathbf{s}$:	Power vector at the object side (incoming wavefront)
$\mathbf{s}'$:	Power vector at the image side (outgoing wavefront)
$\bar{\mathbf{s}}$:	Power vector of the surface
Sph :	Spherical Power of the incoming wavefront, outgoing wavefront or refractive/reflective surface
Cyl :	Cylindrical Power of the incoming wavefront, outgoing wavefront or refractive/reflecting surface
α :	Axis of the cylindrical Power of the incoming wavefront, outgoing wavefront or refractive/reflective surface
$\mathbf{S}_o$:	Vergence matrix of the original wavefront
$\mathbf{S}_p$:	Vergence matrix of the propagated wavefront
$\mathbf{C}, \mathbf{C}'$:	Incidence matrix and emergent matrix
$\mathbf{e}_k, \mathbf{e}'_k, \bar{\mathbf{e}}_k$:	Error vectors for aberrations of higher order, analogously to the definition of the Power vectors
$E, E', \bar{E}$:	Generally aberrations of the incoming and outgoing wavefront and the refractive/reflective surface.

1. Introduction

Aberrations play a decisive role in optics. In this PhD study, it is dealt with them in the framework of geometrical optics in which the wavelength is neglected $(\lambda \to 0)$ with respect to diffraction effects [1,2]. Also in this case, still the notions of both rays and wavefronts 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.

With the help of the Coddington equation and the vertex correction formula the analytical calculation of local Power and Astigmatism of a wavefront after reflection, refraction and also propagation can be accomplished. In three recent publications the author extended the refraction, propagation and reflection equations to HOA [25,26,27].

1.1. Rays, Wavefronts and Aberrations

An imagery will be said to be free from 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 paraxial conjugate image point. In terms of rays, this image point serves as a reference point which any ray starting from the object point through the aperture has to hit. In terms of waves, the image point serves as 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.

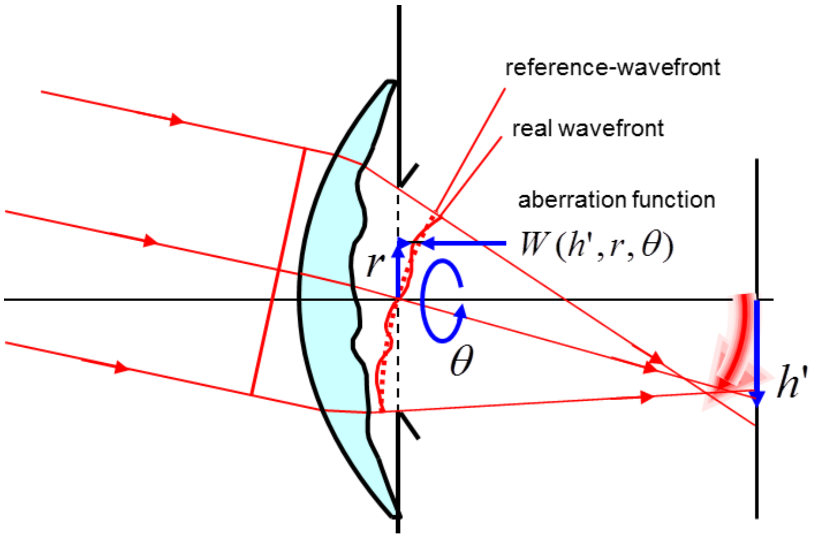

Figure 2: Caculation of the wavefront aberration function using numerical ray tracing. The aberration function can be written as a power series expansion in both the image coordinates (h') and the pupil coordinates (r,θ) or some combinations of these. The *wave aberration function* is defined by the optical path differences (OPD) between the real wavefronts and the reference sphere along the real occurring rays.

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

Throughout the PhD thesis, it will be referred to wave aberrations. A wavefront based description of these aberrations can either refer to the geometrical shape of the real *wavefronts* in space (as it will be done in the PhD thesis), or by a *wave aberration function* which describes the optical path differences (OPD) between the real wavefronts and the reference sphere along the real occurring rays [see Figure 2].

1.2. 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 either case 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 only meaningful in connection with the underlying aberration scheme.

While the treatment of rotationally symmetric systems is well established in literature [2,3], there exist rather few publications about non-symmetric systems. Thompson has treated the third-order aberrations [28] and the fifth-order aberrations [29] (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 [30].

It is a very interesting subtopic to consider the aberration function for fixed image point and consequently as a function of the pupil coordinates only [2], but without any restrictions to the symmetries of surfaces or wavefronts. In this case, which is the focus of the present PhD study, 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 [10]. It will also be done 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 define the order of an aberration as the highest number of added powers of x and y [10,11]. It is well accepted that there is no one-to-one correspondence between the order used in this work and the more general one described above [2]. This arises since different orders concerning the image coordinates are summarized within one order of pupil coordinates. Throughout the PhD thesis, we will summarize 1st order aberrations (tilt) and 2nd order aberrations (comprising Defocus and Astigmatism) as *Lower Order Aberrations* (LOA), and all aberrations of 3rd order (Coma, Trefoil), 4th order (e.g. Spherical Aberration) and higher will be summarized as *Higher Order Aberrations* (HOA) [see Figure 3], as also done in Ref. [10,12].

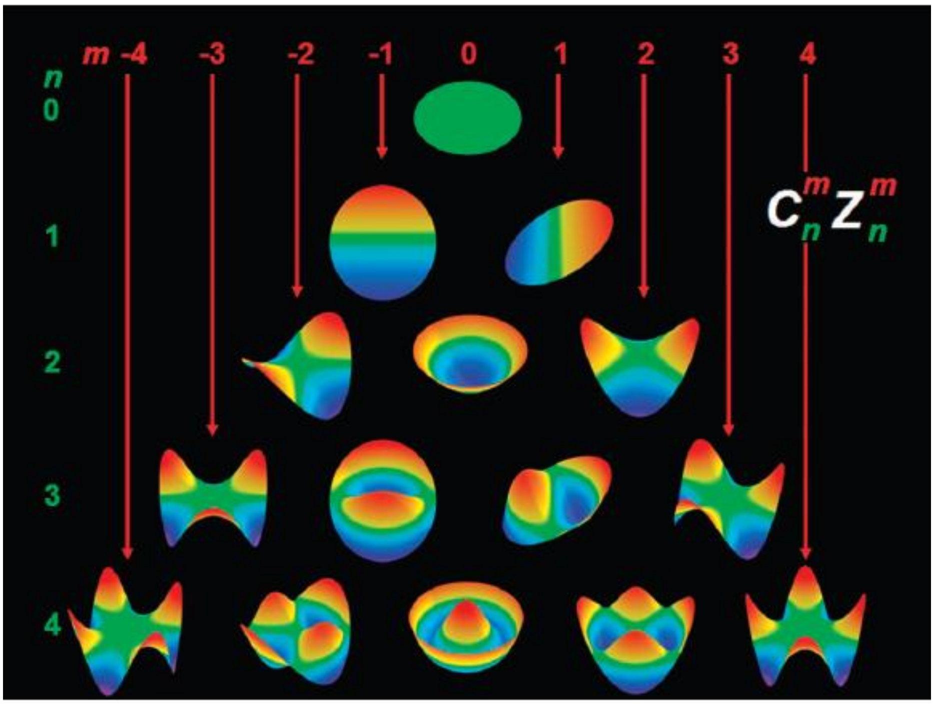

Figure 3: Illustration of the wavefront aberrations by Zernike-polynomials up to the radial order $n = 4$ and the angular frequency m. Throughout the PhD thesis, aberrations of radial order $n = 1$ (tilt) and $n = 2$ (Defocus and Astigmatism) as *Lower Order Aberrations* (LOA), and all aberrations of radial order $n = 3$ (Coma, Trefoil) and $n = 4$ (e.g. Spherical Aberration) and higher will be summarized as *Higher Order Aberrations* (HOA). Figure from [13]

Wavefront aberrations are the starting point for computing the image quality. Although it is not in the focus of this PhD thesis, the image quality is often represented by the Point-Spread-Function (PSF), which is computed from the wave aberration in the exit pupil and from its interference pattern taking into account the finite wavelength of light [1,31]. In particular there exist well-known features of the Point-Spread-Functions (see Figure 4) assigned to the elementary aberrations shown in Figure 3. Until now the aberrations in the exit pupil had to be calculated by ray tracing. The purpose of this PhD is to provide a method for calculating the wavefront aberrations in the pupil plane by analytical wavefront tracing. The higher the radial order of the aberration is the higher is the asymmetry of the PSF. Usually only the aberrations of first order (prism) and second order (power and astigmatism) are corrected by contact lenses and spectacle lenses.

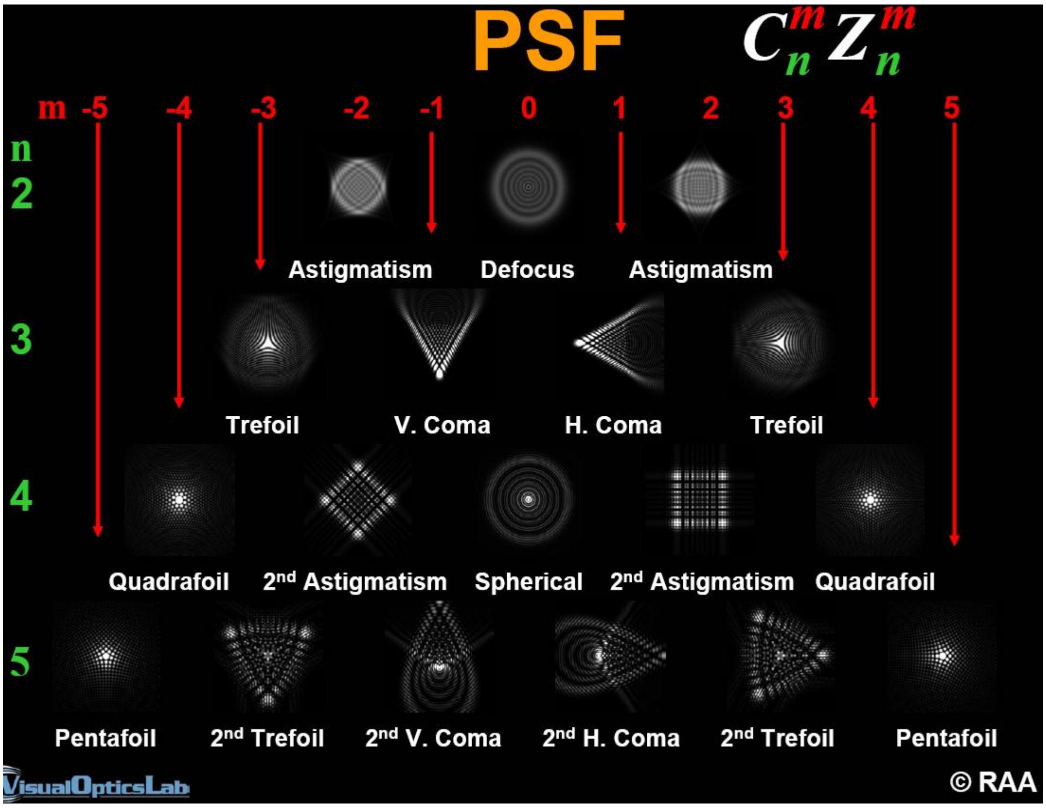

Figure 4: Illustration of the Point-Spread-Function (PSF) pattern taking into account the finite wavelength of light and their influence on the image quality by Zernike-polynomials up to the radial order $n = 5$ and the angular frequency m. As higher the radial order of the aberration is as higher is the asymmetry of the aberration. Figure from [14].

1.3. General context and scope of the work

The awareness of the role of HOA has increased in optometry and ophthalmology [10,11,12,13 ,15,16,17,18]. Figure 5 shows the influence of each aberration with the same Root-Mean-Square (RMS) on the imaging of an optotype. The quality of the image is worse at the center of the Zernike-Pyramid than at the edges even though the RMS is equal. HOA 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 based on local derivatives, but which is nevertheless suitable for describing all effects of a large pupil. It will be shown that this description is indeed fully equivalent to the usual approaches which are tailored for describing the entire pupil (e.g. by means of Zernike polynomials). The local description has the advantage to permit the derivation of analytical formulas for computing HOA, which represents a significant progress in the general understanding and in a reduced numerical effort.

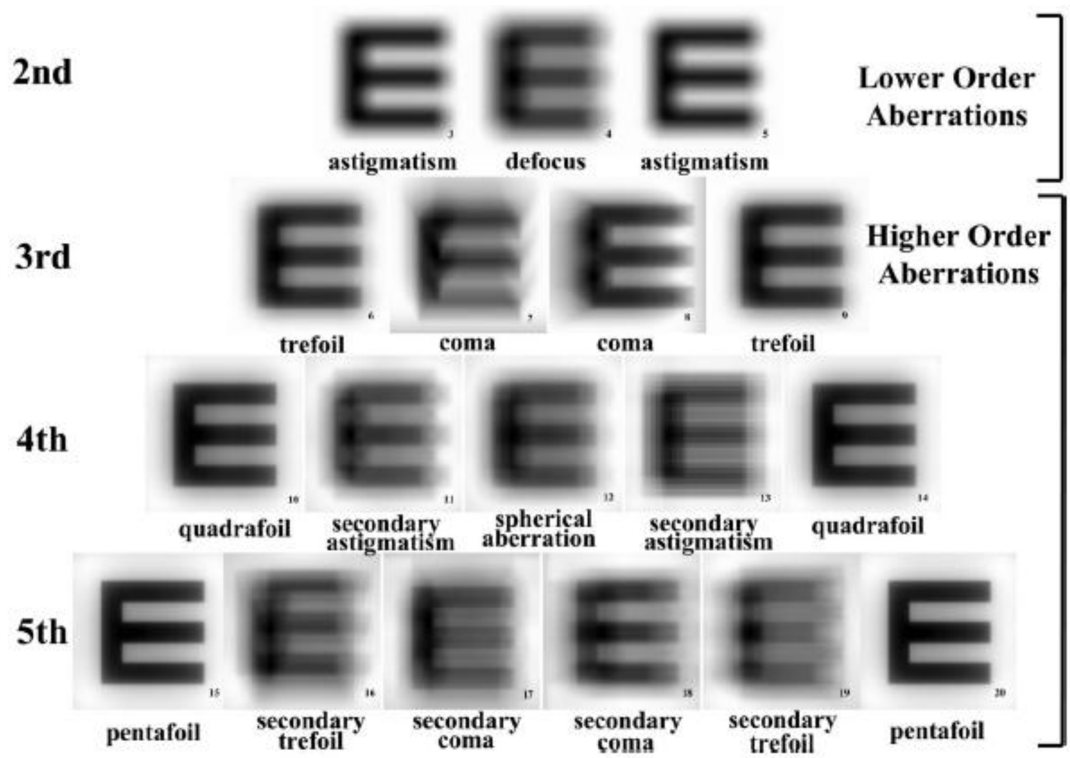

Figure 5: Influence of each aberration (Zernike-coefficient) with the same Root-Mean-Square (RMS) on the imaging of an optotype. The quality of the image is worse at the center of the Zernike-Pyramid than at the edges even though the RMS is equal. Figure from [18].

Hitherto for determining HOA, the wavefront in the pupil was calculated by ray-tracing [1,8,20 ,21,28,29,30] a precise method when a large number of rays are used but then being 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 [3,4,5,6,7,22,23]. Wavefront tracing is a very fast semi-analytical method [22,23]. 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 [32,33,34].

The importance of wavefront driven correction of ocular aberrations which are often measured by an aberrometer has increased rapidly in recent years. The wavefront data are determined at some device-specific plane and by the diameter of the evaluated ray bundle. Depending on the desired application, it is usually necessary to transform these raw data to some other plane, e.g. the entrance pupil of the eye, the cornea (as is relevant for LASIK or contact lenses) or the vertex plane of a spectacle lens. The ray bundle's diameter, in turn, is determined by the pupil size of the eye.

Figure 6 shows the mean value and standard deviation of the Root-Mean-Square (RMS) of the wavefront aberration of 18 Zernike-coefficients. 109 subjects were measured by an aberrometer and the Zernike-coefficients were determined at a pupil size of 5.7 mm [12]. The first three Zernike-coefficients describe the aberrations of second order (power and astigmatism). It is obvious that these aberrations are dominating but individually also the Higher Order Aberrations can reach high values. The small picture shows the Higher Order Aberrations magnified. The Zernike-coefficient Z_4^0 (spherical aberration) is significant different from zero.

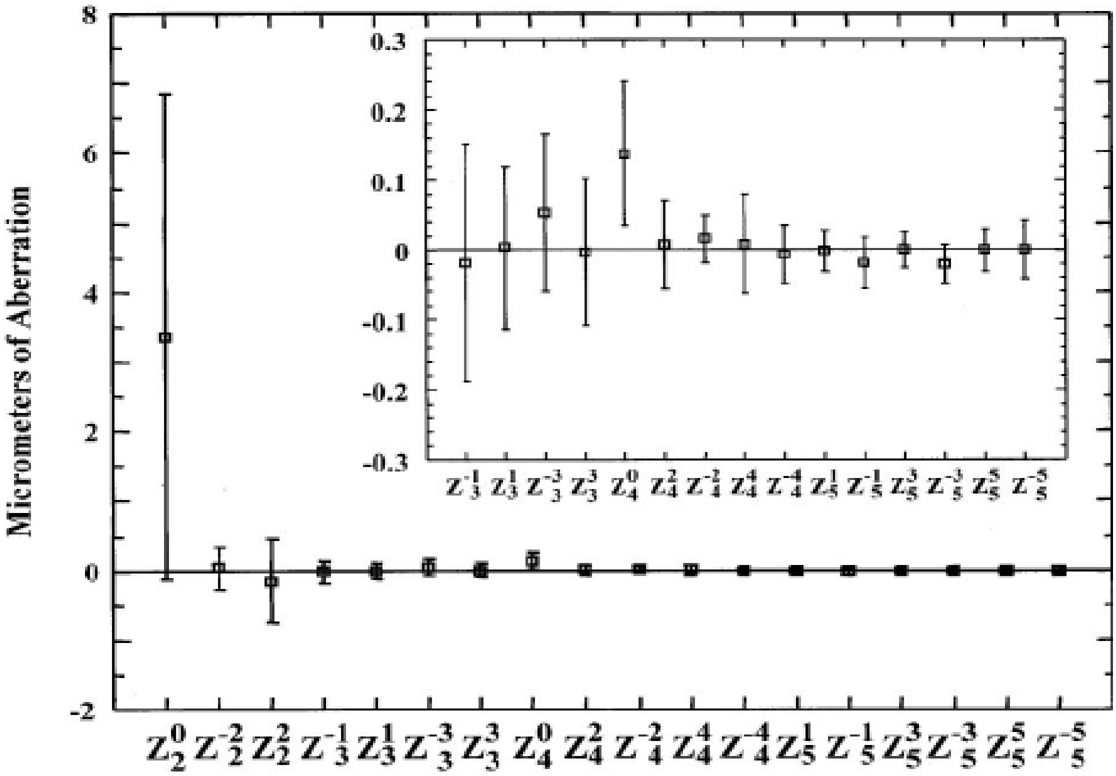

Figure 6: Mean value and standard deviation of the Root-Mean-Square (RMS) of the wavefront aberration of 18 Zernike-coefficients at a pupil size of 5.7 mm (109 subjects). The first three Zernike-coefficients describe the aberrations of second order (power and astigmatism). It is obvious that these aberrations are dominating but individually also the Higher Order Aberrations can reach high values. The small picture shows the Higher Order Aberrations magnified. Figure from [12]

While there exist various publications dealing with analytical scaling transformations to a different pupil size [35,36,37,38,39,40,41,42] rotating the pupil [36,41,42,43] displacing the pupil [35,36 ,41,42,43] or deforming the pupil [42] only a few publications can be found which attempt to treat the wavefront propagation in an analytical way. In [36,44] an analytical method is described to calculate the propagation of a wavefront, but the method is still restricted by some approximations. As is written there, further study is necessary to obtain a unified formulation for wavefronts containing both low-order and high-order aberrations. <u>In this PhD thesis we have developed such a novel unified analytical propagation method in homogenous material.</u>

It is known from literature how to calculate Power and Astigmatism of a local wavefront after the refraction or reflection 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 [1,4,5,8].

For calculating the wavefront aberrations of an entire lens, especially of a spectacle lens, it is necessary to propagate the wavefront from the intersection point of the chief ray at the first surface along the chief ray to the intersection point at the next surface and so on. In the special case of a spectacle lens this means the propagation from the front to the rear surface and further to the vertex point sphere or the entrance pupil of the eye.

Further, it is necessary to describe the wavefront in different (rotated) coordinate systems, because the refracting planes, e.g. the refracting plane at the front surface and at the rear surface of a spectacle lens, are not identical. They are rotated around the chief ray. A rotation is also necessary to describe the aberrations relating to the horizontal or vertical axis or the axis defined by Listing’s law. Listing’s law describes the three dimensional eye movement when viewing in a diagonal gaze direction (tertiary position). It says that the rotation takes place around an axis which is perpendicular to the plane spanned by the vector in primary gaze direction and the vector in tertiary gaze direction [45,46]. The goal and also the advantage of the method is that the derived equations allow calculating the coefficients of the wavefront in the rotated coordinate system relating to the coefficients of the original wavefront directly without a coordinate transformation.

For second order aberrations (Power and Astigmatism) the propagation and rotation of the coefficients of the wavefront is known and described by the analytical transfer equation, which can be described either in matrix form [7,24,32,47,48] or by power vectors [49].

The purpose of this PhD thesis is to extend the Generalized Coddington Equation [3,4,5,6,7,8,9] and Transfer Equation [7,32,24,47,48,49] 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. Theoretical background

It turns out to be very practical to establish the treatment of refraction, propagation and reflection 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 A: Relation between sagitta derivatives and OPD derivatives). Refraction equations are a set of relations between the incoming wavefront, the outgoing wavefront and the refractive surface. Regardless 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 two other ones.

2.1. Coordinate Systems

In order to describe the incoming wavefront, the refractive or reflective surface and the outgoing or reflected wavefront, three different local Cartesian coordinate systems (x, y, z), $(\bar{x}, \bar{y}, \bar{z})$ and (x', y', z') are used, respectively (see Figure 7 for refraction and Figure 8 for reflection). 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 or reflective surface. The systems possess as common axis $x = x' = \bar{x}$ the normal of the refracting or reflecting plane, which is the plane containing the normals of the incoming wavefront, the refractive or reflective surface and the outgoing or reflected 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 or reflecting plane. The z axis points along the incoming chief ray, the z' axis points along the outgoing or reflected chief ray, and the $\bar{z}$ axis points along the normal of the refractive or reflecting surface. The orientations of the y axis, the y' axis and the $\bar{y}$ axis are such that each system is right-handed.

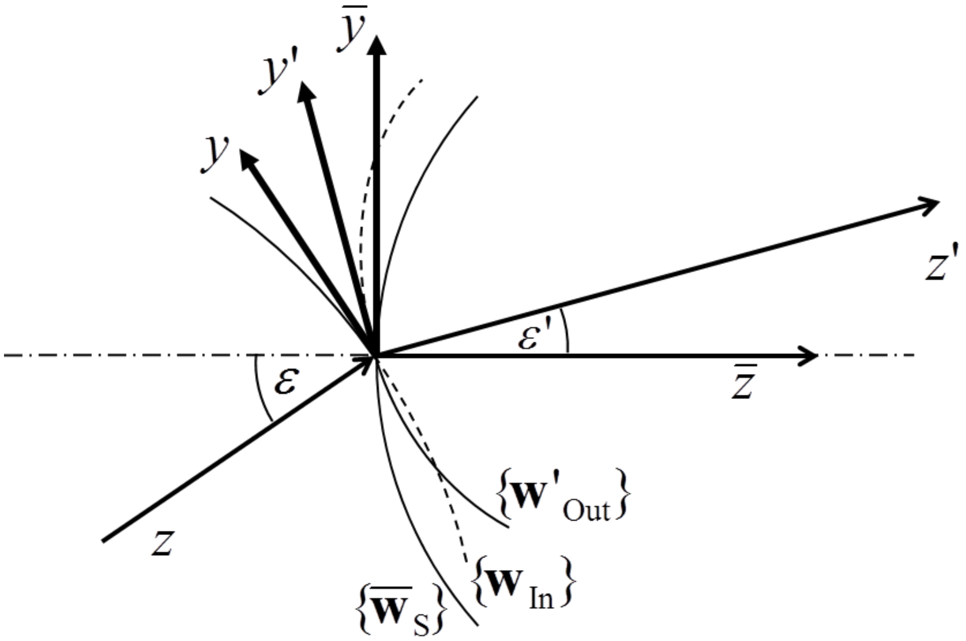

Figure 7: Local coordinates systems $(\bar{x}, \bar{y}, \bar{z})$ of the refractive surface $\{\overline{\mathbf{w}}_{\text{S}}\}$, (x, y, z) of the incoming wavefront $\{\mathbf{w}_{\text{In}}\}$and (x', y', z') of the outgoing wavefront $\{\mathbf{w'}_{\text{Out}}\}$ where the brackets $\{.\}$ shall denote the entity of vectors. 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. 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.

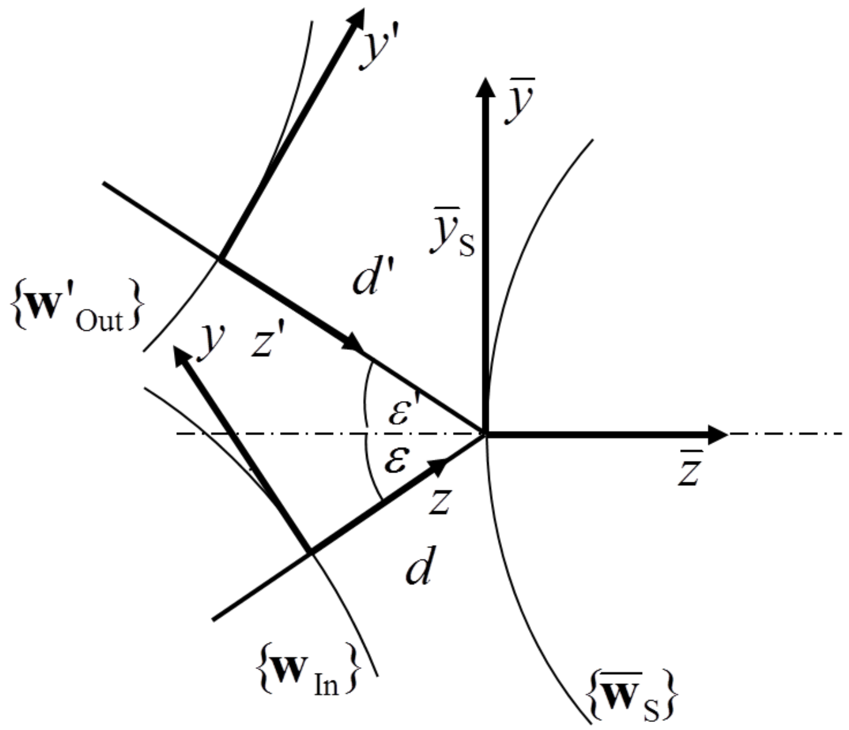

Figure 8: Local coordinates systems $(\bar{x}, \bar{y}, \bar{z})$ of the reflective surface $\{\bar{\mathbf{w}}_S\}$, (x, y, z) of the incoming wavefront $\{\mathbf{w}_{In}\}$and (x', y', z') of the reflected wavefront $\{\mathbf{w}'_{Out}\}$ where the brackets $\{.\}$ shall denote the entity of vectors. The origins of these coordinate systems coincide in the chief ray's intersection point with the reflective surface. The origins are fictitious separated by *d* and *d'* for a better understanding of the nomenclature. The systems possess as common axis $x = x' = \bar{x}$ the normal of the reflecting plane, which is the plane containing the normals of the incoming wavefront, the reflective surface and the reflected wavefront. The z axis points along the incoming chief ray, the z' axis points along the reflected chief ray, and the $\bar{z}$ axis points along the normal of the reflective 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 lower-case letters, such as $\mathbf{r}$ for position or $\mathbf{n}$ for normal vectors, and matrices are written as bold upper-case letters, such as $\mathbf{R}$ for spatial rotations. Any object (i.e. quantity, space point or vector) which is specified in the (x, y, z) frame is represented by an unprimed symbol (e.g. x, $\mathbf{r}$, $\mathbf{n}$,…), whereas the representation of the same object in the primed frame (x', y', z') or in the frame $(\bar{x}, \bar{y}, \bar{z})$ is given by a prime or a bar at 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

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

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

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

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

Additionally to the coordinate notation, we introduce a lower index notation for labeling whether a quantity belongs to the incoming wavefront, the refractive or reflective surface or the outgoing or reflected wavefront. Regardless 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 or reflected wavefront ($\mathbf{n}_{\mathrm{Out}}$, $\mathbf{n}'_{\mathrm{Out}}$, $\bar{\mathbf{n}}_{\mathrm{Out}}$, respectively), and the index "S" stands for the refractive or reflective 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 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.

In contrast to refraction and reflection, where three coordinate systems are appropriate, in the case of propagation where tilt is absent it is practical to use one common global Cartesian coordinate system (x,y,z) in order to describe the original wavefront and the propagated wavefront. The system is defined by the intersection point of the chief ray with the original wavefront and by the direction of the chief ray which defines the z axis. The orientation of the x axis can be freely selected. The orientation of the y axis is such that the system is right-handed (see Figure 9).

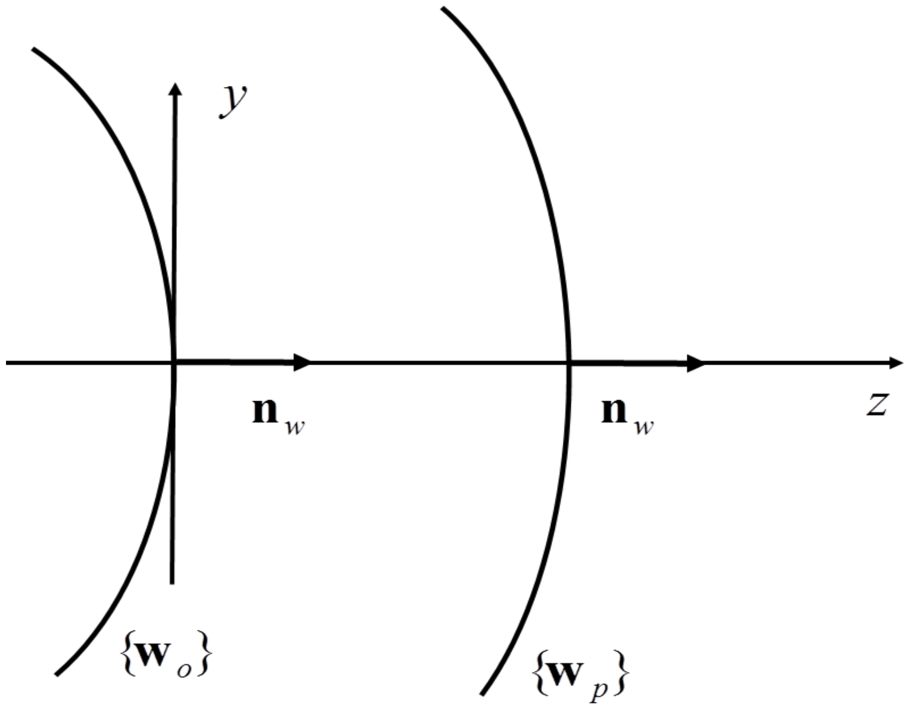

Figure 9: In the case of propagation where tilt is absent it is practical to use one common global Cartesian coordinate system (x, y, z) in order to describe the original wavefront and the propagated wavefront. The system is defined by the intersection point of the chief ray with the original wavefront and by the direction of the chief ray which defines the z axis. The orientation of the x axis can be freely selected. The orientation of the y axis is such that the system is right-handed

2.2. Description of Wavefronts

Since the wavefronts and 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 or the outgoing wavefront, unless those are distinguished explicitly.

Any surface sagitta, provided 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* [2,50]. Even for these polynomials there exist different conventions, indexing schemes and normalizations [1,11]. We use the OSA standard of Zernike polynomials $Z_k^m(\rho, \vartheta)$ of Ref.[11] which describes a surface $w(x, y)$ within a pupil of radius r_0 as the expansion

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

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

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

with $$T_k^m(x,y) = \frac{x^m y^{k-m}}{m!(k-m)!}$$

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

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

By the order of an aberration term we mean the number k, in either of the Eqs. (3) and (4). As long as the series expansion is infinite, i.e. the sum runs to $k \to \infty$, a transformation between any of the representations in Eq. (3) and Eq. (4) is legitimate, well-defined and unique.

In practice, however, an expansion is always truncated at some finite order k_0, justified by the observation that the major part of 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 $C^{\infty}(P)$ which is spanned by the finite (incomplete) basis system of functions underlying the truncated series.

Before proceeding in the reasoning, we consider the first orders $k = 0,1,2$ of Taylor and Zernike basis sets of $V = C^{\infty}(P)$, respectively. We observe that also if the subspaces spanned by these basis functions are identical, the basis vectors of order $k = 2$ will be not identical. For example, in Eq. (3) the Zernike aberration in the term $Z_2^0 = \sqrt{3}\left(2\rho^2 - 1\right) = \sqrt{3}\left(2\left(x^2 + y^2\right)/r_0^2 - 1\right)$ due to $\rho = r/r_0$ with order $k = 2$, usually called Defocus, contains also a constant term, whereas any $k = 2$ term in Eq. (4) is a monomial with pure value $k = 2$ for added x and y powers or similar in the case of higher orders $k = 4$, 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, contains also 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 chapter 4.4 and in [51]. The following Table 1 shows both basis sets of Taylor and Zernike for the first orders $k = 0,1,2$ where for simplicity we use $r_0 = 1$ for the Zernike terms.

#	order k	Taylor T_k^m	Zernike Z_k^m
1	0	$T_0^0 = 1$	$Z_0^0 = 1$
2	1	$T_1^0 = y$	$Z_1^{-1} = 2y$
3	1	$T_1^1 = x$	$Z_1^1 = 2x$
4	2	$T_2^0 = y^2/2$	$Z_2^{-2} = 2\sqrt{6}xy$
5	2	$T_2^1 = xy$	$Z_2^0 = \sqrt{3}\left(2\left(x^2+y^2\right)-1\right)$
6	2	$T_2^2 = x^2/2$	$Z_2^2 = \sqrt{6}\left(x^2-y^2\right)$

Table 1: The first orders $k = 0,1,2$ of Taylor and Zernike basis sets of $V = C^\infty(P)$, as defined in Eq. (3) and Eq. (4), where for simplicity we use $r_0 = 1$ for the Zernike terms

Let us now discuss how a function of order $k = 2$, say $f(x) = 1 + \alpha x^2$, is represented in each system. In Taylor representation, we would obtain (see Eq. (4))

$$f(x) = \sum_{k=0}^{2}\sum_{m=0}^{k} a_{m,k-m} T_k^m(x,y) \tag{6}$$

with

$$a_0^0 = 1, \quad a_2^2 = 2\alpha, \quad a_1^0, a_1^1, a_2^0, a_2^1 = 0$$

Whereas in Zernike representation, we would obtain (see Eq. (3))

$$f(x) = \sum_{k=0}^{2}\sum_{m=-k}^{k} c_k^m Z_k^m \tag{7}$$

with

$$c_0^0 = 1 + \frac{\alpha}{4}, \quad c_2^0 = \frac{\alpha}{4\sqrt{3}}, \quad c_2^2 = \frac{\alpha}{2\sqrt{6}}, \quad c_1^{-1}, c_1^1, c_2^{-2} = 0.$$

Now, if the space allowed for representation is truncated to contain only terms of order $k_0 = 0$, then the approximated Taylor representation would be $f(x) \approx 1$ whereas the approximated Zernike representation would be $f(x) \approx 1 + \alpha/4$. Both approximations are not identical, and they are not very good for $\alpha = 1$ either. However, for $\alpha = 10^{-3}$, they are more similar and also a good approximation to $f(x)$ in the inner parts of the pupil, and for $\alpha = 10^{-6}$, they are almost identical and a very good approximation to $f(x)$ in the whole domain (i.e. the pupil), of course depending on the demanded accuracy.

On a more abstract level, we encounter the following situation. Given is a vector space V (of functions) whose dimension is assumed to be $n = 2$ without loss of generality here. Formally we denote the coordinates of vectors in V by x_1 and x_2. Further two different basis systems $\{\mathbf{v}_1, \mathbf{v}_2\}$ and $\{\mathbf{w}_1, \mathbf{w}_2\}$ of V are given. We can symbolize them as blue and red sets of vectors, as shown in Figure 10. The basis systems are chosen according to our situation concerning the Zernike and the Taylor set in that $\mathbf{v}_1$ spans the same subspace V as $\mathbf{w}_1$ does, i.e. both systems give rise to a common subspace $V_1 = \langle \mathbf{v}_1 \rangle = \langle \mathbf{w}_1 \rangle$ of V. On the other hand, $\mathbf{v}_2$ spans a different subspace of V than $\mathbf{w}_2$ does.

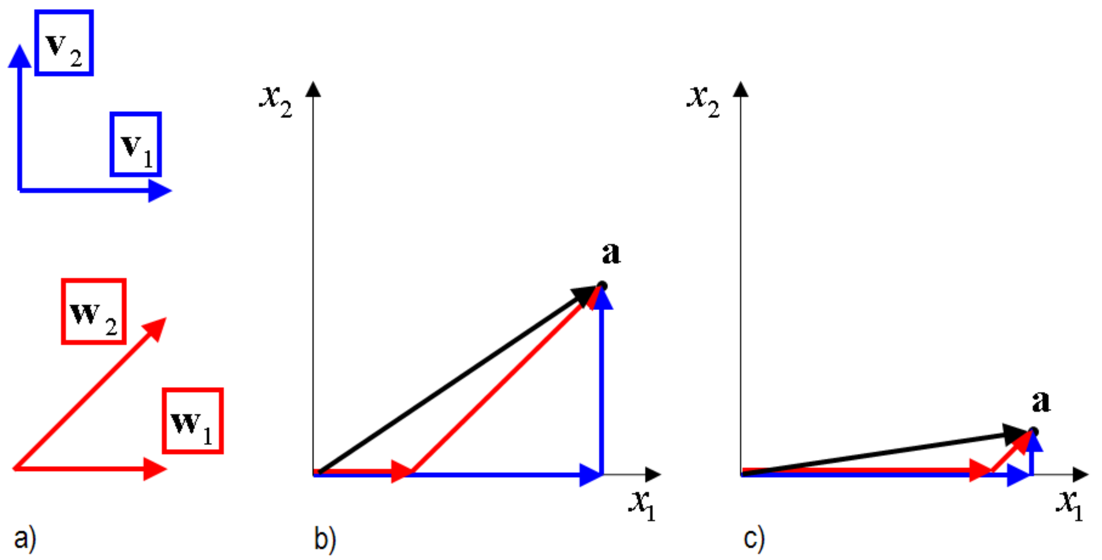

Figure 10: Formally the coordinates of vectors in V are denoted by x_1 and x_2. Further two different basis systems $\{\mathbf{v}_1, \mathbf{v}_2\}$ and $\{\mathbf{w}_1, \mathbf{w}_2\}$ of V are given as shown in a). They are symbolized as blue and red sets of vectors. We consider a given vector $\mathbf{a}$ shown as black arrow in b) and c). Then we obtain different representations depending on if the red basis set or the blue one is used. If the basis set is truncated, i.e. $\mathbf{v}_2$ and $\mathbf{w}_2$ have to be omitted, then the representation of $\mathbf{a}$ in the subspace V_1 corresponds to the blue horizontal arrow for the blue basis set and to the red one in the case of the red one. The horizontal vectors can be interpreted as the projections of $\mathbf{a}$ onto V_1 or W_1. In the blue case the projection takes place along the direction of $\mathbf{v}_2$ whereas in the red case it is performed along $\mathbf{w}_2$. Since $\mathbf{v}_2$ and $\mathbf{w}_2$ are not parallel, those projections are different, which is directly dependent on the distance of $\mathbf{a}$ in relation to V_1 or W_1. b) Vector $\mathbf{a}$ far away from the subspace $V_1 = \langle \mathbf{v}_1 \rangle = \langle \mathbf{w}_1 \rangle$ spanned by $\mathbf{v}_1$ or $\mathbf{w}_1$ c) Vector $\mathbf{a}$ close to the subspace spanned by $\mathbf{v}_1$ or $\mathbf{w}_1$

Now, if we consider a given vector $\mathbf{a}$ (black arrow in Figure 10b,c), then we will obtain different representations depending on if the red basis set or the blue one is used. If the basis set is truncated, i.e. $\mathbf{v}_2$ and $\mathbf{w}_2$ have to be omitted, then the representation of $\mathbf{a}$ in the subspace V_1 will correspond to the blue horizontal arrow for the blue basis set and to the red one in the case of the red one. The horizontal vectors can be interpreted as the projections of $\mathbf{a}$ onto V_1, and in the blue case the projection takes place along the direction of $\mathbf{v}_2$ whereas in the red case it is performed along $\mathbf{w}_2$. Since $\mathbf{v}_2$ and $\mathbf{w}_2$ are not parallel, those projections are different. In the case of Figure 10b), where $\mathbf{a}$ is far away from V_1, the projections are even very different, and both are no good approximation to $\mathbf{a}$. On the other hand, if $\mathbf{a}$ is lying close to V_1 (Figure 10c), then the projections are quite similar, and both are good approximations to $\mathbf{a}$ itself.

Our conclusion is the following. In contrast to the Zernike polynomials, which are tailored for a surface description over a finite pupil size, it seems only at first glance that a description of local derivatives at the pupil might only be valid 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

$$\begin{aligned} w_{\mathrm{In}}(x,y) &= \sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a_{\mathrm{In},m,k-m}}{m!(k-m)!}x^m y^{k-m} \\ w'_{\mathrm{Out}}(x',y') &= \sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a'_{\mathrm{Out},m,k-m}}{m!(k-m)!}x'^m y'^{k-m} \end{aligned} \tag{8}$$

and

$$\overline{w}_{\mathrm{S}}(\overline{x},\overline{y}) = \sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{\overline{a}_{m,k-m}}{m!(k-m)!}\overline{x}^m \overline{y}^{k-m} \tag{9}$$

for describing the incoming wavefront, the outgoing or reflected wavefront and the refractive or reflective surface, respectively.

Analogously we introduce for describing the original wavefront and the propagated wavefront

$$\begin{aligned} w_{\mathrm{o}}(x,y) &= \sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a_{\mathrm{o},m,k-m}}{m!(k-m)!}x^m y^{k-m} \\ w_{\mathrm{p}}(x,y) &= \sum_{k=0}^{\infty}\sum_{m=0}^{k}\frac{a_{\mathrm{p},m,k-m}}{m!(k-m)!}x^m y^{k-m} \end{aligned} \tag{10}$$

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.

2.3. 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)[1].

2.3.1. Refraction

For the aberrations of second order the refraction of a spherical wavefront with orthogonal incidence onto a spherical surface with the Surface Power $\bar{S}$ (see Figure 11) is described by the vergence equation [1,2]:

$$S' = S + \bar{S} \tag{11}$$

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 the refractive surface to the center point of 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

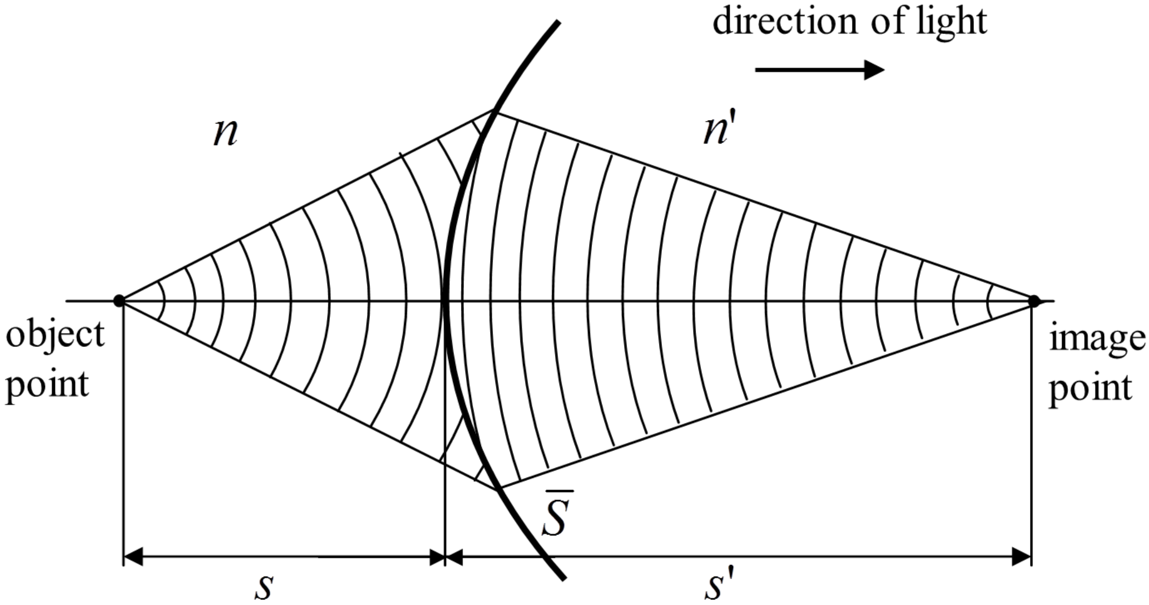

Figure 11: For the aberrations of second order the refraction of a spherical wavefront with vergence $S = n/s$ with orthogonal incidence onto a spherical surface with the Surface Power $\bar{S} = (n'-n)/r$ is described by the vergence equation. The vergence $S' = n'/s'$ of the outgoing wavefront is equal to the sum of the vergence of the incoming wavefront and the Surface Power $S' = S + \bar{S}$.

In literature, the notion of vergences is usually extended to 3-dimensional space for describing the sphero-cylindrical power of a surface by the following steps. First, the curvatures $1/s$, $1/s'$ and $1/r$ in Eq. (11) are identified with the second derivatives of the sagittas of the incoming wavefront, the outgoing wavefront and the surface, respectively. Further, in 3-dimensional space the second derivatives $w_{\text{In}}^{(2,0)} = \partial^2 w_{\text{In}} / \partial x^2$, $w_{\text{In}}^{(1,1)} = \partial^2 w_{\text{In}} / \partial x \partial y$, $w_{\text{In}}^{(0,2)} = \partial^2 w_{\text{In}} / \partial y^2$, are summarized in terms of 2×2 vergence matrices [8,24] in the shape $n \begin{pmatrix} w_{\text{In}}^{(2,0)} & w_{\text{In}}^{(1,1)} \\ w_{\text{In}}^{(1,1)} & w_{\text{In}}^{(2,0)} \end{pmatrix}$, and similarly for $w'_{\text{Out}}(x', y')$ and $\bar{w}_{\text{S}}(\bar{x}, \bar{y})$, 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.

Additionally to the description in terms of vergence matrices, an equivalent description is common in the 3-dimensional vector space of power vectors [52,53,54], which we will apply throughout the thesis. For the incoming and the outgoing wavefront, as well as the refractive surface we introduce the power vectors

$$\mathbf{s} = \begin{pmatrix} S_{xx} \\ S_{xy} \\ S_{yy} \end{pmatrix} = n \begin{pmatrix} w_{\text{In}}^{(2,0)} \\ w_{\text{In}}^{(1,1)} \\ w_{\text{In}}^{(0,2)} \end{pmatrix}, \qquad \mathbf{s}' = \begin{pmatrix} S'_{xx} \\ S'_{xy} \\ S'_{yy} \end{pmatrix} = n' \begin{pmatrix} w'^{(2,0)}_{\text{Out}} \\ w'^{(1,1)}_{\text{Out}} \\ w'^{(0,2)}_{\text{Out}} \end{pmatrix}, \qquad \bar{\mathbf{s}} = \begin{pmatrix} \bar{S}_{xx} \\ \bar{S}_{xy} \\ \bar{S}_{yy} \end{pmatrix} = (n'-n) \begin{pmatrix} \bar{w}_{\text{S}}^{(2,0)} \\ \bar{w}_{\text{S}}^{(1,1)} \\ \bar{w}_{\text{S}}^{(0,2)} \end{pmatrix} \qquad (12)$$

The symbolism S_{xx}, etc. is merely understood as component labeling of the vector $\mathbf{s}$. Nevertheless, it shall remind the reader to the fact that the value of S_{xx} is proportional to the second derivative $w_{\text{In}}^{(2,0)}$ of the wavefront sagitta. It is well-known that the components of Eq. (12) are in ophthalmic terms given by

$$\begin{aligned} S_{xx} &= \left(Sph + \frac{Cyl}{2} \right) - \frac{Cyl}{2} \cos 2\alpha \\ S_{xy} &= -\frac{Cyl}{2} \sin 2\alpha \\ S_{yy} &= \left(Sph + \frac{Cyl}{2} \right) + \frac{Cyl}{2} \cos 2\alpha \end{aligned} \tag{13}$$

where

Sph is the spherical Power of the incoming wavefront

Cyl is the cylindrical Power of the incoming wavefront

α 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. (11) relating the components of Eq. (12) to each other 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 [1,4,5,8].

The most general case is characterized by an astigmatic wavefront hitting an astigmatic surface under oblique incidence, but such that no special orientation between the refracting plane, the directions of principle Power of the incoming wavefront and those of the refractive surface has to be assumed at all. This is the most complex case, described by the "Generalized Coddington Equation" [3,4,5,6,7,8,9], in compact form written in terms of power vectors

$$\mathbf{C}'\mathbf{s}' = \mathbf{C}\mathbf{s} + \nu\bar{\mathbf{s}} \tag{14}$$

where we have introduced the matrices

$$\mathbf{C}' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varepsilon' & 0 \\ 0 & 0 & \cos^2\varepsilon' \end{pmatrix}, \qquad \mathbf{C} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varepsilon & 0 \\ 0 & 0 & \cos^2\varepsilon \end{pmatrix} \tag{15}$$

and the factor

$$\nu = \frac{n'\cos\varepsilon' - n\cos\varepsilon}{n' - n}. \tag{16}$$

2.3.2. Propagation

For the aberrations of second order the propagation of a spherical wavefront with the Vergence S_o (see Figure 12) is described by the propagation or Transfer equation [7,24,32,47,48,49]

$$S_p = \frac{1}{1-\frac{d}{n}S_o} S_o \tag{17}$$

where

$S_o = n/s_o$ is the Vergence of the original wavefront

$S_p = n/s_p$ is the Vergence of the propagated wavefront

s_o is the vertex distance of the original wavefront (distance along the chief ray from the wavefront to the image point), which is equivalent to the radius of curvature of the original wavefront

s_p is the vertex distance of the propagated wavefront (distance along the chief ray from the wavefront to the image point), which is equivalent to the radius of curvature of the propagated wavefront

n is the refractive index

d is the propagation distance

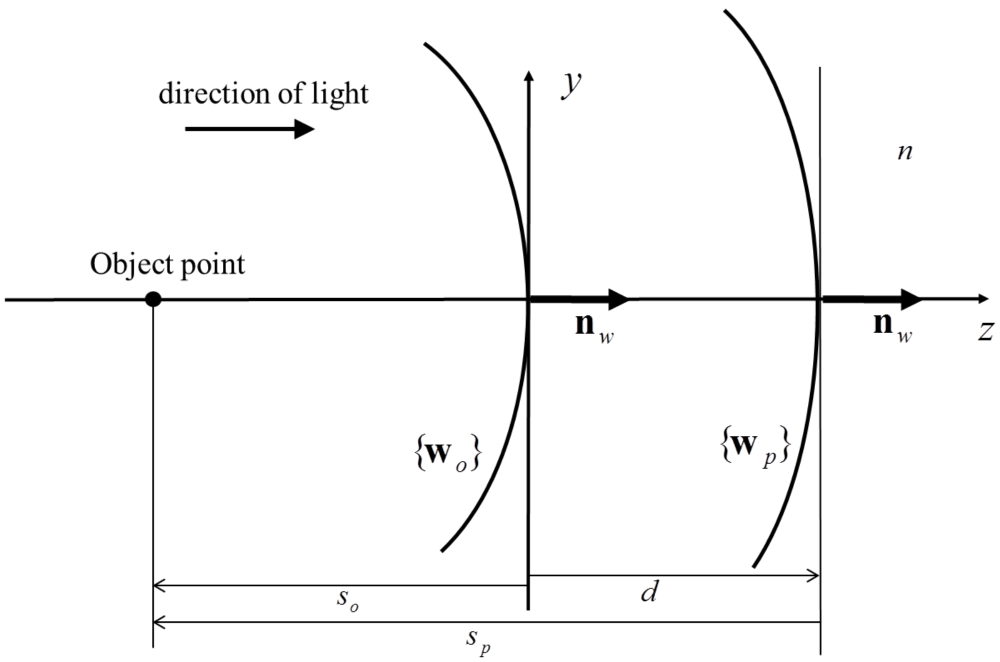

Figure 12: Propagation of a spherical wavefront $\mathbf{w}_o$ with a vergence distance s_o about the distance d to the propagated wavefront $\mathbf{w}_p$ with a vergence distance $s_p = s_o - d$. For the aberrations of second order the propagation of a spherical wavefront with the Vergence $S_o = n/s_o$ is described by the propagation or Transfer equation $S_p = \frac{1}{1-\frac{d}{n}S_o} S_o$.

In literature, the notion of vergences is usually extended to 3-dimensional space for describing the sphero-cylindrical power of a wavefront in terms of 2×2 vergence matrices [25,52,53] of the shape $n\begin{pmatrix} w_o^{(2,0)} & w_o^{(1,1)} \\ w_o^{(1,1)} & w_o^{(2,0)} \end{pmatrix}$, for $w_o(x,y)$ and similarly for $w_p(x,y)$.

$$\mathbf{S}_o = \begin{pmatrix} S_{o,xx} & S_{o,xy} \\ S_{o,xy} & S_{o,yy} \end{pmatrix} = n\begin{pmatrix} w_o^{(2,0)} & w_o^{(1,1)} \\ w_o^{(1,1)} & w_o^{(0,2)} \end{pmatrix}, \qquad \mathbf{S}_p = \begin{pmatrix} S_{p,xx} & S_{p,xy} \\ S_{p,xy} & S_{p,yy} \end{pmatrix} = n\begin{pmatrix} w_p^{(2,0)} & w_p^{(1,1)} \\ w_p^{(1,1)} & w_p^{(0,2)} \end{pmatrix} \tag{18}$$

The relation between the components of Eq. (18) and the ophthalmic terms $sph, cyl, axis$ are well known [25] and described in Chapter 2.3.1 by Eq. (13).

One well-established generalization of Eq. (11) relating the components of Eq. (18) to each other is the "Generalized Propagation Equation". It describes the propagation of an astigmatic wavefront [7,24 ,32,47,48] written in compact form in terms of vergence matrices,

$$\mathbf{S}_p = \frac{1}{\mathbf{1} - \frac{d}{n}\mathbf{S}_o}\mathbf{S}_o, \tag{19}$$

where we have introduced the unit matrix

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{20}$$

Additionally to the description in terms of vergence matrices, an equivalent description is common in the 3-dimensional vector space of power vectors [47,54]. In [49] also the "Generalized Propagation Equation" in terms of power vectors is described.

2.3.3. Reflection

For the aberrations of second order the reflection of a spherical wavefront with orthogonal incidence onto a spherical surface with the Surface Power $\bar{S}$ (see Figure 13) is described by the vergence equation:

$$S' = S + \bar{S} \tag{21}$$

which is equivalent to

$$\frac{1}{s} + \frac{1}{s'} = \frac{2}{r} \tag{22}$$

where

$S = n/s$ is the Vergence of the incoming wavefront

$S' = -n/s'$ is the Vergence of the reflected wavefront

$\bar{S} = -2n/r$ is the Surface Power

s is the vertex distance at the object side (Axial distance from the reflective 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 reflective surface to the image point), which is equivalent to the radius of curvature of the reflected wavefront

r is the radius of curvature of the reflective surface (distance from the reflective surface to the center point of the reflective surface)

n is the refractive index

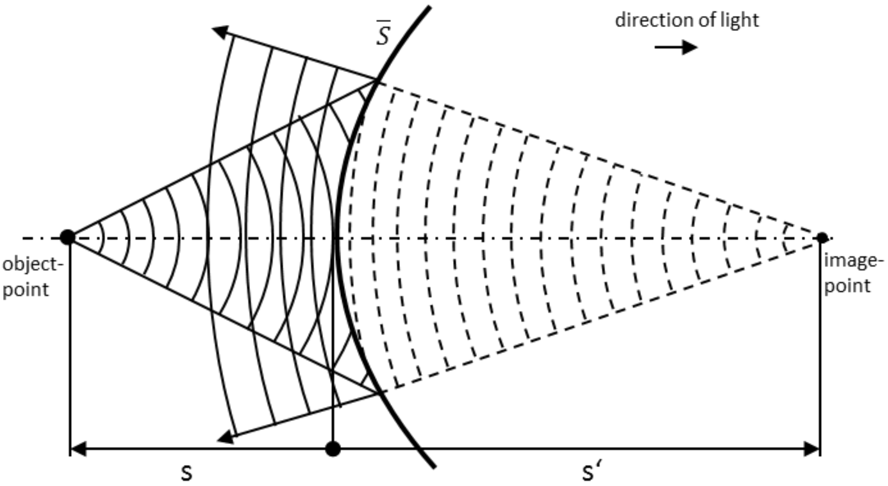

Figure 13: For the aberrations of second order the reflection of a spherical wavefront with vergence $S = n/s$ with orthogonal incidence onto a spherical surface with the Surface Power $\bar{S} = -2n/r$ is described by the vergence equation. The vergence $S' = -n/s'$ of the reflected wavefront is equal to the sum of the vergence of the incoming wavefront and the Surface Power $S' = S + \bar{S}$.

For the incoming and the reflected wavefront, as well as the reflective surface we introduce the power vectors

$$\mathbf{s} = \begin{pmatrix} S_{xx} \\ S_{xy} \\ S_{yy} \end{pmatrix} = n \begin{pmatrix} w_{\text{In}}^{(2,0)} \\ w_{\text{In}}^{(1,1)} \\ w_{\text{In}}^{(0,2)} \end{pmatrix}, \qquad \mathbf{s}' = \begin{pmatrix} S'_{xx} \\ S'_{xy} \\ S'_{yy} \end{pmatrix} = -n \begin{pmatrix} w'^{(2,0)}_{\text{Out}} \\ w'^{(1,1)}_{\text{Out}} \\ w'^{(0,2)}_{\text{Out}} \end{pmatrix}, \qquad \bar{\mathbf{s}} = \begin{pmatrix} \bar{S}_{xx} \\ \bar{S}_{xy} \\ \bar{S}_{yy} \end{pmatrix} = -2n \begin{pmatrix} \bar{w}_{\text{S}}^{(2,0)} \\ \bar{w}_{\text{S}}^{(1,1)} \\ \bar{w}_{\text{S}}^{(0,2)} \end{pmatrix} \tag{23}$$

The relation between the components of Eq. (23) and the ophthalmic terms $sph, cyl, axis$ are well known [25] and described in Chapter 2.3.1 by Eq. (13).

One well-established generalization of Eq. (21) relating the components of Eq. (23) to each other 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 [1,4,5,8].

The most general case is characterized by an astigmatic wavefront hitting an astigmatic surface under oblique incidence, but such that no special orientation between the refracting plane, the directions of principle Power of the incoming wavefront and those of the reflective surface has to be assumed at all. This is the most complex case in compact form written in terms of power vectors

$$\bar{\mathbf{s}} = \tilde{\mathbf{C}}(\mathbf{s}' - \mathbf{s}) \tag{24}$$

where we have introduced the matrices

$$\tilde{\mathbf{C}} = \begin{pmatrix} \cos^{-1}\varepsilon & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \cos\varepsilon \end{pmatrix} \tag{25}$$

2.3.4. Power Vectors

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

$$\mathbf{e}_k = \begin{pmatrix} E_{x\ldots xx} \\ E_{x\ldots xy} \\ \vdots \\ E_{y\ldots yy} \end{pmatrix} := n \begin{pmatrix} w_{\mathrm{In}}^{(k,0)} \\ w_{\mathrm{In}}^{(k-1,1)} \\ \vdots \\ w_{\mathrm{In}}^{(0,k)} \end{pmatrix}, \quad \mathbf{e}'_k = \begin{pmatrix} E'_{x\ldots xx} \\ E'_{x\ldots xy} \\ \vdots \\ E'_{y\ldots yy} \end{pmatrix} := n' \begin{pmatrix} w'^{(k,0)}_{\mathrm{Out}} \\ w'^{(k-1,1)}_{\mathrm{Out}} \\ \vdots \\ w'^{(0,k)}_{\mathrm{Out}} \end{pmatrix}, \quad \bar{\mathbf{e}}_k = \begin{pmatrix} \bar{E}_{x\ldots xx} \\ \bar{E}_{x\ldots xy} \\ \vdots \\ \bar{E}_{y\ldots yy} \end{pmatrix} := (n'-n) \begin{pmatrix} \bar{w}_{\mathrm{S}}^{(k,0)} \\ \bar{w}_{\mathrm{S}}^{(k-1,1)} \\ \vdots \\ \bar{w}_{\mathrm{S}}^{(0,k)} \end{pmatrix}, \tag{26}$$

in the case of refraction and

$$\mathbf{e}_k = \begin{pmatrix} E_{x\ldots xx} \\ E_{x\ldots xy} \\ \vdots \\ E_{y\ldots yy} \end{pmatrix} := n \begin{pmatrix} w_{\mathrm{In}}^{(k,0)} \\ w_{\mathrm{In}}^{(k-1,1)} \\ \vdots \\ w_{\mathrm{In}}^{(0,k)} \end{pmatrix}, \quad \mathbf{e}'_k = \begin{pmatrix} E'_{x\ldots xx} \\ E'_{x\ldots xy} \\ \vdots \\ E'_{y\ldots yy} \end{pmatrix} := -n \begin{pmatrix} w'^{(k,0)}_{\mathrm{Out}} \\ w'^{(k-1,1)}_{\mathrm{Out}} \\ \vdots \\ w'^{(0,k)}_{\mathrm{Out}} \end{pmatrix}, \quad \bar{\mathbf{e}}_k = \begin{pmatrix} \bar{E}_{x\ldots xx} \\ \bar{E}_{x\ldots xy} \\ \vdots \\ \bar{E}_{y\ldots yy} \end{pmatrix} := -2n \begin{pmatrix} \bar{w}_{\mathrm{S}}^{(k,0)} \\ \bar{w}_{\mathrm{S}}^{(k-1,1)} \\ \vdots \\ \bar{w}_{\mathrm{S}}^{(0,k)} \end{pmatrix}, \tag{27}$$

in the case of reflection, 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. (15) can also be extended to all $k \geq 2$ by the definition

$$\mathbf{C}'_k = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \cos\varepsilon' & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cos^k \varepsilon' \end{pmatrix}, \qquad \mathbf{C}_k = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \cos\varepsilon & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cos^k \varepsilon \end{pmatrix}. \tag{28}$$

and Eq. (25) can also be extended to all $k \geq 2$ by the definition

$$\tilde{\mathbf{C}}_k = \begin{pmatrix} \cos^{-1}\varepsilon & 0 & \cdots & 0 \\ 0 & 1 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & \cos^{k-1}\varepsilon \end{pmatrix}. \tag{29}$$

3. Derivation of the Refraction Equations

3.1. Mathematical Approach in the 2D Case

3.1.1. Coordinates in the 2D case

For giving insight into the method with smallest possible effort, we first treat in detail a fictitious two-dimensional problem in which the third space dimension does not exist. Later we will transfer the corresponding approach to the three-dimensional case, i.e. the case of interest, but now we will for an instant 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, shall still be called 'surface'). All rays and normal vectors then lie in that plane, too. We summarize this situation in 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 x-direction, but this is by no means necessary since it is inherent to the mathematics of the two-component system that any ray deflection in a direction other that in the given plane cannot occur.

The two-dimensional version of the rotation matrix takes the form

$$\mathbf{R}(\varepsilon)=\begin{pmatrix}\cos\varepsilon & -\sin\varepsilon\\ \sin\varepsilon & \cos\varepsilon\end{pmatrix}. \tag{30}$$

3.1.2. Description of Wavefronts in the 2D case

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

$$\mathbf{w}_{\mathrm{In}}(y)=\begin{pmatrix} y\\ w_{\mathrm{In}}(y)\end{pmatrix} \tag{31}$$

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

$$w_{\mathrm{In}}(y)=\sum_{k=0}^{\infty}\frac{a_{\mathrm{In},k}}{k!}y^k \tag{32}$$

which corresponds to Eq. (8) in the 3D case. Equivalently, we represent the outgoing wavefront and the refractive surface in their preferred coordinate frames by the vectors

$$\mathbf{w'}_{\text{Out}}(y') = \begin{pmatrix} y' \\ w'_{\text{Out}}(y') \end{pmatrix}, \qquad \bar{\mathbf{w}}_{\text{S}}(\bar{y}) = \begin{pmatrix} \bar{y} \\ \bar{w}_{\text{S}}(\bar{y}) \end{pmatrix} \tag{33}$$

where

$$w'_{\text{Out}}(y') = \sum_{k=0}^{\infty} \frac{a'_{\text{Out},k}}{k!} y'^k, \qquad \bar{w}_{\text{S}}(\bar{y}) = \sum_{k=0}^{\infty} \frac{\bar{a}_{\text{S},k}}{k!} \bar{y}^k, \tag{34}$$

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

$$a_{\text{In},k} = \frac{\partial^k}{\partial y^k} w_{\text{In}}(y)\bigg|_{y=0} = w_{\text{In}}^{(k)}(0) \tag{35}$$

In the 2D case the vector $\mathbf{e}_k$ in Eq. (26) reduces to a scalar $E_k = nw_{\text{In}}^{(k)} = na_{\text{In},k}$, e.g. for second and third-order aberrations, we have $E_2 = nw_{\text{In}}^{(2)} = na_2$, $E_3 = nw_{\text{In}}^{(3)} = na_3$, 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 $a'_{\text{Out},k}$, $\bar{a}_{\text{S},k}$ by multiplication with the refractive index n' for the outgoing wavefront and with 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. Additionally, 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. $a_{\text{In},k} = 0$, $a'_{\text{Out},k} = 0$, $\bar{a}_{\text{S},k} = 0$ for $k < 2$.

3.1.3. 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 introduce the function

$$\mathbf{n}(v) := \frac{1}{\sqrt{1+v^2}} \begin{pmatrix} -v \\ 1 \end{pmatrix}. \qquad (36)$$

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 $\mathbf{n}^{(1)}(0) \equiv \partial/\partial v\, \mathbf{n}(v)\big|_{v=0}$, $\mathbf{n}^{(2)}(0) \equiv \partial^2/\partial v^2\, \mathbf{n}(v)\big|_{v=0}$, etc.:

$$\mathbf{n}(0) := \begin{pmatrix} 0 \\ 1 \end{pmatrix},\ \mathbf{n}^{(1)}(0) := \begin{pmatrix} -1 \\ 0 \end{pmatrix},\ \mathbf{n}^{(2)}(0) := \begin{pmatrix} 0 \\ -1 \end{pmatrix},\ \mathbf{n}^{(3)}(0) := \begin{pmatrix} 3 \\ 0 \end{pmatrix},\ \mathbf{n}^{(4)}(0) := \begin{pmatrix} 0 \\ 9 \end{pmatrix}, \text{ etc.,} \qquad (37)$$

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

$$\begin{aligned}
\frac{\partial}{\partial y}\mathbf{n}_{\mathrm{In}}(y)\Big|_{y=0} &\equiv \mathbf{n}_{\mathrm{In}}^{(1)}(0) = \mathbf{n}^{(1)}(0) w_{\mathrm{In}}^{(2)}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix} w_{\mathrm{In}}^{(2)}(0) \\
\frac{\partial}{\partial y'}\mathbf{n}'_{\mathrm{Out}}(y')\Big|_{y'=0} &\equiv \mathbf{n}'^{(1)}_{\mathrm{Out}}(0) = \mathbf{n}^{(1)}(0) w'^{(2)}_{\mathrm{Out}}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix} w'^{(2)}_{\mathrm{Out}}(0) \qquad (38) \\
\frac{\partial}{\partial \bar{y}}\overline{\mathbf{n}}_{\mathrm{S}}(\bar{y})\Big|_{\bar{y}=0} &\equiv \overline{\mathbf{n}}_{\mathrm{S}}^{(1)}(0) = \mathbf{n}^{(1)}(0) \overline{w}_{\mathrm{S}}^{(2)}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \overline{w}_{\mathrm{S}}^{(2)}(0),
\end{aligned}$$

and similarly for the higher derivatives.

3.1.4. 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. (32)-(35)) are determined for all orders $2 \le k \le k_0$ for the order k_0 of interest, and to assign values to its corresponding local aberrations.

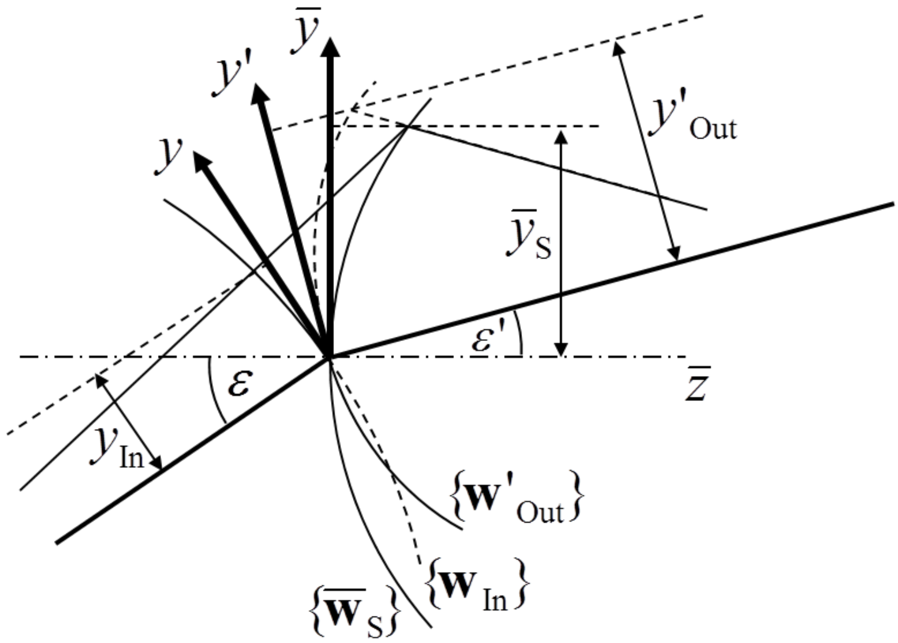

Figure 14: Shown are the local coordinates systems of the refractive surface, of the incoming wavefront and of the outgoing wavefront in the true situation in which the origins of all coordinate systems coincide. While the chief ray and the coordinate systems are fixed, a neighboring ray scans the incoming 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 $\{\mathbf{w}'_{\mathrm{Out}}\}$. Except for the limiting case $y_{\mathrm{In}} \to 0$, the three points in space, $\mathbf{w}_{\mathrm{In}}, \mathbf{w}'_{\mathrm{Out}}, \bar{\mathbf{w}}_{\mathrm{S}}$, do in general not coincide. Consistently with our notation, we denote as y_{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'_{Out}, and the projection of the intersection with $\{\bar{\mathbf{w}}_{\mathrm{S}}\}$ onto the $\bar{y}$ axis is called $\bar{y}_{\mathrm{S}}$.

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 $\{.\}$ shall denote the entity of vectors described by Eqs. (31),(33) (see Figure 14 and Figure 15). Except for the limiting case $y_{\mathrm{In}} \to 0$, the three points in space, $\mathbf{w}_{\mathrm{In}}, \mathbf{w}'_{\mathrm{Out}}, \bar{\mathbf{w}}_{\mathrm{S}}$, do in general not coincide. As shown in Figure 14 and Figure 15, and consistently with our notation, we denote as y_{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'_{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 Figure 14. 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 Figure 14).

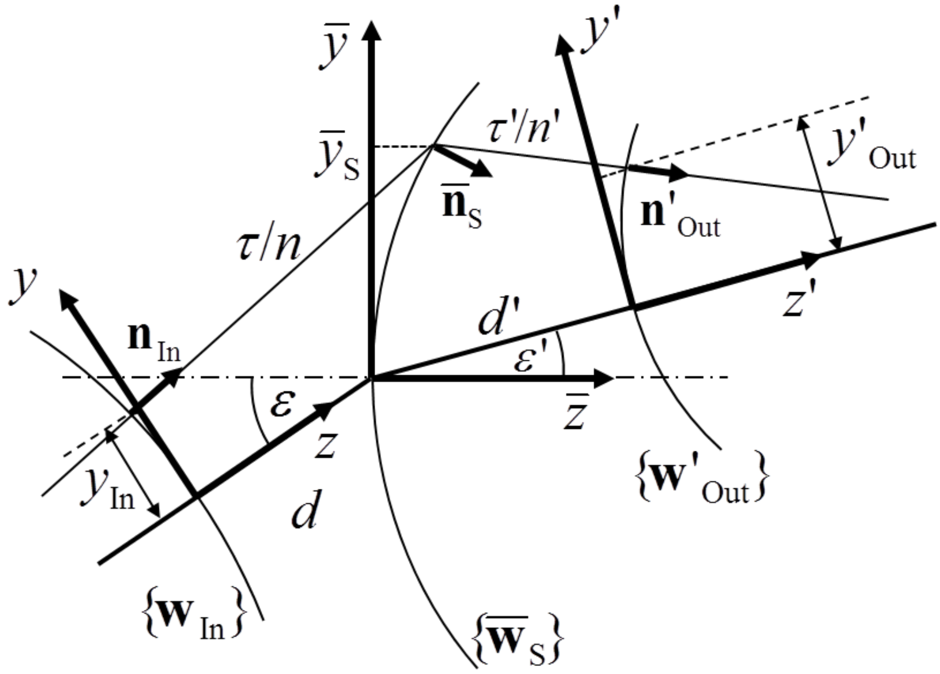

Figure 15: Shown is a fictitious situation of separated origins by *d* and *d'* for a better understanding of the nomenclature. The surface normal vectors along the neighboring ray are also drawn, referred to as $\bar{\mathbf{n}}_{\mathrm{In}}$, $\bar{\mathbf{n}}_{\mathrm{S}}$, $\bar{\mathbf{n}}_{\mathrm{Out}}$ in the common global system $(\bar{x}, \bar{y}, \bar{z})$. 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.

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 Figure 15. The true situation is $d = d' = 0$, which is relevant throughout the thesis.

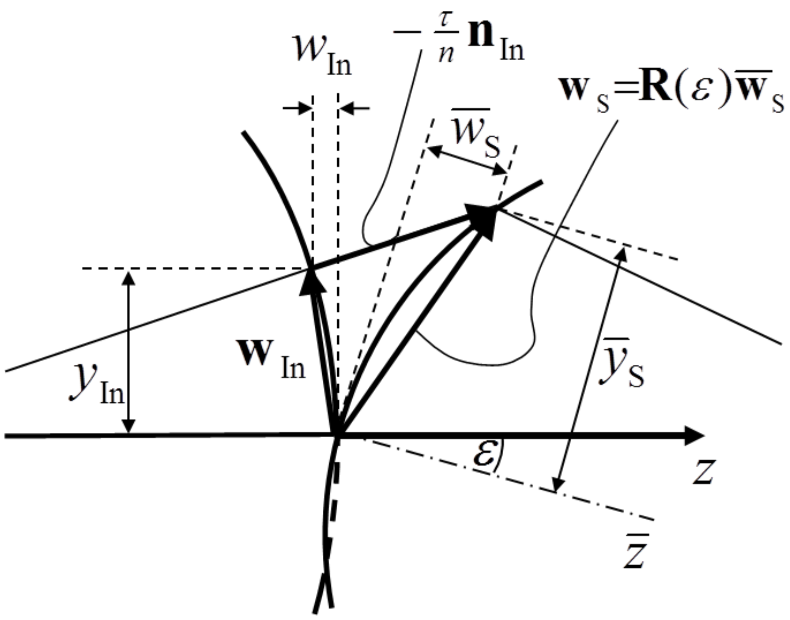

Figure 16: The vector $\mathbf{w}_{\mathrm{In}} = \mathbf{w}_{\mathrm{In}}(y_{\mathrm{In}})$ (see Eq. (31)) points to the neighboring ray's intersection point with the incoming wavefront, and the wavefront's OPD referred to the refractive surface along the ray is denoted by τ, correspondingly the vector 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 $\mathbf{w}_{\mathrm{S}} = \mathbf{R}(\varepsilon)\overline{\mathbf{w}}_{\mathrm{S}}$ (see Eq. (1)) yields the first one of the fundamental equations in Eq. (39).

While in Figure 14 and Figure 15 all quantities are drawn in their preferred frames, Figure 16 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. (31)) 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 τ, whereas the absolute value τ is defined by the optical path distance between the neighboring ray's intersection point with the incoming wavefront and the refractive surface and the sign of τ is determined by the relative position of the these intersection points. If the intersection point of the ray with the wavefront is before the intersection point of the ray with the refractive surface the OPD will be negative $(\tau < 0)$, and if the ray first intersects the refractive surface the OPD will be positive $(\tau > 0)$. Therefore the vector from the incoming wavefront to the surface is $-\tau/n\mathbf{n}_{\mathrm{In}}$, determined by the product of the OPD and the normal unit vector of the incoming wavefront. 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 $\mathbf{w}_{\mathrm{S}} = \mathbf{R}(\varepsilon)\overline{\mathbf{w}}_{\mathrm{S}}$ (see Eq. (1)) yields the first one of the fundamental equations in Eq. (39).

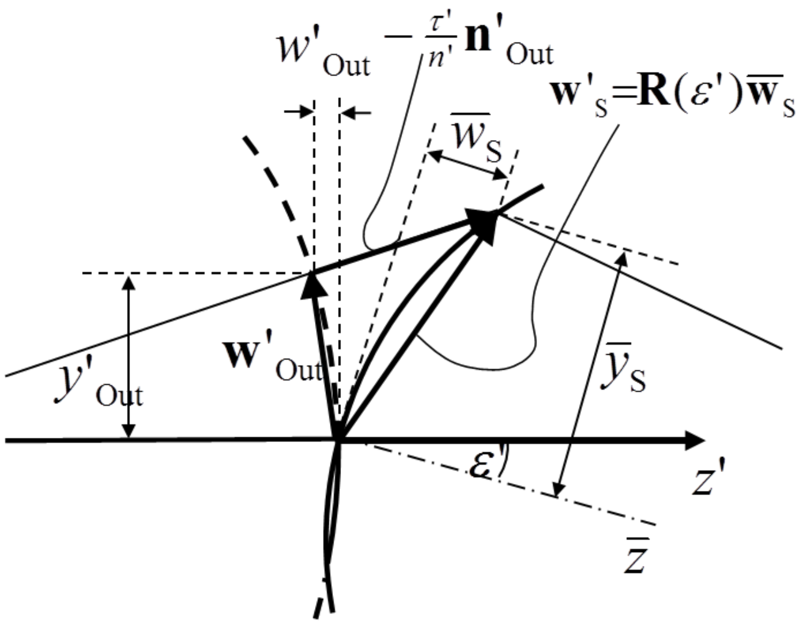

Figure 17: The vector $\mathbf{w'}_{\text{Out}} = \mathbf{w'}_{\text{Out}}(y'_{\text{Out}})$ (see Eq. (33)) points to the neighboring ray's intersection point with the outgoing wavefront, and the wavefront's OPD referred to the refractive surface along the ray is denoted by τ', correspondingly the vector from the wavefront to the surface is $-\tau'/n'\mathbf{n'}_{\text{Out}}$. Hence, the vector to the point on the surface itself, $\mathbf{w'}_{\text{S}}$, must be equal to the vector sum $\mathbf{w'}_{\text{S}} = \mathbf{w'}_{\text{Out}} - \tau'/n'\,\mathbf{n'}_{\text{Out}}$. Transforming $\mathbf{w'}_{\text{S}}$ to its preferred frame by $\mathbf{w}_{\text{S}} = \mathbf{R}(\varepsilon')\overline{\mathbf{w}}_{\text{S}}$ (see Eq. (1)) yields the second one of the fundamental equations in Eq. (39).

Analogously we have $\mathbf{w'}_{\text{Out}} - \tau'/n'\mathbf{n'}_{\text{Out}} = \mathbf{w'}_{\text{S}}$ for the outgoing wavefront in the frame (y', z'), yielding the second equation in Eq. (39) (see Figure 17). The sum of the OPD from the ray's intersection point with the incoming wavefront to the refractive surface $(-\tau)$ and the OPD from the refractive surface to the ray's intersection point with the outgoing wavefront (τ') has to be constant, and in the true situation with $d = d' = 0$ yields $-\tau + \tau' = 0$. Therefore the 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.

$$\begin{aligned} \begin{pmatrix} y_{\text{In}} \\ w_{\text{In}}(y_{\text{In}}) \end{pmatrix} - \frac{\tau}{n}\mathbf{n}_{\text{In}} &= \mathbf{R}(\varepsilon)\begin{pmatrix} \bar{y}_{\text{S}} \\ \bar{w}_{\text{S}}(\bar{y}_{\text{S}}) \end{pmatrix} \\ \begin{pmatrix} y'_{\text{Out}} \\ w'_{\text{Out}}(y'_{\text{Out}}) \end{pmatrix} - \frac{\tau}{n'}\mathbf{n'}_{\text{Out}} &= \mathbf{R}(\varepsilon')\begin{pmatrix} \bar{y}_{\text{S}} \\ \bar{w}_{\text{S}}(\bar{y}_{\text{S}}) \end{pmatrix} \end{aligned} \tag{39}$$

From Eq. (39), 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 $\bar{w}_{\text{S}}(\bar{y}_{\text{S}})$ as the unknown function. Although only the surface is of interest, in Eq. (39) additionally the four quantities τ , y_{In} , y'_{Out} , $\bar{y}_{\mathrm{S}}$ are also unknown. However, they are not independent from each other: if any one of them is given, the other three ones can no longer be chosen independently. We use $\bar{y}_{\mathrm{S}}$ as independent variable and to consider the three other unknowns τ , y_{In} , y'_{Out} as functions of it.

Eq. (39) 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 only interested in a solution 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

$$\mathbf{p}(\bar{y}_{\mathrm{S}}) = \begin{pmatrix} y_{\mathrm{In}}(\bar{y}_{\mathrm{S}}) \\ y'_{\mathrm{Out}}(\bar{y}_{\mathrm{S}}) \\ \tau(\bar{y}_{\mathrm{S}}) \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix} \tag{40}$$

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 these Eq. (39) 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. (39), we distinguish if the independent variable $\bar{y}_{\mathrm{S}}$ enters into Eq. (39) explicitly like 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. (40). To this end, we define the function $\left(\mathrm{IR}^4 \times \mathrm{IR}\right) \mapsto \mathrm{IR}^4 : (\mathbf{p}, \bar{y}_{\mathrm{S}}) \mapsto \mathbf{f}$ by

$$\mathbf{f}(\mathbf{p}, \bar{y}_{\mathrm{S}}) = \begin{pmatrix} y_{\mathrm{In}} - \frac{\tau}{n} n_y\left(w_{\mathrm{In}}^{(1)}(y_{\mathrm{In}})\right) \quad -\left(\bar{y}_{\mathrm{S}} \cos\varepsilon - \bar{w}_{\mathrm{S}} \sin\varepsilon\right) \\ w_{\mathrm{In}}(y_{\mathrm{In}}) - \frac{\tau}{n} n_z\left(w_{\mathrm{In}}^{(1)}(y_{\mathrm{In}})\right) \quad -\left(\bar{y}_{\mathrm{S}} \sin\varepsilon + \bar{w}_{\mathrm{S}} \cos\varepsilon\right) \\ y'_{\mathrm{Out}} - \frac{\tau}{n'} n'_y\left(w'^{(1)}_{\mathrm{Out}}(y'_{\mathrm{Out}})\right) - \left(\bar{y}_{\mathrm{S}} \cos\varepsilon' - \bar{w}_{\mathrm{S}} \sin\varepsilon'\right) \\ w'_{\mathrm{Out}}(y'_{\mathrm{Out}}) - \frac{\tau}{n'} n'_z\left(w'^{(1)}_{\mathrm{Out}}(y'_{\mathrm{Out}})\right) - \left(\bar{y}_{\mathrm{S}} \sin\varepsilon' + \bar{w}_{\mathrm{S}} \cos\varepsilon'\right) \end{pmatrix}, \tag{41}$$

where $(p_1, p_2, p_3, p_4) = (y_{\mathrm{In}}, y'_{\mathrm{Out}}, \tau, \bar{w}_{\mathrm{S}})$ are the components of $\mathbf{p}$. Setting now $\mathbf{p} = \mathbf{p}(\bar{y}_{\mathrm{S}})$, Eq. (41) allows rewriting the fundamental system of Eq. (39) in a more compact way as

$$\mathbf{f}\left(\mathbf{p}(\bar{y}_{\mathrm{S}}), \bar{y}_{\mathrm{S}}\right) = \mathbf{0} \tag{42}$$

as can be verified explicitly by component wise comparison with Eq. (39).

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. (42) with respect to $\bar{y}_{\mathrm{S}}$, evaluated in the origin. The advantage of the form of Eq. (42) using Eq. (41) is that the various terms can be tracked in a fairly compact manner.

The total derivative of $\mathbf{f}\left(\mathbf{p}(\bar{y}_{\mathrm{S}}), \bar{y}_{\mathrm{S}}\right)$ in Eq. (42) 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 $p_i(\bar{y}_{\mathrm{S}})$, plus the partial derivative of $\mathbf{f}$ with respect to the explicit dependence on $\bar{y}_{\mathrm{S}}$. This transforms the system of algebraic equations in Eq. (39) to the system of differential equations

$$\sum_{j=1}^{4} \frac{\partial f_i}{\partial p_j} p_j^{(1)}(\bar{y}_{\mathrm{S}}) + \frac{\partial f_i}{\partial \bar{y}_{\mathrm{S}}} = 0, \quad i = 1,...,4, \tag{43}$$

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 $\mathbf{p} = \mathbf{p}(\bar{y}_{\mathrm{S}})$. The Jacobian $\mathbf{A}$ reads

$$\mathbf{A} := \begin{pmatrix} \frac{\partial f_1}{\partial y_{\mathrm{In}}} & \frac{\partial f_1}{\partial y'_{\mathrm{Out}}} & \frac{\partial f_1}{\partial \tau} & \frac{\partial f_1}{\partial \bar{w}_{\mathrm{S}}} \\ \frac{\partial f_2}{\partial y_{\mathrm{In}}} & \frac{\partial f_2}{\partial y'_{\mathrm{Out}}} & \frac{\partial f_2}{\partial \tau} & \frac{\partial f_2}{\partial \bar{w}_{\mathrm{S}}} \\ \frac{\partial f_3}{\partial y_{\mathrm{In}}} & \frac{\partial f_3}{\partial y'_{\mathrm{Out}}} & \frac{\partial f_3}{\partial \tau} & \frac{\partial f_3}{\partial \bar{w}_{\mathrm{S}}} \\ \frac{\partial f_4}{\partial y_{\mathrm{In}}} & \frac{\partial f_4}{\partial y'_{\mathrm{Out}}} & \frac{\partial f_4}{\partial \tau} & \frac{\partial f_4}{\partial \bar{w}_{\mathrm{S}}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\tau}{n} n_{\mathrm{In},y}^{(1)} w_{\mathrm{In}}^{(2)} & 0 & -\frac{1}{n} n_{\mathrm{In},y} & \sigma \\ w_{\mathrm{In}}^{(1)} - \frac{\tau}{n} n_{\mathrm{In},z}^{(1)} w_{\mathrm{In}}^{(2)} & 0 & -\frac{1}{n} n_{\mathrm{In},z} & -\chi \\ 0 & 1 - \frac{\tau}{n'} n'^{(1)}_{\mathrm{Out},y} w'^{(2)}_{\mathrm{Out}} & -\frac{1}{n'} n'_{\mathrm{Out},y} & \sigma' \\ 0 & w'^{(1)}_{\mathrm{Out}} - \frac{\tau}{n'} n'^{(1)}_{\mathrm{Out},z} w'^{(2)}_{\mathrm{Out}} & -\frac{1}{n'} n'_{\mathrm{Out},z} & -\chi' \end{pmatrix} \tag{44}$$

where for convenience we have introduced $\sigma = \sin\varepsilon$, $\chi = \cos\varepsilon$, and similar for ε'. In Eq. (44), the occurring expressions are understood as $w_{\mathrm{In}}^{(1)} \equiv w_{\mathrm{In}}^{(1)}(y_{\mathrm{In}})$, $w_{\mathrm{In}}^{(2)} \equiv w_{\mathrm{In}}^{(2)}(y_{\mathrm{In}})$, $n_{\mathrm{In},y} \equiv n_{\mathrm{In},y}(w_{\mathrm{In}}^{(1)}(y_{\mathrm{In}}))$, $n_{\mathrm{In},y}^{(1)} \equiv n_{\mathrm{In},y}^{(1)}(w_{\mathrm{In}}^{(1)}(y_{\mathrm{In}}))$, etc, and analogously for the 'Out' quantities, and additionally $y_{\mathrm{In}}, y'_{\mathrm{Out}}, \tau, \bar{w}_{\mathrm{S}}$ are themselves functions of $\bar{y}_{\mathrm{S}}$.

The derivative vector $\partial f_i / \partial \bar{y}_{\mathrm{S}}$ in Eq. (43) shall be summarized as

$$\mathbf{b} := -\frac{\partial \mathbf{f}}{\partial \bar{y}_{\mathrm{S}}} = \begin{pmatrix} \chi \\ \sigma \\ \chi' \\ \sigma' \end{pmatrix}, \tag{45}$$

Both $\mathbf{A}$ and $\mathbf{b}$ are deduced from $\mathbf{f}\left(\mathbf{p}(\bar{y}_\mathrm{S}), \bar{y}_\mathrm{S}\right)$ and must in general themselves have the same kind of dependence, i.e. $\mathbf{A}\left(\mathbf{p}(\bar{y}_\mathrm{S}), \bar{y}_\mathrm{S}\right)$ and $\mathbf{b}\left(\mathbf{p}(\bar{y}_\mathrm{S}), \bar{y}_\mathrm{S}\right)$. However, due to the special property of $\mathbf{f}$ to be linear in $\bar{y}_\mathrm{S}$, $\mathbf{b}$ is constant. Additionally, $\mathbf{A}$ has no explicit dependence on $\bar{y}_\mathrm{S}$ besides the implicit dependence via $\mathbf{p}(\bar{y}_\mathrm{S})$. Hence we write $\mathbf{b}$ without argument and $\mathbf{A} = \mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))$, and Eq. (43) can be written in the form

$$\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))\mathbf{p}^{(1)}(\bar{y}_\mathrm{S}) = \mathbf{b}\,. \tag{46}$$

3.1.5. Solving techniques for the fundamental equation

Eq. (46) is the derivative of the fundamental equation in Eq. (42), and therefore it is itself a fundamental equation. But additionally, it allows a stepwise solution for the derivatives $\mathbf{p}^{(k)}(\bar{y}_\mathrm{S} = 0)$ for increasing order k. Formally, Eq. (46) can be solved for $\mathbf{p}^{(1)}(\bar{y}_\mathrm{S})$ by

$$\mathbf{p}^{(1)}(\bar{y}_\mathrm{S}) = \mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\mathbf{b}\,. \tag{47}$$

Eq. (47) holds as a function of $\bar{y}_\mathrm{S}$, but of course for arbitrary $\bar{y}_\mathrm{S}$ both sides of Eq. (47) are unknown. However, evaluating Eq. (47) for $\bar{y}_\mathrm{S} = 0$ exploits that then the right-hand side (rhs) is known because $\mathbf{p}(0) = \mathbf{0}$ is known! In the same manner, Eq. (47) serves as starting point for a recursion scheme by repeated total derivative and evaluation for $\bar{y}_\mathrm{S} = 0$. Remembering that $\mathbf{b}$ is constant, we obtain

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \\
\mathbf{p}^{(2)}(0) &= \left(\mathbf{A}^{-1}\right)^{(1)}\mathbf{b} \\
&\;\;\cdots \\
\mathbf{p}^{(k)}(0) &= \left(\mathbf{A}^{-1}\right)^{(k-1)}\mathbf{b},
\end{aligned} \tag{48}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1)} = \left.\frac{d}{d\bar{y}_\mathrm{S}}\mathbf{A}\left(\mathbf{p}(\bar{y}_\mathrm{S})\right)^{-1}\right|_{\bar{y}_\mathrm{S}=0}$, …, $\left(\mathbf{A}^{-1}\right)^{(k-1)} = \left.\frac{d^{k-1}}{d\bar{y}_\mathrm{S}^{k-1}}\mathbf{A}\left(\mathbf{p}(\bar{y}_\mathrm{S})\right)^{-1}\right|_{\bar{y}_\mathrm{S}=0}$ are total derivatives of the function $\mathbf{A}\left(\mathbf{p}(\bar{y}_\mathrm{S})\right)^{-1}$. The reason why Eq. (48) really does provide solutions for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$ is that in any row of Eq. (48) the entries on the rhs are all known assuming that the equations above are already solved. Although on the rhs there occur implicit derivatives $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, … as well, they are always of an order less than on the left-hand side (lhs). For example, the second row in Eq. (48) reads in explicit form $\mathbf{p}^{(2)}(0)=\sum_{i=1}^{4}\left(\frac{\partial}{\partial p_i}\mathbf{A}(\mathbf{p})^{-1}\right)p_i^{(1)}\Big|_{\bar{y}_\mathrm{S}=0}\cdot\mathbf{b}$ where $\bar{y}_\mathrm{S}=0$ 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 due to the first row in Eq. (48). Generally, the highest derivative of $\mathbf{p}$ occurring in $\left(\frac{d^{k-1}}{d\bar{y}_\mathrm{S}^{k-1}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\right)\Big|_{\bar{y}_\mathrm{S}=0}$ is $\mathbf{p}^{(k-1)}(0)$, which is already known at the stage when $\mathbf{p}^{(k)}(0)$ is to be computed by Eq. (48).

Although looking attractive and formally simple, applying Eq. (48) in practice requires still 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 $\partial^2/\partial p_i \partial p_j$. Both tasks are straightforward to be executed by a computer algebra package but nevertheless lengthy and not the best way how 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! To this purpose, we start the recursion scheme from Eq. (46) instead of Eq. (47). The first $(k-1)$ total derivatives of Eq. (46) are

$$\begin{aligned}
\mathbf{A}\mathbf{p}^{(1)}(0)&=\mathbf{b} &&\text{(a)}\\
\mathbf{A}^{(1)}\mathbf{p}^{(1)}(0)+\mathbf{A}\mathbf{p}^{(2)}(0)&=\mathbf{0} &&\text{(b)}\\
\mathbf{A}^{(2)}\mathbf{p}^{(1)}(0)+2\mathbf{A}^{(1)}\mathbf{p}^{(2)}(0)+\mathbf{A}\mathbf{p}^{(3)}(0)&=\mathbf{0} &&\text{(c)}\\
&\cdots\\
\sum_{j=1}^{k}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0)&=\mathbf{0},\quad k\geq 2 &&\text{(d)}
\end{aligned}\tag{49}$$

where $\mathbf{A}=\mathbf{A}(\mathbf{p}(0))=\mathbf{A}(\mathbf{0})$, and $\mathbf{A}^{(1)}=\frac{d}{d\bar{y}_\mathrm{S}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))\Big|_{\bar{y}_\mathrm{S}=0}$, …, $\mathbf{A}^{(k-j)}=\frac{d^{k-j}}{d\bar{y}_\mathrm{S}^{k-j}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))\Big|_{\bar{y}_\mathrm{S}=0}$ are total derivatives of the function $\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))$. For the last line of Eq. (49) we have applied the formula for the p-th derivative of a product, $(fg)^{(p)}=\sum_{j=0}^{p}\binom{p}{j}f^{(p-j)}g^{(j)}$. Eq. (49) represents a recursion scheme where in each equation containing $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$, only $\mathbf{p}^{(k)}(0)$ (in the last term for

$j = k$) is unknown provided that all previous equations for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k-1)}(0)$ are already solved. A formal solution for $\mathbf{p}^{(k)}(0)$, expressed in terms of its predecessors, is

$$\begin{aligned} \mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \qquad\qquad\qquad , \quad k=1 \\ \mathbf{p}^{(k)}(0) &= -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), \quad k \geq 2. \end{aligned} \tag{50}$$

Although quite different in appearance at first glance, Eq. (50) yields exactly the same solutions as Eq. (48).

3.1.6. Solutions for the General Refraction Equations

In the result for $\mathbf{p}^{(1)}(0)$, the first rows of both Eqs. (48),(50) involve $\mathbf{A}(\mathbf{0})^{-1}$. For obtaining $\mathbf{A}(\mathbf{0})^{-1}$, we evaluate Eq. (44) for $\mathbf{p} = \mathbf{0}$ and apply Eqs. (37), yielding

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1 & 0 & 0 & \sigma \\ 0 & 0 & -1/n & -\chi \\ 0 & 1 & 0 & \sigma' \\ 0 & 0 & -1/n' & -\chi' \end{pmatrix} \Rightarrow \mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} 1 & -n\sigma/\eta & 0 & n'\sigma/\eta \\ 0 & -n\sigma'/\eta & 1 & n'\sigma'/\eta \\ 0 & -nn'\chi'/\eta & 0 & nn'\chi/\eta \\ 0 & n/\eta & 0 & -n'/\eta \end{pmatrix} \text{ with } \eta = n'\chi' - n\chi \tag{51}$$

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

$$\mathbf{p}^{(1)}(0) = \begin{pmatrix} \chi \\ \chi' \\ -n\sigma \\ 0 \end{pmatrix} \tag{52}$$

For the orders $k \geq 2$ we apply Eqs. (50). The derivatives $\mathbf{A}^{(1)} = \left.\frac{d}{d\bar{y}_{\mathrm{S}}}\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))\right|_{\bar{y}_{\mathrm{S}}=0}$, etc. are directly obtained by total derivative of Eq. (44) with respect to $\bar{y}_{\mathrm{S}}$, evaluating for $\bar{y}_{\mathrm{S}} = 0$ and again applying Eqs. (37). For the orders $k \geq 2$ only the results $\overline{w}_{\mathrm{S}}^{(k)}(0)$ for the refractive surface are interesting, therefore we directly provide those results. The resulting second-order law is (omitting the argument '(0)')

$$\eta \cdot \overline{w}_{\mathrm{S}}^{(2)} = \chi'^2\, n' w'^{(2)}_{\mathrm{Out}} - \chi^2 n w^{(2)}_{\mathrm{In}} \tag{53}$$

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

$$\begin{aligned} \eta \cdot \overline{w}_{\mathrm{S}}^{(3)} &= \chi'^3\, n' w'^{(3)}_{\mathrm{Out}} - \chi^3 n w^{(3)}_{\mathrm{In}} + R_3 \\ \eta \cdot \overline{w}_{\mathrm{S}}^{(4)} &= \chi'^4\, n' w'^{(4)}_{\mathrm{Out}} - \chi^4 n w^{(4)}_{\mathrm{In}} + R_4 \\ &\dots \\ \eta \cdot \overline{w}_{\mathrm{S}}^{(k)} &= \chi'^k\, n' w'^{(k)}_{\mathrm{Out}} - \chi^k n w^{(k)}_{\mathrm{In}} + R_k \end{aligned} \tag{54}$$

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

$$R_3 = -\frac{3n\sigma\chi\chi'}{\eta}\left(n\, w'^{(2)}_{\mathrm{Out}} - n' w^{(2)}_{\mathrm{In}}\right)\left(\chi' w'^{(2)}_{\mathrm{Out}} - \chi w^{(2)}_{\mathrm{In}}\right) \tag{55}$$

$$\begin{aligned} R_4 = {}& \left(\alpha\, w'^{(2)}_{\mathrm{Out}} + \beta w^{(2)}_{\mathrm{In}}\right) w'^{(3)}_{\mathrm{Out}} + \left(\beta' w'^{(2)}_{\mathrm{Out}} + \alpha' w^{(2)}_{\mathrm{In}}\right) w^{(3)}_{\mathrm{In}} \\ & + \gamma'\left(w'^{(2)}_{\mathrm{Out}}\right)^3 + \delta'\left(w'^{(2)}_{\mathrm{Out}}\right)^2 w^{(2)}_{\mathrm{In}} + \delta w'^{(2)}_{\mathrm{Out}}\left(w^{(2)}_{\mathrm{In}}\right)^2 + \gamma\left(w^{(2)}_{\mathrm{In}}\right)^3 \end{aligned} \tag{56}$$

with

$$\begin{aligned} \alpha &= \frac{2n\sigma\chi'^3}{\eta}\left(n'\chi' - 6n\chi\right) \\ \beta &= \frac{2n\sigma\chi\chi'^2}{\eta}\left(2n'\chi' + 3n\chi\right) \\ \gamma &= \frac{3n\chi^2}{\eta^2}\left(2n'\chi^2\chi'\eta - \sigma^2(n^2\chi^2 + 4n'^2\chi'^2)\right) \\ \delta &= \frac{3n'\chi}{n\eta^2}\left((2n'\chi' + n\chi)(n^2\chi^2 + 2nn'\chi\chi' + 2n'^2\chi'^2)\sigma'^2 - 2\eta(n\chi\chi')^2\right) \end{aligned} \tag{57}$$

and α', β', γ', δ' are obtained from $-\alpha$, $-\beta$, $-\gamma$, $-\delta$, respectively, by interchanging $n \leftrightarrow n'$, $\chi \leftrightarrow \chi'$, $\sigma \leftrightarrow \sigma'$, $\eta \leftrightarrow -\eta$.

Eq. (54) holds likewise for the derivatives and for the coefficients $a_{\mathrm{In},k}$, $a'_{\mathrm{Out},k}$, $\overline{a}_{\mathrm{S},k}$ due to Eqs. (32)-(35). In terms of local aberrations, Eq. (54) reads (after substituting χ, χ' by the cosines)

$$\nu \cdot \overline{E}_k = E'_k \cos^k \varepsilon' - E_k \cos^k \varepsilon + R_k\,, \tag{58}$$

where in R_k all wavefront derivatives are expressed in terms of local aberrations, which describes **for the first time** the relation between the local aberrations of the refracting surface and the incoming and outgoing wavefront.

3.1.7. Generalization of the Coddington Equation

Although application of Eq. (48) or Eq. (50) 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. (55),(56) for R_3 (or R_4) will vanish if we set $w_{\mathrm{In}}^{(j)}=0$ and $w'^{(j)}_{\mathrm{Out}}=0$ 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 only aberrations for one single given order k are present while for all lower orders $j<k$ we have $w_{\mathrm{In}}^{(j)}=0$ and $w'^{(j)}_{\mathrm{Out}}=0$, then $R_k=0$, which means for fixed order k that Eq. (54) will be valid for vanishing remainder term. This assumption can in fact be shown to hold generally.

To this purpose, we start from the recursion scheme in Eq. (50) and show that only the term containing $\mathbf{p}^{(1)}$ can contribute to the sum if all aberrations vanish for order less than k. For doing so, it is necessary to exploit two basic properties of the derivatives $\mathbf{A}^{(m)}=\left.\frac{d^m}{d\bar{y}_{\mathrm{S}}^m}\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))\right|_{\bar{y}_{\mathrm{S}}=0}$ of the matrix $\mathbf{A}$ for the orders $1\le m\le k-1$. As can be shown by element wise differentiation of the matrix $\mathbf{A}$, the highest wavefront derivatives present in $\mathbf{A}^{(m)}(\mathbf{p}(\bar{y}_{\mathrm{S}}))$ (see Eq. (44)) occur in the terms proportional to τ , and those are proportional to either $w_{\mathrm{In}}^{(m+2)}$ or $w'^{(m+2)}_{\mathrm{Out}}$. 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 $w'^{(m+1)}_{\mathrm{Out}}$. It follows that

- i) The highest possible wavefront derivatives present in $\mathbf{A}^{(m)}$ are $w_{\mathrm{In}}^{(m+1)}$ or $w'^{(m+1)}_{\mathrm{Out}}$.
- 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. (50), we notice that the occurring derivatives of the matrix $\mathbf{A}$ are $\mathbf{A}^{(k-1)}$, $\mathbf{A}^{(k-2)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ for $j=1,2,...,(k-1)$, respectively. It follows from property i) that the highest occurring wavefront derivatives in these terms are $k,(k-1),...,3,2$, respectively. Now, if all wavefront derivatives up to order $(k-1)$ vanish, it will follow from property ii) that all the matrix derivatives $\mathbf{A}^{(k-2)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ must vanish, leaving only $\mathbf{A}^{(k-1)}$. Therefore all terms in Eq. (50) vanish, excluding only the contribution for $j=1$. We directly conclude that

$$\begin{aligned}\mathbf{p}^{(k)} &= -\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{p}^{(1)} \\ &= -\left(\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{A}^{-1}\right)\cdot\mathbf{b}\end{aligned}, \qquad k \geq 2 \tag{59}$$

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

$$\mathbf{A}^{(m)} = \begin{pmatrix} -m\chi^{m-1}\sigma w_{\text{In}}^{(m+1)} & 0 & \frac{\chi^m}{n} w_{\text{In}}^{(m+1)} & 0 \\ \chi^m w_{\text{In}}^{(m+1)} & 0 & 0 & 0 \\ 0 & -m\chi'^{m-1}\sigma' w'^{(m+1)}_{\text{Out}} & \frac{\chi'^m}{n'} w_{\text{In}}^{(m+1)} & 0 \\ 0 & \chi'^m w_{\text{In}}^{(m+1)} & 0 & 0 \end{pmatrix}, \tag{60}$$

where $y_{\text{In}}^{(1)}$, $y'^{(1)}_{\text{Out}}$ and $\tau^{(1)}$ have been substituted by their solutions χ, χ' and ns wherever they occur, respectively (see Eq. (52)). Inserting $\mathbf{A}^{(m)}(0)$ for $m = k-1$ and $\mathbf{A}(0)^{-1}$ from Eq. (51) into Eq. (59) yields directly that

$$\eta \cdot \bar{s}^{(k)}(0) = \chi'^k n' w'^{(k)}_{\text{Out}}(0) - \chi^k n w_{\text{In}}^{(k)}(0) \tag{61}$$

for all orders $k \geq 2$.

The resulting refraction equation in the situation of Eq. (61) in terms of local aberrations reads

$$\nu \cdot \overline{E}_k = E'_k \cos^k \varepsilon' - E_k \cos^k \varepsilon, \tag{62}$$

which is indeed Eq. (58) for $R_k = 0$.

3.2. Mathematical Approach in the 3D Case

3.2.1. 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 only report the most important differences. Analogously to Eq. (31), the incoming wavefront is now represented by the 3D vector

$$\mathbf{w}_{\text{In}}(x,y) = \begin{pmatrix} x \\ y \\ w_{\text{In}}(x,y) \end{pmatrix} \tag{63}$$

where $w_{\mathrm{In}}(x, y)$ is given by Eq. (8), 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. (26) for $\mathbf{e}_k$). The outgoing wavefront and the refractive surface are treated similarly.

For treating the normal vectors, we introduce the analogous functions to Eq. (36) as

$$\mathbf{n}(u,v) := \frac{1}{\sqrt{1+u^2+v^2}} \begin{pmatrix} -u \\ -v \\ 1 \end{pmatrix}, \tag{64}$$

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

$$\frac{\mathbf{w}^{(1,0)} \times \mathbf{w}^{(0,1)}}{\left|\mathbf{w}^{(1,0)} \times \mathbf{w}^{(0,1)}\right|} = \frac{1}{\sqrt{1+w^{(1,0)2}+w^{(0,1)2}}} \begin{pmatrix} -w^{(1,0)} \\ -w^{(0,1)} \\ 1 \end{pmatrix} = \mathbf{n}\left(w^{(1,0)}, w^{(0,1)}\right) = \mathbf{n}(\nabla w), \tag{65}$$

In the intersection point we have now $\mathbf{n}_{\mathrm{In}}(0,0) = (0,0,1)^T$, $\mathbf{n}'_{\mathrm{Out}}(0,0) = (0,0,1)^T$, $\bar{\mathbf{n}}_{\mathrm{S}}(0,0) = (0,0,1)^T$, and the derivatives corresponding to Eq. (37) can directly be obtained from Eq. (64).

3.2.2. 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. (39), 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

$$\mathbf{p}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) = \begin{pmatrix} x_{\mathrm{In}}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \\ y_{\mathrm{In}}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \\ x'_{\mathrm{Out}}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \\ y'_{\mathrm{Out}}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \\ \tau(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \\ \bar{s}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}) \end{pmatrix} \tag{66}$$

and the 3D analogue to Eq. (39) leads now to

$$\mathbf{f}\left(\mathbf{p}(\bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}), \bar{x}_{\mathrm{S}}, \bar{y}_{\mathrm{S}}\right) = \mathbf{0} \tag{67}$$

where $\mathbf{f}$ is the 3D analogue to Eq. (41).

One important difference compared to 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

$$\begin{aligned} \mathbf{A}\big(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S})\big)\mathbf{p}^{(1,0)}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S}) &= \mathbf{b}_x \\ \mathbf{A}\big(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S})\big)\mathbf{p}^{(0,1)}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S}) &= \mathbf{b}_y \end{aligned} \tag{68}$$

where the different inhomogeneities are given as column vectors

$$\mathbf{b}_x = -\frac{\partial \mathbf{f}}{\partial \bar{x}_\mathrm{S}} = \begin{pmatrix}1 & 0 & 0 & 1 & 0 & 0\end{pmatrix}^T, \quad \mathbf{b}_y = -\frac{\partial \mathbf{f}}{\partial \bar{y}_\mathrm{S}} = \begin{pmatrix}0 & \chi & \sigma & 0 & \chi' & \sigma'\end{pmatrix}^T. \tag{69}$$

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 $\mathbf{A}(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S}))$ with elements $A_{ij} := \partial f_i / \partial p_j$ is the same for both equations and analogous to Eq. (44) but now of size 6×6. It is practical to provide it in block structure notation

$$\mathbf{A}\big(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S})\big) = \left(\begin{array}{cc|cc} \mathbf{A}_\mathrm{In} & \mathbf{0} & \mathbf{A}_\tau & \overline{\mathbf{A}}_\mathrm{S} \\ \mathbf{0} & \mathbf{A'}_\mathrm{Out} & & \end{array}\right) \tag{70}$$

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

$$\mathbf{A}_\mathrm{In} = \begin{pmatrix} 1-\frac{\tau}{n}\left(n_{\mathrm{In},x}^{(0,1)} w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},x}^{(1,0)} w_\mathrm{In}^{(2,0)}\right) & -\frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)} w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},z}^{(1,0)} w_\mathrm{In}^{(1,1)}\right) \\ -\frac{\tau}{n}\left(n_{\mathrm{In},y}^{(0,1)} w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},y}^{(1,0)} w_\mathrm{In}^{(2,0)}\right) & 1-\frac{\tau}{n}\left(n_{\mathrm{In},y}^{(0,1)} w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},y}^{(1,0)} w_\mathrm{In}^{(1,1)}\right) \\ w_\mathrm{In}^{(1,0)} - \frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)} w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},z}^{(1,0)} w_\mathrm{In}^{(2,0)}\right) & w_\mathrm{In}^{(0,1)} - \frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)} w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},z}^{(1,0)} w_\mathrm{In}^{(1,1)}\right) \end{pmatrix} \tag{71}$$

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

$$\mathbf{A}_\tau = -\begin{pmatrix} n_{\mathrm{In},x}/n \\ n_{\mathrm{In},y}/n \\ n_{\mathrm{In},z}/n \\ n'_{\mathrm{Out},x}/n' \\ n'_{\mathrm{Out},y}/n' \\ n'_{\mathrm{Out},z}/n' \end{pmatrix}, \quad \overline{\mathbf{A}}_\mathrm{S} = \begin{pmatrix} 0 \\ \sigma \\ -\chi \\ 0 \\ \sigma' \\ -\chi' \end{pmatrix} \tag{72}$$

3.2.3. Solutions for the General Refraction Equations

The direct solutions analogously to Eq. (48) are now given by

$$\begin{aligned}
&\mathbf{p}^{(1,0)}(0,0) = \mathbf{A}^{-1}\mathbf{b}_x \\
&\mathbf{p}^{(0,1)}(0,0) = \mathbf{A}^{-1}\mathbf{b}_y \\
&\mathbf{p}^{(2,0)}(0,0) = \left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_x \\
&\mathbf{p}^{(1,1)}(0,0) = \left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_x = \left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_y \\
&\mathbf{p}^{(0,2)}(0,0) = \left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_y \\
&\qquad\ldots \\
&\mathbf{p}^{(k_x,k_y)}(0,0) = \begin{cases} \left(\mathbf{A}^{-1}\right)^{(k_x-1,0)}\mathbf{b}_x & ,\quad k_x \neq 0, k_y = 0 \\ \left(\mathbf{A}^{-1}\right)^{(k_x-1,k_y)}\mathbf{b}_x = \left(\mathbf{A}^{-1}\right)^{(k_x,k_y-1)}\mathbf{b}_y & ,\quad k_x \neq 0, k_y \neq 0 \\ \left(\mathbf{A}^{-1}\right)^{(0,k_y-1)}\mathbf{b}_y & ,\quad k_x = 0, k_y \neq 0 \end{cases}
\end{aligned} \tag{73}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0,0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1,0)} = \frac{d}{d\bar{x}_\mathrm{S}}\mathbf{A}(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S}))^{-1}\Big|_{\bar{x}_\mathrm{S}=0,\bar{y}_\mathrm{S}=0}$,

$\left(\mathbf{A}^{-1}\right)^{(k_x,k_y)} = \frac{d^{k_x}}{d\bar{x}_\mathrm{S}^{k_x}}\frac{d^{k_y}}{d\bar{x}_\mathrm{S}^{k_y}}\mathbf{A}(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S}))^{-1}\Big|_{\bar{x}_\mathrm{S}=0,\bar{y}_\mathrm{S}=0}$, etc. The fact that there are two starting equations (68) 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. (67), for each $\mathbf{p}^{(k_x,k_y)}$ both 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. (51),(52) for the 2D case, we provide here the explicit results

$$\mathbf{A}(\mathbf{0})=\begin{pmatrix}1&0&0&0&0&0\\0&1&0&0&0&\sigma\\0&0&0&0&-1/n&-\chi\\0&0&1&0&0&0\\0&0&0&1&0&\sigma'\\0&0&0&0&-1/n'&-\chi'\end{pmatrix}\Rightarrow\mathbf{A}(\mathbf{0})^{-1}=\begin{pmatrix}1&0&0&0&0&0\\0&1&-n\sigma/\eta&0&0&n'\sigma/\eta\\0&0&0&1&0&0\\0&0&-n\sigma'/\eta&0&1&n'\sigma'/\eta\\0&0&-nn'\chi'/\eta&0&0&nn'\chi/\eta\\0&0&n/\eta&0&0&-n'/\eta\end{pmatrix} \quad (74)$$

and, after application of Eqs. (69),(73) the solutions

$$\mathbf{p}^{(1,0)}(0,0)=\begin{pmatrix}1\\0\\1\\0\\0\\0\end{pmatrix},\qquad \mathbf{p}^{(0,1)}(0,0)=\begin{pmatrix}0\\\chi\\0\\\chi'\\-n\sigma\\0\end{pmatrix} \quad (75)$$

<u>The general result for the refraction equation can be written in the way</u>

$$\eta\overline{w}_{\mathrm{S}}^{(k_x,k_y)}=\chi'^{k_y}\,n'w'^{(k_x,k_y)}_{\mathrm{Out}}-\chi^{k_y}\,nw^{(k_x,k_y)}_{\mathrm{In}}+R_{k_x,k_y}\,, \quad (76)$$

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 x the direction no tilting cosines occur at all. Summarizing all components of Eq. (76) for a fixed value of $k=k_x+k_y$ and applying Eqs. (5),(28),(26) yields the refraction equation in terms of local aberrations,

$$\nu\cdot\overline{\mathbf{e}}_k=\mathbf{C}'_k\,\mathbf{e}'_k-\mathbf{C}_k\mathbf{e}_k+\mathbf{r}_k\,, \quad (77)$$

where $\mathbf{r}_k$ is a vector collecting the remainder terms R_{k_x,k_y} in Eq. (76) analogously to R_k in Eq. (58). Eq. (77) is the general refraction equation for aberrations of any order in the 3D case.

3.2.4. Generalization of the Coddington Equation

Although Eq. (73) 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 $w^{(j_x,j_y)}_{\mathrm{In}}$, $w'^{(j_x,j_y)}_{\mathrm{Out}}$ for all lower orders, i.e. for $j_x+j_y<k_x+k_y$. This works analogously to the treatment of Eqs. (49)-(61), with the only difference that the notation requires more effort.

Analogously to Eq. (50) we obtain as result that

$$\begin{aligned}
\mathbf{p}^{(k_x,0)}(0,0) &= -\mathbf{A}^{-1}\sum_{j_x=1}^{k_x-1}\binom{k_x-1}{j_x-1}\mathbf{A}^{(k_x-j_x,0)}\mathbf{p}^{(j_x,0)}, \qquad k_x \geq 2, k_y = 0 \quad (a)\\
\mathbf{p}^{(k_x,k_y)}(0,0) &= -\mathbf{A}^{-1}\sum_{\substack{j_x\geq 1,\, j_y\geq 0\\ j_x+j_y<k_x+k_y}}\binom{k_x-1}{j_x-1}\binom{k_y}{j_y}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)} \qquad (b)\\
&= -\mathbf{A}^{-1}\sum_{\substack{j_x\geq 0,\, j_y\geq 1\\ j_x+j_y<k_x+k_y}}\binom{k_x}{j_x}\binom{k_y-1}{j_y-1}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)}, \quad k_x \neq 0, k_y \neq 0 \quad (c)\\
\mathbf{p}^{(0,k_y)}(0,0) &= -\mathbf{A}^{-1}\sum_{j_y=1}^{k_y-1}\binom{k_y-1}{j_y-1}\mathbf{A}^{(0,k_y-j_y)}\mathbf{p}^{(0,j_y)}, \qquad k_x = 0, k_y \geq 2 \quad (d)
\end{aligned} \tag{78}$$

where again for $\mathbf{p}^{(k_x,k_y)}$ two formally different solutions occur which are essentially identical. We recognize that Eq. (78) (a) is a special case of Eq. (78) (b) for $k_y = 0$, $j_y = 0$, and similarly Eq. (78) (d) is a special case of Eq. (78) (c) for $k_x = 0$, $j_x = 0$. By means of a similar reasoning as 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. (78) will reduce to the lowest term, yielding

$$\begin{aligned}
\mathbf{p}^{(k_x,0)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,0)}\mathbf{p}^{(1,0)}, \quad k_x \geq 2, k_y = 0 \quad (a)\\
\mathbf{p}^{(k_x,k_y)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,k_y)}\mathbf{p}^{(1,0)} \quad (b)\\
&= -\mathbf{A}^{-1}\mathbf{A}^{(k_x,k_y-1)}\mathbf{p}^{(0,1)}, \quad k_x \neq 0, k_y \neq 0 \quad (c)\\
\mathbf{p}^{(0,k_y)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(0,k_y-1)}\mathbf{p}^{(0,1)}, \quad k_x = 0, k_y \geq 2 \quad (d)
\end{aligned} \tag{79}$$

For finally evaluating Eqs. (78) 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 is given as

$$\mathbf{A}^{(m_x,m_y)} = \left(\begin{array}{cc|cc} \mathbf{A}_{\text{In}}^{(m_x,m_y)} & \mathbf{0} & \mathbf{A}_{\tau}^{(m_x,m_y)} & \overline{\mathbf{A}}_{\text{S}}^{(m_x,m_y)} \\ \mathbf{0} & \mathbf{A'}_{\text{Out}}^{(m_x,m_y)} & & \end{array}\right) \tag{80}$$

with the block

$$\mathbf{A}_{\text{In}}^{(m_x,m_y)} = \begin{pmatrix} -m_y\chi^{m_y-1}\sigma w_{\text{In}}^{(m_x+2,m_y-1)} & -m_y\chi^{m_y-1}\sigma w_{\text{In}}^{(m_x+1,m_y)} \\ -m_y\chi^{m_y-1}\sigma w_{\text{In}}^{(m_x+1,m_y)} & -m_y\chi^{m_y-1}\sigma w_{\text{In}}^{(m_x,m_y+1)} \\ \chi^{m_y} w_{\text{In}}^{(m_x+1,m_y)} & \chi^{m_y} w_{\text{In}}^{(m_x,m_y+1)} \end{pmatrix} \tag{81}$$

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

$$\mathbf{A}_\tau = \begin{pmatrix} \chi^{m_y} w_{\text{In}}^{(m_x+1,m_y)} / n \\ \chi^{m_y} w_{\text{In}}^{(m_x,m_y+1)} / n \\ 0 \\ \chi'^{m_y} w'^{(m_x+1,m_y)}_{\text{Out}} / n' \\ \chi'^{m_y} w'^{(m_x,m_y+1)}_{\text{Out}} / n' \\ 0 \end{pmatrix}, \qquad \overline{\mathbf{A}}_\text{S} = \mathbf{0}, \tag{82}$$

where $x_{\text{In}}^{(1,0)}$, $x_{\text{In}}^{(0,1)}$, $y_{\text{In}}^{(1,0)}$, $y_{\text{In}}^{(0,1)}$, etc. have been substituted by their solutions according to Eq. (75). Inserting $\mathbf{A}^{(m_x,m_y)}$ from Eqs. (80)-(82) and $\mathbf{A}(\mathbf{0})^{-1}$ from Eq. (74) into Eqs. (79) yields one common relation for $\overline{w}_\text{S}^{(k_x,k_y)}$ for the various subcases in Eqs. (79) (omitting the argument ‘ $(0,0)$ ’):

$$\eta\, \overline{w}_\text{S}^{(k_x,k_y)} = \chi'^{k_y}\, n' w'^{(k_x,k_y)}_{\text{Out}} - \chi^{k_y} n\, w_{\text{In}}^{(k_x,k_y)} \tag{83}$$

for all orders $k \geq 2$.

Eq. (83) can be summarized in a similar fashion as Eq. (76) to a vector equation in the very appealing form

$$\nu\, \overline{\mathbf{e}}_k = \mathbf{C}'_k\, \mathbf{e}'_k - \mathbf{C}_k \mathbf{e}_k \tag{84}$$

which is Eq. (77) for $\mathbf{r}_k = \mathbf{0}$. Eq. (84), an interesting result of the present thesis, is the refraction equation for aberrations of fixed order $k \geq 2$ under the assumption that all aberrations with order lower than k vanish.

3.3. Results and Discussion

The derived equations in the previous chapters 3.1 and 3.2 describe the solution for the refractive surface if the incoming and outgoing wavefront is given. Although this is a very interesting topic, as will be shown by example 3.4.1, another 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.

3.3.1. 2D Case

Eq. (62) describes the special case that for given order k the aberrations of the incoming and 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. (62) can be transformed to

$$E'_k \cos^k \varepsilon' = E_k \cos^k \varepsilon + \nu \cdot \overline{E}_k \,. \qquad (85)$$

We could generally show this statement to hold for all orders $k \geq 2$ including as a special case for $k = 2$ the well-known Coddington and Vergence equation. Therefore Eq. (85) represents an interesting result of the present thesis.

Also Eq. (58) 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

$$E'_k \cos^k \varepsilon' = E_k \cos^k \varepsilon + \nu \cdot \overline{E}_k - R_k \,. \qquad (86)$$

Eq. (86) 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. (86) for lower orders.

E.g., 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 the aberrations E_k of the incoming wavefront and $\overline{E}_k$ of the refractive surface are given (see Figure 18). In a first step the aberrations of order $k = 2$ are calculated using Eq. (86), which is in this case identical with the well-known Coddington equation

$$S' \cos^2 \varepsilon' = S \cos^2 \varepsilon + \frac{n' \cos \varepsilon' - n \cos \varepsilon}{n' - n} \cdot \overline{S} \,. \qquad (87)$$

In a second step the aberrations of order $k = 3$ are calculated using Eq. (86) and the results of Eq. (87)

$$E'_3 \cos^3 \varepsilon' = E_3 \cos^3 \varepsilon + \frac{n' \cos \varepsilon' - n \cos \varepsilon}{n' - n} \cdot \overline{E}_3 - R_3 \qquad (88)$$

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

In Figure 18 is the relation described by Eq. (88) exemplified. The incoming wavefront $\{\mathbf{w}_{\mathrm{In}}\}$ hits the refractive surface $\{\overline{\mathbf{w}}_{\mathrm{S}}\}$ by the angle of incidence ε and the outgoing wavefront $\{\mathbf{w}'_{\mathrm{Out}}\}$ emerges with the angle ε'. The incoming wavefront, the refractive surface and the outgoing wavefront show aberrations of second order $(S, \overline{S}, S')$ and third order $(E_3, \overline{E}_3, E'_3)$. The origins of these coordinate systems coincide in the chief ray's intersection point with the refractive surface but they are fictitious separated for a better understanding.

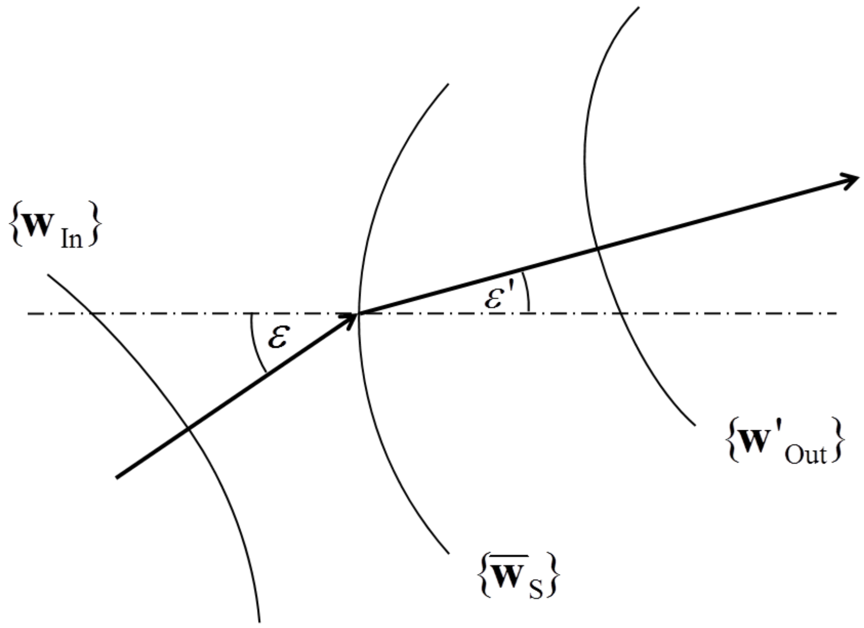

Figure 18: The incoming wavefront $\{\mathbf{w}_{\text{In}}\}$ hits the refractive surface $\{\overline{\mathbf{w}}_{\text{S}}\}$ by the angle of incidence ε and the outgoing wavefront $\{\mathbf{w}'_{\text{Out}}\}$ emerges with the angle ε'. The incoming wavefront, the refractive surface and the outgoing wavefront show aberrations of second order $(S, \bar{S}, S')$ and third order $(E_3, \bar{E}_3, E'_3)$. The origins of these coordinate systems coincide in the chief ray's intersection point with the refractive surface but they are fictitious separated in this figure for a better understanding.

3.3.2. 3D Case

Equivalently to the 2D case transforming Eq. (84) 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 which we could generally show to hold for all orders $k \geq 2$ including the special case of the Coddington equation.

In the general case Eq. (77) 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.

$$\mathbf{C}'_k\,\mathbf{e}'_k = \mathbf{C}_k\mathbf{e}_k + \nu \cdot \bar{\mathbf{e}}_k - \mathbf{r}_k\,, \tag{89}$$

where in $\mathbf{r}_k$ only aberrations of order $j < k$ occur. Therefore, $\mathbf{r}_k$ can be determined by successively solving of Eq. (89) for lower orders. Eq. (89) is the general refraction equation for aberrations of any order in the 3D case.

3.4. Examples and Applications

Two examples are provided, which demonstrate the advantage of the analytical nature of the derived equations. The first example reflects the interesting topic that a refractive surface has to be determined, which images an axial object point perfectly without any aberrations (up to the order $k = 6$). In this example a very big aperture-stop with a low f-number is chosen to demonstrate that the derived equations are suitable for describing the effects of a large pupil. The second example deals with another standard situation in optics that the incoming waverfront and the refractive surface are given and the outgoing wavefront is the unknown quantity. In this example a big angle of incidence is chosen to demonstrate that the derived equations can be used by oblique incidence.

3.4.1. Aspherical Surface Correction up to Sixth Order

One important application of the derived equations is that they allow determining a refractive surface, which not only has a defined Power $\bar{S}$, but also generates an outgoing wavefront which 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 (see Figure 19).

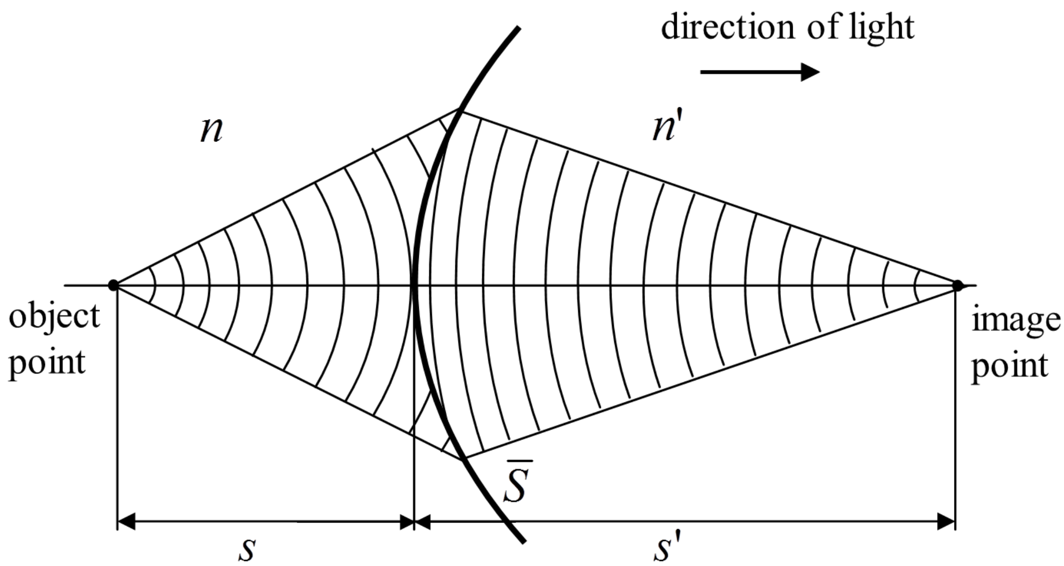

Figure 19: One important application of the derived equations is that they allow determining a refractive surface, which not only has a defined Power $\bar{S}$, but also generates an outgoing wavefront which shows no deviation from an ideal sphere up to the order $k = 6$. The task is to determine a rotationally 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.

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

$$f(y) = r\left(1 - \sqrt{1 - y^2/r^2}\right), \tag{90}$$

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

$$f(y) = \frac{1}{2r}y^2 + \frac{1}{8r^3}y^4 + \frac{1}{16r^5}y^6 + \dots. \tag{91}$$

Applying Eq. (91) once on $f(y) = w_{\text{In}}(y)$, $r = s$ and secondly on $f(y') = w'_{\text{Out}}(y')$, $r = s'$ (including in both cases the sign of s or s') allows us to identify the wavefronts' coefficients in the sense of Eqs. (32)-(35):

$$\begin{aligned} &a_{\text{In},2} = \frac{1}{s} = \frac{S}{n}, \quad a_{\text{In},4} = 3\frac{1}{s^3} = 3\left(\frac{S}{n}\right)^3, \quad a_{\text{In},6} = 45\frac{1}{s^5} = 45\left(\frac{S}{n}\right)^5 \\ &a'_{\text{Out},2} = \frac{1}{s'} = \frac{S'}{n'}, \quad a'_{\text{Out},4} = 3\frac{1}{s'^3} = 3\left(\frac{S'}{n'}\right)^3, \quad a'_{\text{Out},6} = 45\frac{1}{s'^5} = 45\left(\frac{S'}{n'}\right)^5. \end{aligned} \tag{92}$$

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

$$\bar{s}(y) = \frac{\bar{a}_{\text{S},2}}{2}y^2 + \frac{\bar{a}_{\text{S},4}}{24}y^4 + \frac{\bar{a}_{\text{S},6}}{720}y^6 + \dots \tag{93}$$

as in Eq. (34), will be found up to the order $k = 6$ if we provide expression for the three coefficients $\bar{a}_{\text{S},2}$, $\bar{a}_{\text{S},4}$ and $\bar{a}_{\text{S},6}$ (the odd coefficients for $k = 3,5,7,\dots$ 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 $\bar{a}_{\text{S},2}$ can be directly determined by Eq. (53). In the present case of orthogonal incidence we exploit that $\sigma = \sigma' = 0$, $\chi = \chi' = 1$ and $\eta = n' - n$, such that Eq. (53) reads as $(n' - n)\bar{a}_{S,2} = n'a'_{\text{Out},2} - n\,a_{\text{In},2}$ (equivalent to the vergence equation $\bar{S} = S' - S$ in Eq. (11)), yielding

$$\bar{a}_{\text{S},2} = \frac{S' - S}{n' - n}. \tag{94}$$

For finding $\bar{a}_{\mathrm{S},4}$, we have to apply Eqs. (54)-(57). Due to the orthogonal incidence Eq. (57) simplifies to

$$\alpha = 0, \beta = 0, \gamma = \frac{6nn'}{n'-n}, \delta = -\frac{6nn'}{n'-n}, \tag{95}$$

and consequently Eq. (56) simplifies to

$$R_4 = \frac{6nn'}{n'-n}\left(w'^{(2)}_{\mathrm{Out}} - w^{(2)}_{\mathrm{In}}\right)^2\left(w'^{(2)}_{\mathrm{Out}} + w^{(2)}_{\mathrm{In}}\right). \tag{96}$$

Inserting Eq. (96) into Eq. (54) and substituting $w^{(2)}_{\mathrm{In}}$, $w'^{(2)}_{\mathrm{Out}}$ by the coefficients in Eq. (92) yields

$$\begin{aligned}\bar{a}_{\mathrm{S},4} = \bar{w}^{(4)}_{\mathrm{S}} &= \frac{1}{n'-n}\left(n'\,w'^{(4)}_{\mathrm{Out}} - n\,w^{(4)}_{\mathrm{In}} + R_4\right)\\ &= \frac{1}{n'-n}\left(n'\,a'_{\mathrm{Out},4} - n a_{\mathrm{In},4} + \frac{6nn'}{n'-n}\left(a'_{\mathrm{Out},2} - a_{\mathrm{In},2}\right)^2\left(a'_{\mathrm{Out},2} + a_{\mathrm{In},2}\right)\right)\\ &= \frac{3}{(n'-n)^2}\left(\frac{(n'+n)S^3}{n^2} - \frac{2S^2S'}{n} - \frac{2SS'^2}{n'} + \frac{(n'+n)S'^3}{n'^2}\right).\end{aligned} \tag{97}$$

Similarly, we find that

$$\begin{aligned}\bar{a}_{\mathrm{S},6} = \bar{w}^{(6)}_{\mathrm{S}} = \frac{45}{(n'-n)^3}\Bigg(&-\frac{(n'+n)^2S^5}{n^4} + \frac{3(n'+n)S^4S'}{n^3} - \frac{(n'-3n)S^3S'^2}{n^2n'}\\ &+ \frac{(n'+n)S'^5}{n'^4} - \frac{3(n'+n)S'S'^4}{n'^3} + \frac{(n-3n')S^2S'^3}{nn'^2}\Bigg).\end{aligned} \tag{98}$$

Eqs. (97), (98) complete the demanded solution, 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. (94), (97), (98) can be illustrated by a numerical example in which the refractive index of the first medium is $n = 1$, the one of the second medium is $n' = 1.5168$, and the object and image distance are given by $s = -50.0mm$ and $s' = 60.0mm$, respectively. Eqs. (94), (97), (98) then yield $\bar{a}_{\mathrm{S},2} = 0.0876161 mm^{-1}$, $\bar{a}_{\mathrm{S},4} = -0.00006550\, mm^{-3}$, $\bar{a}_{\mathrm{S},6} = 0.00002147\, mm^{-5}$. 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 $r = 1/\bar{a}_{\mathrm{S},2} = 11.4134mm$ (see Figure 20). Paraxial 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 Figure 21), but now we have chosen a stop with semi-diameter

$r_{\text{stop}} = 16.0mm$ which is considerably larger than the surface radius in Figure 20. Again, the peripheral rays introduce large errors.

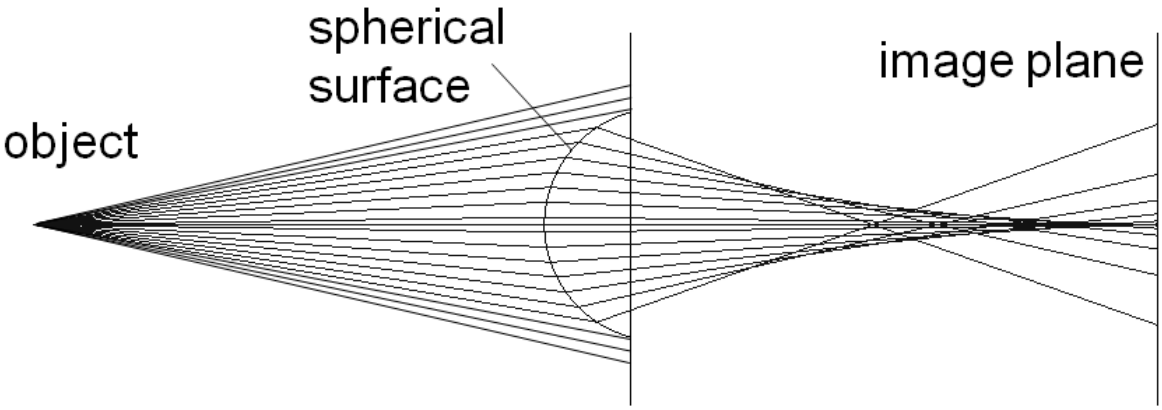

Figure 20: Numerical example in which the refractive index of the first medium is $n = 1$, the one of the second medium is $n' = 1.5168$, and the object and image distance are given by $s = -50.0mm$ and $s' = 60.0mm$. Ray-tracing generated by the optical design package ZEMAX® : Spherical surface with radius $r = 1/\bar{a}_{S,2} = 11.4134mm$ and a aperture stop with a semi-diameter $r_{\text{stop}} = 16.0mm$. Paraxial the imaging is perfect, but the peripheral rays introduce large errors. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context.

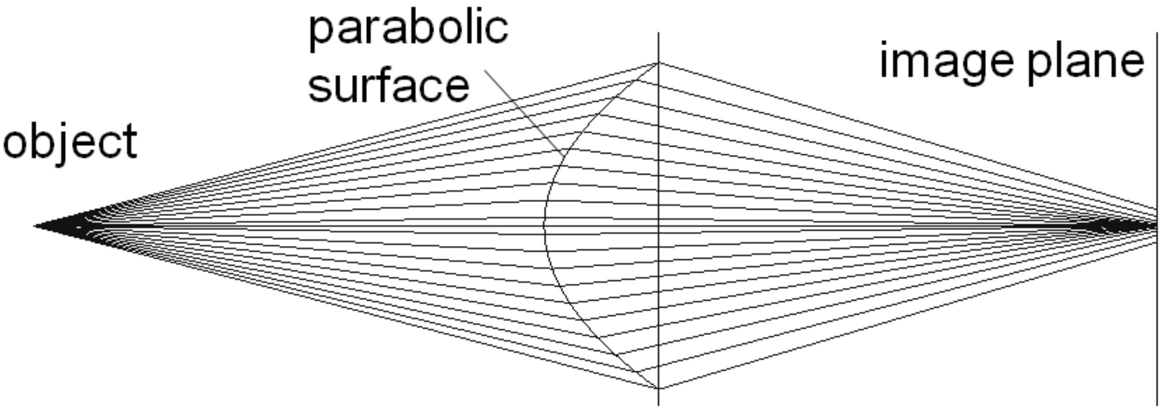

Figure 21: Numerical example in which the refractive index of the first medium is $n = 1$, the one of the second medium is $n' = 1.5168$, and the object and image distance are given by $s = -50.0mm$ and $s' = 60.0mm$. Ray-tracing generated by the optical design package ZEMAX® : Parabolic surface with local curvature $\bar{a}_{S,2}$ and a aperture stop with a semi-diameter $r_{\text{stop}} = 16.0mm$. Paraxial the imaging is perfect, but the peripheral rays introduce large errors. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context.

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 $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$. Figure 22 shows that the errors are reduced to a level which is no longer visible on the scale of the plot.

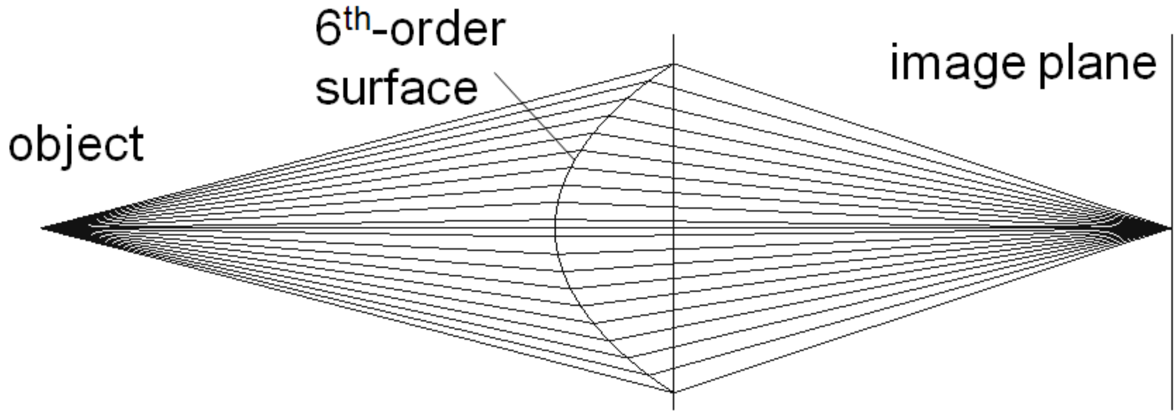

Figure 22: Numerical example in which the refractive index of the first medium is $n = 1$, the one of the second medium is $n' = 1.5168$, and the object and image distance are given by $s = -50.0mm$ and $s' = 60.0mm$. Ray-tracing generated by the optical design package ZEMAX® : Strongly reduced aberrations due to aspherical surface of 6th order with coefficients $\bar{a}_{S,2} = 0.0876161 mm^{-1}$, $\bar{a}_{S,4} = -0.00006550 mm^{-3}$, and $\bar{a}_{S,6} = 0.00002147 mm^{-5}$ and a aperture stop with a semi-diameter $r_{stop} = 16.0mm$. The errors are reduced to a level which is no longer visible on the scale of the plot. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context

3.4.2. A spherical incoming wavefront hits a spherical refractive surface by 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 $n = 1$, the one of the second medium is $n' = 1.5168$, and the angle of incidence is $\varepsilon = 40°$. 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. (14) $\mathbf{C}'\mathbf{s}' = \mathbf{C}\mathbf{s} + \nu\bar{\mathbf{s}}$, 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 2.

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. (89) simplifies to $\mathbf{C}'_3\mathbf{e}'_3 = -\mathbf{r}_3$ (the vector $\mathbf{r}_3$ is shown in Appendix B 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 2.

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. (89)

leads to the resulting error vector of fourth order whose values are again given in Table 2. The 5th and 6th order aberrations for the local wavefront aberrations are also numerically provided in Table 2.

order	wavefront aberration (sagitta)		wave aberration (OPD)	
	symbol	$value \times 1000$	symbol	$value \times 1000$
$k=2$	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	$E'^{\mathrm{OPD}}_{xxxxx}$	0
	E'_{xxxxy}	$0.000713\ mm^{-4}$	$E'^{\mathrm{OPD}}_{xxxxy}$	$0.000010\ mm^{-4}$
	E'_{xxxyy}	0	$E'^{\mathrm{OPD}}_{xxxyy}$	0
	E'_{xxyyy}	$-0.000946\ mm^{-4}$	$E'^{\mathrm{OPD}}_{xxyyy}$	$-0.002170\ mm^{-4}$
	E'_{xyyyy}	0	$E'^{\mathrm{OPD}}_{xyyyy}$	0
	E'_{yyyyy}	$-0.013123\ mm^{-4}$	$E'^{\mathrm{OPD}}_{yyyyy}$	$-0.023830\ mm^{-4}$
$k=6$	E'_{xxxxxx}	$0.000339\ mm^{-5}$	$E'^{\mathrm{OPD}}_{xxxxxx}$	$-0.000078\ mm^{-5}$
	E'_{xxxxxy}	0	$E'^{\mathrm{OPD}}_{xxxxxy}$	0
	E'_{xxxxyy}	$-0.000294\ mm^{-5}$	$E'^{\mathrm{OPD}}_{xxxxyy}$	$-0.000563\ mm^{-5}$
	E'_{xxxyyy}	0	$E'^{\mathrm{OPD}}_{xxxyyy}$	0
	E'_{xxyyyy}	$-0.000663\ mm^{-5}$	$E'^{\mathrm{OPD}}_{xxyyyy}$	$-0.001228\ mm^{-5}$
	E'_{xyyyyy}	0	$E'^{\mathrm{OPD}}_{xyyyyy}$	0
	E'_{yyyyyy}	$-0.004746\ mm^{-5}$	$E'^{\mathrm{OPD}}_{yyyyyy}$	$-0.009508\ mm^{-5}$

Table 2: Numerical results for the local aberrations up to the radial order 6 of the outgoing wavefront calculated by the analytical equation (89) derived in this PhD thesis. Left column: values based on the wavefront sagitta; right column: OPD-based values, as defined by equation (96), and derived from the wavefront sagitta results shown in the left column using equation (324).

As mentioned at the beginning of this thesis, our whole treatment is based on the description of aberrations by their wavefront sagitta. For completeness, it is important to provide also aberration results in the OPD picture. In Appendix A: Relation between sagitta derivatives and OPD derivatives, we provide relations between sagitta derivatives and OPD derivatives. Analogously to Eq. (26), we define OPD-based vectors of aberrations for the wavefronts by

$$\mathbf{e}_k^{\mathrm{OPD}} = \begin{pmatrix} E_{x\ldots xx}^{\mathrm{OPD}} \\ E_{x\ldots xy}^{\mathrm{OPD}} \\ \vdots \\ E_{y\ldots yy}^{\mathrm{OPD}} \end{pmatrix} = \begin{pmatrix} \tau_{\mathrm{In}}^{(k,0)} \\ \tau_{\mathrm{In}}^{(k-1,1)} \\ \vdots \\ \tau_{\mathrm{In}}^{(0,k)} \end{pmatrix}, \quad \mathbf{e'}_k^{\mathrm{OPD}} = \begin{pmatrix} E'^{\mathrm{OPD}}_{x\ldots xx} \\ E'^{\mathrm{OPD}}_{x\ldots xy} \\ \vdots \\ E'^{\mathrm{OPD}}_{y\ldots yy} \end{pmatrix} = \begin{pmatrix} \tau'^{(k,0)}_{\mathrm{Out}} \\ \tau'^{(k-1,1)}_{\mathrm{Out}} \\ \vdots \\ \tau'^{(0,k)}_{\mathrm{Out}} \end{pmatrix}, \tag{99}$$

where $\tau_{\mathrm{In}}^{(k_x,k_y)}, \tau'^{(k_x,k_y)}_{\mathrm{Out}}$ are in this context OPD derivatives of the incoming and the outgoing wavefront which play the role of the generically used symbol $\tau_w^{(k_x,k_y)}$ in Appendix A. 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 A, $\mathbf{e'}_k^{\mathrm{OPD}}$ 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 $k \geq 5$, the deviations between the two pictures are considerable. We remark that this is the reason why it was necessary to treat the relations between the different coordinates simultaneously with the wavefront derivatives from the very beginning (see Eqs. (40), (66)). This confirms that the vector of six unknowns in Eq. (66) does not introduce additional complexity to the problem, but it is rather the only consistent way how to treat carefully the inherent complexity in such a way that numbers like in Table 2 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 chapter. 2.2. In Table 3, we provide the Zernike coefficients up to order $k=6$ for our example assuming a pupil with semi-diameter $r_0 = 3.0mm$. The coefficients have been computed using Eqs. (115) and (116) for the order $k=6$.

order	Symbol (OSA standard)	Zernike coefficients (our method)	Zernike coefficients (ZEMAX®)
		$value/\mu m$	$value/\mu m$
$k=2$	c_2^{-2}	0	-2.4×10^{-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	-2.9×10^{-8}
	c_3^{3}	0	-5.8×10^{-9}
$k=4$	c_4^{-4}	0	-2.4×10^{-8}
	c_4^{-2}	0	-1.8×10^{-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	1.2×10^{-8}
	c_5^{3}	0	1.2×10^{-8}
	c_5^{5}	0	1.8×10^{-8}
$k=6$	c_6^{-6}	0	-1.2×10^{-8}
	c_6^{-4}	0	0.000000
	c_6^{-2}	0	1.2×10^{-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

Table 3: Zernike coefficients of the outgoing wavefront up to order $k=6$ assuming a pupil with semi-diameter $r_0 = 3.0mm$. Left column: values based on our analytical method computed using Eqs. (115) and (116); right column: values based on numerical ray-tracing (ZEMAX®). The agreement between both results is obvious. Apart from yielding exact values for the local derivatives, the derived analytical method is also be suitable for computing Zernike coefficients over a full pupil size if local aberrations up to sufficiently high order are involved.

For comparison, we have also calculated the solution of the same problem with a ray-tracing approach using ZEMAX® (see Figure 23) followed by a Zernike analysis. Those values are provided in Table 3 as a reference. **The consistency of the 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 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 by its nature resulting in small deviations from zero (see Table 3).

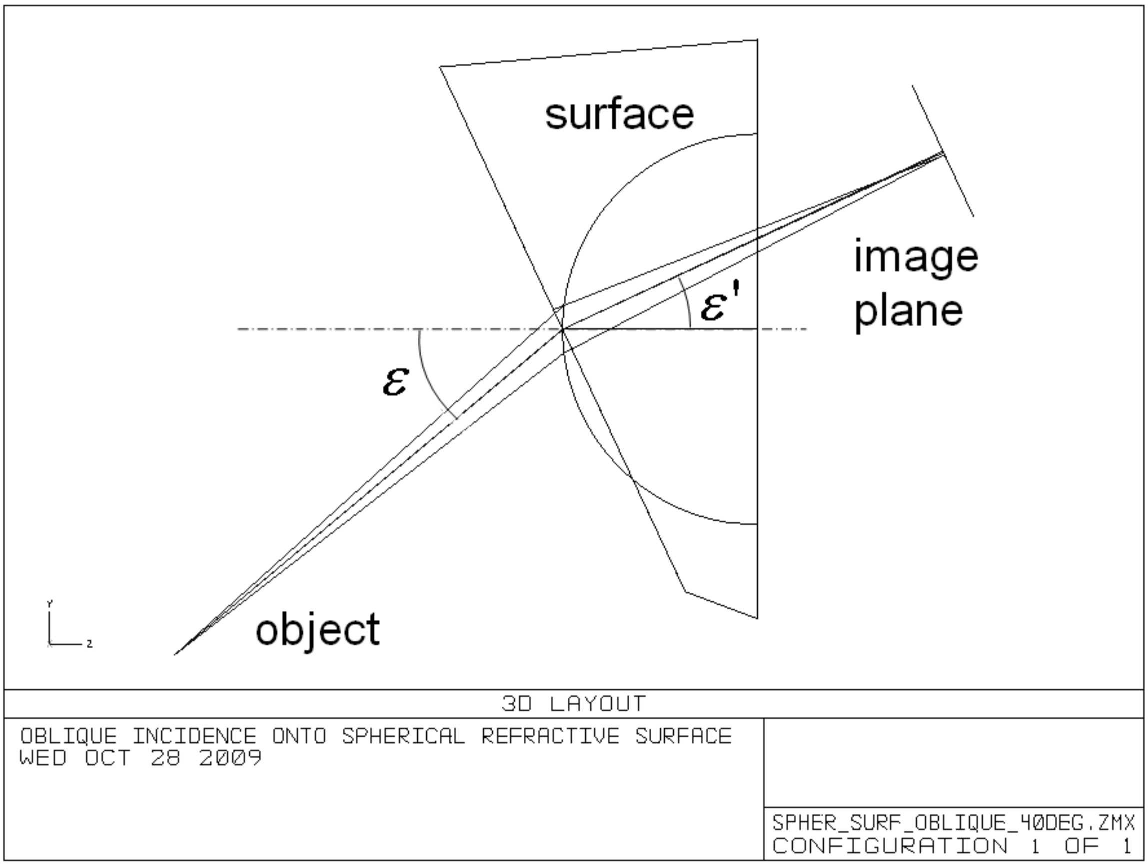

Figure 23: Ray-tracing plot for example B generated by the optical design package ZEMAX®. Given are the spherical incoming wavefront with a vergence $S = 10D$ and a spherical refractive surface with power $\bar{S} = 20D$. The refractive index of the first medium is $n = 1$, the one of the second medium is $n' = 1.5168$, and the angle of incidence is $\varepsilon = 40°$ .A spherical wavefront is refracted by a spherical surface under oblique incidence, giving rise for Coma in the outgoing wavefront. The box drawn around the refractive object are construction lines of ZEMAX® and have no relevance in our context.

4. Description of a Wavefront in a rotated Coordinate System

For calculating the aberrations of a spectacle lens or an entire optical system, it is necessary to describe the wavefront in different (rotated) coordinate systems, because the refracting planes, e.g. the refracting plane at the front surface and at the rear surface e.g. of a spectacle lens, are not identical. They are rotated around the chief ray. A rotation is also necessary to describe the aberrations relating to the horizontal or vertical axis or the axis defined by Listing's law. Listing's law describes the three dimensional eye movement when viewing in a diagonal gaze direction (tertiary position). It says that the rotation takes place around an axis which is perpendicular to the plane spanned by the vector in primary gaze direction and the vector in tertiary gaze direction [45,46]. The goal and also the advantage of the method is that the derived equations allow calculating the coefficients of the wavefront in the rotated coordinate system relating to the coefficients of the original wavefront directly without a coordinate transformation.

4.1. Rotated coordinate system

By rotating the coordinate system about the angle α (see Figure 24), the coordinate transformation is described by

$$\begin{aligned}\tilde{x} &= x\cos\alpha - y\sin\alpha \\ \tilde{y} &= x\sin\alpha + y\cos\alpha\end{aligned} \qquad \text{or} \qquad \begin{pmatrix}\tilde{x}\\ \tilde{y}\end{pmatrix} = \mathbf{R}(\alpha)\begin{pmatrix}x\\ y\end{pmatrix} \tag{100}$$

with the rotation matrix

$$\mathbf{R}(\alpha) = \begin{pmatrix}\cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha\end{pmatrix} \tag{101}$$

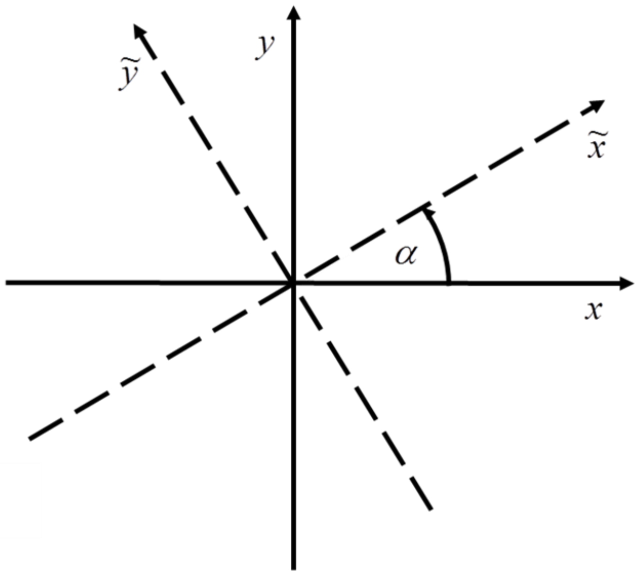

Figure 24: Relation between the coordinates $\tilde{x}, \tilde{y}$ and x, y. By rotating the coordinate system about the angle α, the coordinate transformation is described by $\begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = \mathbf{R}(\alpha) \begin{pmatrix} x \\ y \end{pmatrix}$ with the rotation matrix $\mathbf{R}(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$

Therefore the wavefront $\tilde{w}$ in the rotated coordinate system $\tilde{x}, \tilde{y}$ is defined by

$$\tilde{w}(\tilde{x}, \tilde{y}) = w(x(\tilde{x}, \tilde{y}), y(\tilde{x}, \tilde{y})) \tag{102}$$

By taking the derivative of the wavefront $\tilde{w}$ with respect to $\tilde{x}, \tilde{y}$, the new coefficients $\tilde{a}_{m,k-m}$ are determined in relation to the coefficients $a_{m,k-m}$.

$$\tilde{a}_{m,k-m} = \frac{\partial^k}{\partial \tilde{x}^m \partial \tilde{y}^{k-m}} w(x(\tilde{x}, \tilde{y}), y(\tilde{x}, \tilde{y}))\Big|_{\tilde{x}=0, \tilde{y}=0} \tag{103}$$

4.2. Second order aberrations

For second order aberrations, it is known how to calculate directly the coefficients $\tilde{a}_{m,k-m}$ of the wavefront $\tilde{\mathbf{w}}(\tilde{x}, \tilde{y})$ in the rotated coordinate system $(\tilde{x}, \tilde{y})$ [7,8].

The vector of second order aberrations is

$$\mathbf{s} = \begin{pmatrix} S_{xx} \\ S_{xy} \\ S_{yy} \end{pmatrix} \tag{104}$$

If the coordinate system is rotated by the angle α, the new second order aberrations $\tilde{\mathbf{s}}$ (in the rotated coordinate system $(\tilde{x},\tilde{y})$) will be calculated by

$$\tilde{\mathbf{s}} = \mathbf{R}_2(\alpha)\mathbf{s} \tag{105}$$

with

$$\mathbf{R}_2(\alpha) = \begin{pmatrix} \cos^2\alpha & -2\cos\alpha\sin\alpha & \sin^2\alpha \\ \cos\alpha\sin\alpha & \cos^2\alpha - \sin^2\alpha & -\cos\alpha\sin\alpha \\ \sin^2\alpha & 2\cos\alpha\sin\alpha & \cos^2\alpha \end{pmatrix} \tag{106}$$

4.3. Higher order aberrations

The dependence of the new coefficients $\tilde{a}_{m,k-m}$ on the old coefficients $a_{m,k-m}$ can be described by

$$\begin{pmatrix} \tilde{a}_{00} \\ \tilde{a}_{01} \\ \tilde{a}_{10} \\ \tilde{a}_{02} \\ \tilde{a}_{11} \\ \tilde{a}_{20} \\ \tilde{a}_{03} \\ \tilde{a}_{12} \\ \tilde{a}_{21} \\ \vdots \end{pmatrix} = \mathbf{R}_{Pot}(N,\alpha) \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{02} \\ a_{11} \\ a_{20} \\ a_{03} \\ a_{12} \\ a_{21} \\ \vdots \end{pmatrix} \tag{107}$$

The resulting rotation matrix has a block structure, which shows that the coefficients $\tilde{a}_{m,k-m}$ of order k depend only on the coefficients $a_{m,k-m}$ also of order k. The rotation matrix for the first 15 coefficients $(N=15)$ up to order $(k=4)$ is

$$\mathbf{R}_{Pot}(15,\alpha) = \begin{pmatrix} 1 & 0 & & \cdots & 0 \\ 0 & \mathbf{R}_1(\alpha) & & & \vdots \\ & & \mathbf{R}_2(\alpha) & & \\ \vdots & & & \mathbf{R}_3(\alpha) & 0 \\ 0 & \cdots & & 0 & \mathbf{R}_4(\alpha) \end{pmatrix} \tag{108}$$

The matrix elements of the block structures $\mathbf{R}_k(\alpha)$ for the first order $(k=1)$ is the known rotation matrixes $\mathbf{R}_1(\alpha)$

$$\mathbf{R}_1(\alpha) = \mathbf{R}(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \tag{109}$$

and for the second order aberrations $(k{=}2)$ the known rotation matrixes $\mathbf{R}_2(\alpha)$

$$\mathbf{R}_2(\alpha) = \begin{pmatrix} \cos^2\alpha & -2\cos\alpha\sin\alpha & \sin^2\alpha \\ \cos\alpha\sin\alpha & \cos^2\alpha - \sin^2\alpha & -\cos\alpha\sin\alpha \\ \sin^2\alpha & 2\cos\alpha\sin\alpha & \cos^2\alpha \end{pmatrix} \tag{110}$$

For third order $(k{=}3)$, the rotation matrixes is given by $\mathbf{R}_3(\alpha)$

$$\mathbf{R}_3(\alpha) = \begin{pmatrix} \cos^3\alpha & -3\cos^2\alpha\sin\alpha & 3\cos\alpha\sin^2\alpha & -\sin^3\alpha \\ \cos^2\alpha\sin\alpha & -2\cos\alpha\sin^2\alpha + \cos^3\alpha & \sin^3\alpha - 2\cos^2\alpha\sin\alpha & \cos\alpha\sin^2\alpha \\ \cos\alpha\sin^2\alpha & -\sin^3\alpha + 2\cos^2\alpha\sin\alpha) & \cos^3\alpha - 2\cos\alpha\sin^2\alpha & -\cos^2\alpha\sin\alpha \\ \sin^3\alpha & 3\cos\alpha\sin^2\alpha & 3\cos^2\alpha\sin\alpha & \cos^3\alpha \end{pmatrix} \tag{111}$$

and for fourth order $(k{=}4)$, the rotation matrixes is given by $\mathbf{R}_4(\alpha)$

$$\mathbf{R}_4(\alpha) = \begin{pmatrix} \cos^4\alpha & -4\cos^3\alpha\sin\alpha & 6\cos^2\alpha\sin^2\alpha & -4\cos\alpha\sin^3\alpha & \sin^4\alpha \\ \cos^3\alpha\sin\alpha & \cos^4\alpha - 3\cos^2\sin^2\alpha & -3(\cos^3\alpha\sin\alpha - \cos\alpha\sin^3\alpha) & 3\cos^2\sin^2\alpha - \sin^4\alpha & -\cos\alpha\sin^3\alpha \\ \cos^2\alpha\sin^2\alpha & 2(\cos^3\alpha\sin\alpha - \cos\alpha\sin^3\alpha) & \cos^4\alpha - 4\cos^2\alpha\sin^2\alpha + \sin^4\alpha & -2(\cos^3\alpha\sin\alpha - \cos\alpha\sin^3\alpha) & \cos^2\alpha\sin^2\alpha \\ \cos\alpha\sin^3\alpha & 3\cos^2\sin^2\alpha - \sin^4\alpha & 3(\cos^3\alpha\sin\alpha - \cos\alpha\sin^3\alpha) & \cos^4\alpha - 3\cos^2\sin^2\alpha & -\cos^3\alpha\sin\alpha \\ \sin^4\alpha & 4\cos\alpha\sin^3\alpha & 6\cos^2\alpha\sin^2\alpha & 4\cos^3\alpha\sin\alpha & \cos^4\alpha \end{pmatrix} \tag{112}$$

The equations (109) to (112) show that the block matrix elements $e_{i,j}(\alpha)$ of the rotation matrixes $\mathbf{R}_k(\alpha)$ have a point symmetry with $e_{i,j}(\alpha) = e_{k+2-i,k+2-j}(-\alpha)$.

With $c = \cos\alpha, \quad s = \sin\alpha$ the block matrixes can be simplified to

$$\mathbf{R}_1(\alpha) = \begin{pmatrix} c^k s^0 & * \\ c^0 s^k & * \end{pmatrix}$$

$$\mathbf{R}_2(\alpha) = \begin{pmatrix} c^k s^0 & * & * \\ c^1 s^1 & c^2 - s^2 & * \\ c^0 s^k & k c^1 s^1 & * \end{pmatrix}$$

$$\mathbf{R}_3(\alpha) = \begin{pmatrix} c^k s^0 & * & * & * \\ c^{k-1} s^1 & c^k - (k-1) c^1 s^{k-1} & * & * \\ c^1 s^{k-1} & (k-1) c^{k-1} s^1 - s^k & * & * \\ c^0 s^k & k c^1 s^{k-1} & k c^{k-1} s^1 & * \end{pmatrix}$$

$$\mathbf{R}_4(\alpha) = \begin{pmatrix} c^k s^0 & * & * & * & * \\ c^{k-1} s^1 & c^k - (k-1) c^2 s^2 & * & * & * \\ c^2 s^2 & 2(c^{k-1} s^1 - c^1 s^{k-1}) & c^k - 4c^2 s^2 + s^k & * & * \\ c^1 s^{k-1} & (k-1) c^2 s^2 - s^k & (k-1)(c^{k-1} s^1 - c^1 s^{k-1}) & * & * \\ c^0 s^k & k c^1 s^{k-1} & 2(k-1) c^2 s^2 & k c^{k-1} s^1 & * \end{pmatrix}$$

$$\mathbf{R}_5(\alpha) = \begin{pmatrix} c^k s^0 & * & * & * & * & * \\ c^{k-1} s^1 & c^k - (k-1) c^{k-2} s^2 & * & * & * & * \\ c^{k-2} s^2 & 2c^{k-1} s^1 - 3c^2 s^{k-2} & c^k - 2(k-2) c^{k-2} s^2 + 2(k-2) c^1 s^{k-1} & * & * & * \\ c^2 s^{k-2} & 3c^{k-2} s^2 - 2c^1 s^{k-1} & (k-2) c^{k-1} s^1 - 2(k-2) c^2 s^{k-2} + s^k & * & * & * \\ c^1 s^{k-1} & (k-1) c^2 s^{k-2} - s^k & -(k-1) c^1 s^{k-1} + 2(k-2) c^{k-2} s^2) & (k-1) c^{k-1} s^1 - 2(k-2) c^2 s^{k-2} & * & * \\ c^0 s^k & k c^1 s^{k-1} & 2k c^2 s^{k-2} & 2k c^{k-2} s^2 & k c^{k-1} s^1 & * \end{pmatrix} \quad (113)$$

4.4. Relation between Zernike series and power series

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

$$c_k^m = \frac{1}{\pi r_0^2} \iint_{\text{pupil}} Z_k^m\left(\frac{x}{r_0}, \frac{y}{r_0}\right) w(x,y)\,dxdy\ , \tag{114}$$

where $r := \sqrt{x^2+y^2}$ e, $x = \rho\cos\varphi$, $y = \rho\sin\varphi$ and r_0 is the pupil size.

If the wavefront is given as a series like in Eqs. (8), (9), then the integral in Eq. (114) 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

$$\begin{pmatrix} c_0^0 \\ c_1^{-1} \\ c_1^1 \\ c_2^{-2} \\ c_2^0 \\ c_2^2 \\ c_3^{-3} \\ c_3^{-1} \\ \vdots \\ c_k^k \end{pmatrix} = \mathbf{T}(k) \begin{pmatrix} E \\ r_0 E_x \\ r_0 E_y \\ r_0^2 E_{xx} \\ r_0^2 E_{xy} \\ r_0^2 E_{yy} \\ r_0^3 E_{xxx} \\ r_0^3 E_{xxy} \\ \vdots \\ r_0^k E_{yy\ldots y} \end{pmatrix} = n\mathbf{T}(k) \begin{pmatrix} a_{00} \\ r_0 a_{10} \\ r_0 a_{01} \\ r_0^2 a_{20} \\ r_0^2 a_{11} \\ r_0^2 a_{02} \\ r_0^3 a_{30} \\ r_0^3 a_{21} \\ \vdots \\ r_0^k a_{0k} \end{pmatrix} \tag{115}$$

Also if representations of such a matrix are given in a similar form also in the literature [2,35,51], the prefactors of the underlying power series in literature will not be in detail the same as in our case. Therefore we provide an explicit expression for $\mathbf{T}^{-1}$ here for order $k = 3$, given by

$$\mathbf{T}^{-1}(3)=\begin{pmatrix} 1 & 0 & 0 & 0 & -\sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & -4\sqrt{2} & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & -4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 4\sqrt{3} & -2\sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4\sqrt{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4\sqrt{3} & 2\sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -12\sqrt{2} & 36\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12\sqrt{2} & -12\sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 12\sqrt{2} & 12\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36\sqrt{2} & 12\sqrt{2} \end{pmatrix} \tag{116}$$

The rotation can also be executed in the Zernike space. Therefore the wavefront (Eq. (63)) has to be expanded with Zernike polynomials (Eq. (117)) in polar coordinates.

$$\begin{aligned} Z_{0,0}(\rho,\varphi) &= 1 \\ Z_{1,1}(\rho,\varphi) &= 2\rho\cos\varphi \\ Z_{1,-1}(\rho,\varphi) &= 2\rho\sin\varphi \\ Z_{2,0}(\rho,\varphi) &= \sqrt{3}\left(2\rho^2-1\right) \\ Z_{2,2}(\rho,\varphi) &= \sqrt{6}\rho^2\cos 2\varphi \\ Z_{2,-2}(\rho,\varphi) &= \sqrt{6}\rho^2\sin 2\varphi \\ &\vdots \end{aligned} \tag{117}$$

with
$$w(x,y)=\sum_{k=0}^{\infty}\sum_{m=-k}^{k} c_k^m Z_k^m(\rho,\vartheta), \quad (m-k)\ \text{even} \tag{118}$$

Because of the representation of the Zernike polynomials in polar coordinates, the rotation rule for Zernike coefficients is very simple [35]. The vector of the Zernike coefficients is transformed by rotation with

$$\begin{pmatrix} \tilde{c}_{0,0} \\ \tilde{c}_{1,1} \\ \tilde{c}_{1,-1} \\ \tilde{c}_{2,0} \\ \tilde{c}_{2,2} \\ \tilde{c}_{2,-2} \\ \tilde{c}_{3,1} \\ \tilde{c}_{3,-1} \\ \tilde{c}_{3,3} \\ \vdots \end{pmatrix} = \mathbf{R}_{Zernike}(N,\alpha) \begin{pmatrix} c_{0,0} \\ c_{1,1} \\ c_{1,-1} \\ c_{2,0} \\ c_{2,2} \\ c_{2,-2} \\ c_{3,1} \\ c_{3,-1} \\ c_{3,3} \\ \vdots \end{pmatrix}, \tag{119}$$

The rotation matrix in block matrix description is directly based on the elementary rotation matrix in Eq. (100). For $N = 15$ the rotation matrix has the form:

$$\mathbf{R}_{Zernike}(15,\alpha) = \begin{pmatrix} \boxed{1} & \cdots & & & & & & & \cdots & 0 \\ \boxed{0 \quad \mathbf{R}(\alpha)} & & & & & & & & & \vdots \\ \vdots & & \boxed{\begin{matrix} 1 & \\ & \mathbf{R}(2\alpha) \end{matrix}} & & & & & & & \\ & & & \boxed{\begin{matrix} \mathbf{R}(\alpha) & \\ & \mathbf{R}(3\alpha) \end{matrix}} & & & & & & \\ \vdots & & & & \boxed{\begin{matrix} 1 & & \\ & \mathbf{R}(2\alpha) & \vdots \\ \cdots & 0 & \mathbf{R}(4\alpha) \end{matrix}} \\ 0 & \cdots & & & \end{pmatrix}, \tag{120}$$

Every block in Eq. (120), which relates to the same radial order, has a frame.

To calculate the rotation matrix $\mathbf{R}_{Pot}(N,\alpha)$, it is necessary to transform $\mathbf{R}_{Zernike}(N,\alpha)$ onto the coefficient system of the power series expansion with Eq. (116)

$$\begin{pmatrix} \tilde{a}_{00} \\ \tilde{a}_{01} \\ \tilde{a}_{10} \\ \tilde{a}_{02} \\ \tilde{a}_{11} \\ \tilde{a}_{20} \\ \tilde{a}_{03} \\ \tilde{a}_{12} \\ \tilde{a}_{21} \\ \vdots \end{pmatrix} = n^{-1}\mathbf{T}^{-1}(N) \begin{pmatrix} \tilde{c}_{0,0} \\ \tilde{c}_{1,1} \\ \tilde{c}_{1,-1} \\ \tilde{c}_{2,0} \\ \tilde{c}_{2,2} \\ \tilde{c}_{2,-2} \\ \tilde{c}_{3,1} \\ \tilde{c}_{3,-1} \\ \tilde{c}_{3,3} \\ \vdots \end{pmatrix} = n^{-1}\mathbf{T}^{-1}(N)\mathbf{R}_{Zernike}(N,\alpha) \begin{pmatrix} c_{0,0} \\ c_{1,1} \\ c_{1,-1} \\ c_{2,0} \\ c_{2,2} \\ c_{2,-2} \\ c_{3,1} \\ c_{3,-1} \\ c_{3,3} \\ \vdots \end{pmatrix} = \mathbf{T}^{-1}(N)\mathbf{R}_{Zernike}(N,\alpha)\mathbf{T}(N) \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{02} \\ a_{11} \\ a_{20} \\ a_{03} \\ a_{12} \\ a_{21} \\ \vdots \end{pmatrix}, \tag{121}$$

It follows, that

$$\mathbf{R}_{Pot}(N,\alpha) = \mathbf{T}^{-1}(N)\mathbf{R}_{Zernike}(N,\alpha)\mathbf{T}(N), \tag{122}$$

with a block structure of the form

$$\mathbf{R}_{Pot}(15) = \begin{pmatrix} 1 & 0 & & \cdots & 0 \\ 0 & \mathbf{R}_1(\alpha) & & & \vdots \\ & & \mathbf{R}_2(\alpha) & & \\ \vdots & & & \mathbf{R}_3(\alpha) & 0 \\ 0 & \cdots & & 0 & \mathbf{R}_4(\alpha) \end{pmatrix} \tag{123}$$

where the block matrixes are identical with the ones of Eq. (113).

5. Derivation of the Propagation Equations

5.1. Mathematical Approach in the 2D Case

5.1.1. Description of Wavefronts in the 2D case

The wavefronts themselves are each described by power series expansions. Any point on the original wavefront is given by the vector

$$\mathbf{w}_o(y) = \begin{pmatrix} y \\ w_o(y) \end{pmatrix} \tag{124}$$

where in the 2D case $w_o(y)$ is the curve defined by

$$w_o(y) = \sum_{k=0}^{\infty} \frac{a_{o,k}}{k!} y^k \tag{125}$$

The normal vectors and their derivatives are described as in chapter 3.1.3 and obey the same relations as Eqs. (36)-(38). Since the normal vector of the original wavefront and the normal vector of the propagated wavefront are equal, the normal vector will be labeled generally with $\mathbf{n}_w$.

In application on the functions of interest, $\mathbf{n}_w(y) = \mathbf{n}(w_o^{(1)}(y))$, this means that $\mathbf{n}_w(0) = (0,1)^T$. Further, the first derivatives are given by

$$\left.\frac{\partial}{\partial y}\mathbf{n}_w(y)\right|_{y=0} \equiv \mathbf{n}_w^{(1)}(0) = \mathbf{n}^{(1)}(0) w_o^{(2)}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix} w_o^{(2)}(0) \tag{126}$$

and similarly for the higher derivatives.

5.1.2. Ansatz for Determining the Propagation Equations

Once the local aberrations of the original wavefront are given, its corresponding coefficients a_k are directly determined, too, and equivalently the wavefront's derivatives. It is our aim to calculate the propagated wavefront in the sense that its derivatives and thus its a_k coefficients (see Eqs. (124),(125)) are determined for all orders $2 \le k \le k_0$ for the order k_0 of interest, and to assign values to its corresponding local aberrations.

In contrast to this general procedure, which is the same as in chapter 3, we consider now the following situation as starting point for treating propagation. While the chief ray and the coordinate system are fixed, a neighboring ray scans the original wavefront $\{\mathbf{w}_o\}$ and hits it at an intercept $y_o \neq 0$, then propagates to the propagated wavefront $\{\mathbf{w}_p\}$, where the brackets $\{.\}$ shall denote the entity of vectors described by Eq. (124). As shown Figure 25, and consistently with our notation, we denote as y_o the projection of the neighboring ray's intersection with $\{\mathbf{w}_o\}$ onto the y axis and analogously, the projection of the intersection with $\{\mathbf{w}_p\}$ onto the y axis is denoted as y_p .

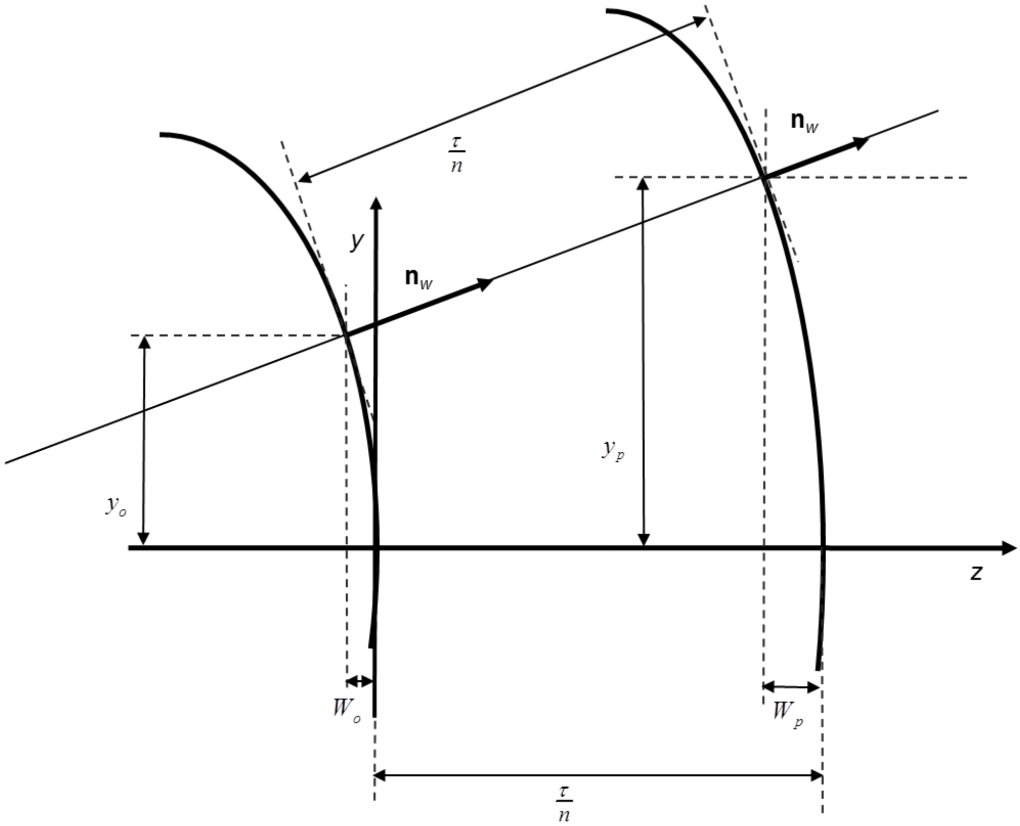

Figure 25: Propagation of a wavefront $\mathbf{w_o}$ about the distance $d = \tau/n$ to the propagated wavefront $\mathbf{w_p}$. The chief ray and the coordinate system are fixed, a neighboring ray scans the original wavefront $\{\mathbf{w}_o\}$ and hits it at an intercept $y_o \neq 0$, then propagates to the propagated wavefront $\{\mathbf{w}_p\}$, where the brackets $\{.\}$ shall denote the entity of vectors described by Eq. (124). Consistently with our notation, we denote as y_o the projection of the neighboring ray's intersection with $\{\mathbf{w}_o\}$ onto the y axis and analogously, the projection of the intersection with $\{\mathbf{w}_p\}$ onto the y axis is denoted as y_p .

The vector $\mathbf{w}_o = \mathbf{w}_o(y_o)$ (see Eq. (124)) points to the neighboring ray's intersection point with the original wavefront, and the propagated wavefront's OPD referred to the original wavefront measured along the ray is denoted by τ . Correspondingly the vector from the original wavefront to the propagated wavefront is $\tau/n\,\mathbf{n}_w$. Hence, the vector to the point on the propagated wavefront itself, $\mathbf{w}_p$, must be equal to the vector sum $\mathbf{w}_p = \mathbf{w}_o + \tau/n\,\mathbf{n}_w$. This yields the fundamental equation:

$$\begin{pmatrix} y_{\text{o}} \\ w_{\text{o}}(y_{\text{o}}) \end{pmatrix} + \frac{\tau}{n}\mathbf{n}_{\text{w}} = \begin{pmatrix} y_{\text{p}} \\ w_{\text{p}}(y_{\text{p}}) \end{pmatrix} \tag{127}$$

From Eq. (127), it is now possible to derive the desired relations order by order. Although only the propagated wavefront is of interest, in Eq. (127) additionally the quantities y_{o} and y_{p} are also unknown. However, those are not independent from each other: if any one of them is given, the other one can no longer be chosen independently. The coordinate y_{p} is used as independent variable, and y_{o} is considered as a function of it.

Eq. (127) represents a nonlinear system of two algebraic equations for the two unknown functions $w_{\text{p}}(y_{\text{p}})$ and $y_{\text{o}}(y_{\text{p}})$. Even if we are only interested in a solution for the function $w_{\text{p}}(y_{\text{p}})$, we cannot obtain it without simultaneously solving the equations for both unknowns order by order. Introducing the vector of unknown functions as

$$\mathbf{p}(y_{\text{p}}) = \begin{pmatrix} y_{\text{o}}(y_{\text{p}}) \\ w_{\text{p}}(y_{\text{p}}) \end{pmatrix} \tag{128}$$

and observing that the initial condition $\mathbf{p}(0) = \begin{pmatrix} 0 \\ \tau/n \end{pmatrix}$ has to be fulfilled, it is now straightforward to compute all the derivatives of Eq. (127) up to some order, which yields relations between the curvatures, third derivatives etc. of the original and propagated wavefront. Rewriting these relations in terms of series coefficients $a_{\text{o},k}$ and solving them for the desired coefficients $a_{\text{p},k}$ yields the desired result.

Rewriting Eq. (127) leads to

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} y_{\text{o}} + \dfrac{\tau}{n} n_{w,y} \quad - y_{\text{p}} \\ w_{\text{o}}(y_{\text{o}}) + \dfrac{\tau}{n} n_{w,z} \quad - w_{\text{p}}(y_p) \end{pmatrix} \tag{129}$$

Before solving Eq. (129), we distinguish if the independent variable y_{p} enters into Eq. (129) explicitly like in the first component of the vector $(y_{\text{p}}, w_{\text{p}}(y_{\text{p}}))^T$, or implicitly via one of the components of Eq. (128). To this end, we follow the concept of chapter 3 and define in this case the function $(\mathbb{R}^2 \times \mathbb{R}) \mapsto \mathbb{R}^2 : (\mathbf{p}, y_{\text{p}}) \mapsto \mathbf{f}$ by

$$\mathbf{f}\left(\mathbf{p}, y_{\mathrm{p}}\right)=\begin{pmatrix} y_{\mathrm{o}}+\frac{\tau}{n} n_{w,y}\left(w_{\mathrm{o}}^{(1)}(y_{\mathrm{o}})\right) & -y_{\mathrm{p}} \\ w_{\mathrm{o}}(y_{\mathrm{o}})+\frac{\tau}{n} n_{w,z}\left(w_{\mathrm{o}}^{(1)}(y_{\mathrm{o}})\right) & -w_{\mathrm{p}} \end{pmatrix}, \tag{130}$$

where $(p_1, p_2)=(y_{\mathrm{o}}, w_{\mathrm{p}})$ are the components of $\mathbf{p}$. Setting now $\mathbf{p}=\mathbf{p}(y_{\mathrm{p}})$, Eq. (130) allows rewriting the fundamental system of Eq. (129) in a more compact way as

$$\mathbf{f}\left(\mathbf{p}(y_{\mathrm{p}}), y_{\mathrm{p}}\right)=\mathbf{0} \tag{131}$$

as can be verified explicitly by component wise comparison with Eq. (129).

Solving Eq. (130), (131) for the function $\mathbf{p}(y_{\mathrm{p}})$ is formally identical to solving Eq. (42) in chapter 3. The only difference is now the name of the independent variable is y_{p} instead of $\bar{y}_{\mathrm{S}}$ in chapter 3. Taking the total derivative of Eq. (131) with respect to y_{p} and applying the principles from the theory of implicit functions leads to the system of differential equations

$$\sum_{j=1}^{2} \frac{\partial f_i}{\partial p_j} p_j^{(1)}(y_{\mathrm{p}})+\frac{\partial f_i}{\partial y_{\mathrm{p}}}=0, \quad i=1,2, \tag{132}$$

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 $\mathbf{p}=\mathbf{p}(y_{\mathrm{p}})$. The Jacobian $\mathbf{A}$ reads

$$\mathbf{A}:=\begin{pmatrix} \frac{\partial f_1}{\partial y_{\mathrm{o}}} & \frac{\partial f_1}{\partial w_{\mathrm{p}}} \\ \frac{\partial f_2}{\partial y_{\mathrm{o}}} & \frac{\partial f_2}{\partial w_{\mathrm{p}}} \end{pmatrix}=\begin{pmatrix} 1+\frac{\tau}{n} n_{w,y}^{(1)} w_{\mathrm{o}}^{(2)} & 0 \\ w_o^{(1)}+\frac{\tau}{n} n_{w,z}^{(1)} w_{\mathrm{o}}^{(2)} & -1 \end{pmatrix} \tag{133}$$

In Eq. (133), the occurring expressions are understood as $w_{\mathrm{o}}^{(1)} \equiv w_{\mathrm{o}}^{(1)}(y_{\mathrm{o}})$, $w_{\mathrm{o}}^{(2)} \equiv w_{\mathrm{o}}^{(2)}(y_{\mathrm{o}})$, $n_{\mathrm{w},y} \equiv n_{\mathrm{w},y}(w_{\mathrm{o}}^{(1)}(y_{\mathrm{o}}))$, $n_{\mathrm{w},y}^{(1)} \equiv n_{\mathrm{w},y}^{(1)}(w_{\mathrm{o}}^{(1)}(y_{\mathrm{o}}))$, etc., and additionally $y_{\mathrm{o}}, w_{\mathrm{p}}$ are themselves functions of y_{p}.

The derivative vector $\partial f_i / \partial y_p$ in Eq. (132) shall be summarized as

$$\mathbf{b}:=-\frac{\partial \mathbf{f}}{\partial y_{\mathrm{p}}}=\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{134}$$

Similarly as in chapter 3 we conclude that we can write $\mathbf{A}$ with argument $\mathbf{A}(\mathbf{p}(y_{\mathrm{p}}))$ only and $\mathbf{b}$ without argument at all because $\mathbf{b}$ is constant.

Eq. (132) can then be written in the form

$$\mathbf{A}(\mathbf{p}(y_{\mathrm{p}}))\mathbf{p}^{(1)}(y_{\mathrm{p}}) = \mathbf{b}\,. \tag{135}$$

5.1.3. Solving techniques for the fundamental equation

For solving Eq. (135) for $\mathbf{p}(y_{\mathrm{p}})$, we can apply identically the same steps as in Eqs. (47)-(50)) in chapter 3, with the only difference that here the independent variable is named y_{p} instead of $\bar{y}_{\mathrm{S}}$, and that the initial condition reads here $\mathbf{p}(0) = \begin{pmatrix} 0 \\ \tau/n \end{pmatrix}$ instead of $\mathbf{p}(0) = 0$ as it was the case in chapter 3. The equations as a function of the independent variable y_{p} are shown in Appendix C (Eqs. (326)-(329)). Hence in this chapter, we directly provide a formal solution for $\mathbf{p}^{(k)}(0)$, expressed in terms of its predecessors, by the equations

$$\begin{aligned} \mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \qquad\qquad\qquad\qquad , \quad k = 1 \\ \mathbf{p}^{(k)}(0) &= -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), \quad k \geq 2. \end{aligned} \tag{136}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$.

5.1.4. Solutions for the General Propagation Equations

In the result for $\mathbf{p}^{(1)}(0)$, the first rows of Eq. (136) involve $\mathbf{A}(\mathbf{0})^{-1}$. For obtaining $\mathbf{A}(\mathbf{0})^{-1}$, we evaluate Eq. (133) for $\mathbf{p} = \mathbf{0}$ and apply Eq. (37) in chapter 3, yielding

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1 - \frac{\tau}{n} w_{\mathrm{o}}^{(2)} & 0 \\ 0 & -1 \end{pmatrix} \Rightarrow \mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} \frac{1}{1 - \tau/n\, w_{\mathrm{o}}^{(2)}} & 0 \\ 0 & -1 \end{pmatrix} \tag{137}$$

The final result for $\mathbf{p}^{(1)}(0)$ is

$$\mathbf{p}^{(1)}(0) = \mathbf{A}^{-1}\mathbf{b} = \begin{pmatrix} \frac{1}{1 - \tau/n\, w_{\mathrm{o}}^{(2)}} \\ 0 \end{pmatrix} \tag{138}$$

The first derivative of the y_o-coordinate, which is the first component p_1 of $\mathbf{p}$, is a dilation depending on the curvature of the original wavefront and the propagated optical path length τ, such that $y_o^{(1)}(0) = \frac{1}{1-\tau/n\, w_o^{(2)}}$. The slope of the propagated wavefront vanishes, $w_p^{(1)}(0)=0$, as does the slope of the original wavefront due to $w_o^{(1)}(0)=0$.

For the orders $k \geq 2$ we apply Eq. (136). The derivatives $\mathbf{A}^{(1)} = \frac{d}{dy_p}\mathbf{A}(\mathbf{p}(y_p))\Big|_{y_p=0}$, etc. are directly obtained by total derivative of Eq. (133) with respect to y_p, evaluating for $y_p = 0$ and again applying Eq. (37). For the orders $k \geq 2$ only the results $w_p^{(k)}(0)$ for the propagated wavefront are of interest, therefore we directly provide those result. The resulting second-order law is (omitting the argument '(0)')

$$w_p^{(2)} = \beta\, w_o^{(2)} \tag{139}$$

with

$$\beta = \frac{1}{1-\tau/n\, w_o^{(2)}} \tag{140}$$

which is well-known as the propagation equation and reveals to be a special case of the results. <u>The novel resulting higher-order laws can be written in a similar fashion</u>

$$\begin{aligned}
w_p^{(3)} &= \beta^3 w_o^{(3)} \\
w_p^{(4)} &= \beta^4\left(w_o^{(4)} + 3\frac{\tau}{n}\left(\beta w_o^{(3)2} - w_o^{(2)4}\right)\right) \\
w_p^{(5)} &= \beta^5\left(w_o^{(5)} + 5\beta\frac{\tau}{n} w_o^{(3)}\left(2w_o^{(4)} + 3\beta\frac{\tau}{n} w_o^{(3)2} - 6w_o^{(2)3}\right)\right) \\
&\ldots
\end{aligned} \tag{141}$$

Eq. (141) can be generalized for $2 < k \leq 6$ to

$$w_p^{(k)} = \beta^k (w_o^{(k)} + R_k) \tag{142}$$

where in R_k the dependence of $w_p^{(k)}$ on all wavefront derivatives $w_o^{(j)}$ of lower order ($j < k$) is summarized.

5.1.5. Special case

Although application of Eq. (136) provides a solution for $w_{\mathrm{p}}^{(k)}(0)$ 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 Eq. (142) for R_k will vanish if we set $w_{\mathrm{o}}^{(j)}=0$ for all lower orders $j<k$ (for $k=3$ or $k=4$, respectively).

This leads to the assumption (for $k>2$) that the following statement is generally true: if only aberrations of one single given order k are present while for all lower orders $j<k$ we have $w_{\mathrm{o}}^{(j)}=0$, then $\left(\frac{1}{1-\tau/n\, w_{\mathrm{o}}^{(2)}}\right)=1$ and $R_k=0$, which means for fixed order k that Eq. (142) will be valid for vanishing remainder term and the aberration of the propagated wavefront will be equal to the aberration of the original wavefront independent of the propagation distance d.

To this purpose, we start from the recursion scheme in Eq. (136) and show that only the term containing $\mathbf{p}^{(1)}$ can contribute to the sum if all aberrations vanish for order less than k. For doing so, it is necessary to exploit two basic properties of the derivatives $\mathbf{A}^{(m)}=\frac{d^m}{dy_{\mathrm{p}}^m}\mathbf{A}(\mathbf{p}(y_{\mathrm{p}}))\Big|_{y_{\mathrm{p}}=0}$ of the matrix $\mathbf{A}$ for the orders $1\le m\le k-1$. As can be shown by element wise differentiation of the matrix $\mathbf{A}$, the highest wavefront derivatives present in $\mathbf{A}^{(m)}(\mathbf{p}(y_{\mathrm{p}}))$ (see Eq. (133)) are proportional to $w_{\mathrm{o}}^{(m+2)}$. Evaluating $\mathbf{A}^{(m)}(\mathbf{p}(y_{\mathrm{p}}))$ at the position $y_{\mathrm{p}}=0$ shows that $\mathbf{A}^{(m)}$ cannot contain any higher wavefront derivatives than $w_{\mathrm{o}}^{(m+2)}$. It follows that

i) The highest possible wavefront derivatives present in $\mathbf{A}^{(m)}$ are $w_{\mathrm{o}}^{(m+2)}$.

ii) If all wavefront derivatives even up to order $(m+2)$ 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. (136), we notice that the occurring derivatives of the matrix $\mathbf{A}$ are $\mathbf{A}^{(k-1)}$, $\mathbf{A}^{(k-2)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ for $j=1,2,...,(k-1)$, respectively. It follows from property i) that the highest occurring wavefront derivatives in these terms are $(k+1),k,(k-1),...,3,2$, respectively. Now, if all wavefront derivatives up to order $(k-1)$ vanish, it will follow from property ii) that all the matrix derivatives $\mathbf{A}^{(k-3)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ must vanish, leaving only $\mathbf{A}^{(k-1)}$ and $\mathbf{A}^{(k-2)}$. Therefore all terms in Eq. (136) vanish, excluding only the contribution for $j=1$ and $j=2$. We directly conclude that

$$\begin{aligned} \mathbf{p}^{(2)} &= \quad -\mathbf{A}^{-1}\mathbf{A}^{(1)}\mathbf{A}^{-1}\mathbf{b} && , \quad k=2 \\ \mathbf{p}^{(k)} &= -\mathbf{A}^{-1}\sum_{j=1}^{2}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)} && , \quad k\geq 3. \end{aligned} \tag{143}$$

This leads directly to

$$\begin{aligned} \mathbf{p}^{(2)} &= \quad -\mathbf{A}^{-1}\mathbf{A}^{(1)}\mathbf{A}^{-1}\mathbf{b} && , \quad k=2 \\ \mathbf{p}^{(k)} &= \mathbf{A}^{-1}\left((k-1)\mathbf{A}^{(k-2)}\mathbf{A}^{-1}\mathbf{A}^{(1)} - \mathbf{A}^{(k-1)}\right)\mathbf{A}^{-1}\mathbf{b} && , \quad k\geq 3 \end{aligned} \tag{144}$$

In the term

$$\mathbf{A}^{(1)} = \begin{pmatrix} \dfrac{-\tau/n}{1-\tau/n\, w_o^{(2)}}\, w_o^{(3)} & 0 \\ w_o^{(2)} & 0 \end{pmatrix} \tag{145}$$

only wavefront derivatives $w_o^{(3)}$ and $w_o^{(2)}$ occur. Therefore $\mathbf{A}^{(1)} = \mathbf{0}$ for $k > 3$ because $w_o^{(3)}$ and $w_o^{(2)}$ vanish. Eq. (144) can then be written in the form

$$\begin{aligned} \mathbf{p}^{(3)} &= \mathbf{A}^{-1}(2\mathbf{A}^{(1)}\mathbf{A}^{-1}\mathbf{A}^{(1)} - \mathbf{A}^{(2)})\mathbf{A}^{-1}\mathbf{b} && , \quad k=3 \\ \mathbf{p}^{(k)} &= \quad -\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{A}^{-1}\mathbf{b} && , \quad \text{otherwise} \end{aligned} \tag{146}$$

To evaluate $\mathbf{p}^{(3)}$ in Eq. (146) the second derivative of $\mathbf{A}$ has to be calculated. $\mathbf{A}^{(2)}$ reads if all derivatives of the wavefront vanish for order less or equal to $m=2$

$$\mathbf{A}^{(2)} = \begin{pmatrix} -\tau/n\left(\tau/n\, w_o^{(3)} + w_o^{(4)}\right) & 0 \\ w_o^{(3)} & 0 \end{pmatrix} \tag{147}$$

For evaluating $\mathbf{A}^{(k-1)}$ for $k-1>2$ we set $k-1 =: m$, and it is straightforward to show by induction that if all aberrations vanish for order less or equal to m, then

$$\mathbf{A}^{(m)} = \begin{pmatrix} -\tau/n\, w_o^{(m+2)} & 0 \\ w_o^{(m+1)} & 0 \end{pmatrix}, \tag{148}$$

where $y_o^{(1)}$ has been substituted by their solution $\dfrac{1}{1-\tau/n\, w_o^{(2)}}$, wherever it occurs, respectively (see Eq.(138)). Inserting $\mathbf{A}^{(m)}(0)$ for $m=k-1$ and $\mathbf{A}(0)^{-1}$ from Eq. (136) into Eq. (146) yields directly that

$$w_{\mathrm{p}}^{(k)} = w_{\mathrm{o}}^{(k)} \tag{149}$$

for all orders $k > 2$.

5.2. Mathematical Approach in the 3D Case

5.2.1. 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 and analogously to Eqs. (63)-(74) in chapter 3. Therefore, we will only report the most important differences. Analogously to Eq. (124), the original wavefront is now represented by the 3D vector

$$\mathbf{w}_o(x, y) = \begin{pmatrix} x \\ y \\ w_{\mathrm{o}}(x, y) \end{pmatrix} \tag{150}$$

where $w_{\mathrm{o}}(x, y)$ and the relation between the coefficients and the derivatives is defined as described in chapter 3. The connection between coefficients and local aberrations is now given by multiplying the coefficient with the refractive index.

For treating the normal vectors, we use the same function

$$\mathbf{n}(u, v) := \frac{1}{\sqrt{1 + u^2 + v^2}} \begin{pmatrix} -u \\ -v \\ 1 \end{pmatrix}, \tag{151}$$

as in chapter 3 and make use of the fact that the normal vector $\mathbf{n}_w(x, y)$ to a surface $\mathbf{w}(x, y) := (x, y, w(x, y))^T$ is given by $\mathbf{n}(\nabla w)$. In the intersection point we have now $\mathbf{n}_w(0,0) = (0,0,1)^T$, and the derivatives corresponding to Eq. (37) can directly be obtained from Eq. (151).

5.2.2. Ansatz for Determining the Propagation Equations

The starting point for establishing the relations between the original and the propagated wavefront is now given by equations analogous to Eq. (127), with the only difference that x and y components are simultaneously present.

The vector of unknown functions is now given by

$$\mathbf{p}(x_\mathrm{p}, y_\mathrm{p}) = \begin{pmatrix} x_\mathrm{o}(x_\mathrm{p}, y_\mathrm{p}) \\ y_\mathrm{o}(x_\mathrm{p}, y_\mathrm{p}) \\ w_p(x_\mathrm{p}, y_\mathrm{p}) \end{pmatrix} \tag{152}$$

and the 3D analogue to Eq. (127) leads now to

$$\mathbf{f}\left(\mathbf{p}(x_\mathrm{p}, y_\mathrm{p}), x_\mathrm{p}, y_\mathrm{p}\right) = \mathbf{0} \tag{153}$$

where $\mathbf{f}$ is the 3D analogue to Eq. (130).

Since Eq. (153) is formally identical to Eq. (67) in chapter 3, the solving procedure from chapter 3 can be directly applied. In particular, we have to deal with two first-order equations

$$\begin{aligned} \mathbf{A}\left(\mathbf{p}(x_\mathrm{p}, y_\mathrm{p})\right)\mathbf{p}^{(1,0)}(x_\mathrm{p}, y_\mathrm{p}) = \mathbf{b}_x \\ \mathbf{A}\left(\mathbf{p}(x_\mathrm{p}, y_\mathrm{p})\right)\mathbf{p}^{(0,1)}(x_\mathrm{p}, y_\mathrm{p}) = \mathbf{b}_y \end{aligned} \tag{154}$$

which correspond exactly to Eq. (68) in chapter 3. Of course, the explicit expressions how $\mathbf{f}$ and $\mathbf{p}$ depend on their arguments now lead to different expressions for the column vectors of the inhomogeneities

$$\mathbf{b}_x = -\frac{\partial \mathbf{f}}{\partial x_\mathrm{p}} = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}^T, \quad \mathbf{b}_y = -\frac{\partial \mathbf{f}}{\partial y_\mathrm{p}} = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix}^T. \tag{155}$$

and for the Jacobian matrix $\mathbf{A}(\mathbf{p}(x_\mathrm{p}, y_\mathrm{p}))$ with elements $A_{ij} := \partial f_i / \partial p_j$ which is now given by

$$\mathbf{A}\left(\mathbf{p}(x_\mathrm{p}, y_\mathrm{p})\right) = \begin{pmatrix} 1 + \frac{\tau}{n}(n_{w,x}^{(0,1)} w_\mathrm{o}^{(1,1)} + n_{w,x}^{(1,0)} w_\mathrm{o}^{(2,0)}) & \frac{\tau}{n}(n_{w,x}^{(0,1)} w_\mathrm{o}^{(0,2)} + n_{w,x}^{(1,0)} w_\mathrm{o}^{(1,1)}) & 0 \\ \frac{\tau}{n}(n_{w,y}^{(0,1)} w_\mathrm{o}^{(1,1)} + n_{w,y}^{(1,0)} w_\mathrm{o}^{(2,0)}) & 1 + \frac{\tau}{n}(n_{w,y}^{(0,1)} w_\mathrm{o}^{(0,2)} + n_{w,y}^{(1,0)} w_\mathrm{o}^{(1,1)}) & 0 \\ w_\mathrm{o}^{(1,0)} + \frac{\tau}{n}(n_{w,z}^{(0,1)} w_\mathrm{o}^{(1,1)} + n_{w,z}^{(1,0)} w_\mathrm{o}^{(2,0)}) & w_\mathrm{o}^{(0,1)} + \frac{\tau}{n}(n_{w,z}^{(0,1)} w_\mathrm{o}^{(0,2)} + n_{w,z}^{(1,0)} w_\mathrm{o}^{(1,1)}) & -1 \end{pmatrix} \tag{156}$$

5.2.3. Solutions for the General Propagation Equations

The formal analogy of Eqs. (49) to Eqs. (69) in chapter 3 can be exploited by making use of the solving techniques developed in chapter 3. Equivalently either Eqs. (73) or Eqs. (78) from chapter 3 can be directly applied. The only difference to chapter 3 is now that again the explicit expressions for the Jacobian and its inverse, which have to be inserted in those Eq. (73) or Eq. (78) from chapter 3, have another appearance, here given by

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1-\tau/_n\, w_{\rm o}^{(2,0)} & -\tau/_n\, w_{\rm o}^{(1,1)} & 0 \\ -\tau/_n\, w_{\rm o}^{(1,1)} & 1-\tau/_n\, w_{\rm o}^{(0,2)} & 0 \\ 0 & 0 & -1 \end{pmatrix} \Rightarrow \mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} \gamma \begin{pmatrix} 1-\tau/_n\, w_{\rm o}^{(0,2)} & \tau/_n\, w_{\rm o}^{(1,1)} \\ \tau/_n\, w_{\rm o}^{(1,1)} & 1-\tau/_n\, w_{\rm o}^{(2,0)} \end{pmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & \quad 0 \end{matrix} & -1 \end{pmatrix} \tag{157}$$

with $\gamma = \dfrac{-1}{\det(\mathbf{A}(\mathbf{0}))} = \dfrac{1}{1-\tau/_n w_{\rm o}^{(2,0)} - (\tau/_n w_{\rm o}^{(1,1)})^2 - \tau/_n\, w_{\rm o}^{(0,2)} + (\tau/_n)^2\, w_{\rm o}^{(2,0)} w_{\rm o}^{(0,2)})}$

and after inserting Eqs. (155) in Eqs. (73), (78), we obtain for the order $k = 2$ the solutions

$$\mathbf{p}^{(1,0)}(0,0) = \gamma \begin{pmatrix} n(n-\tau w_{\rm o}^{(0,2)}) \\ n\tau w_{\rm o}^{(1,1)} \\ 0 \end{pmatrix}, \qquad \mathbf{p}^{(0,1)}(0,0) = \gamma \begin{pmatrix} n\tau w_{\rm o}^{(1,1)} \\ n(n-\tau w_{\rm o}^{(2,0)}) \\ 0 \end{pmatrix} \tag{158}$$

For the orders $k \geq 2$ we apply Eq. (78). The derivatives $\mathbf{A}^{(1,0)} = \dfrac{d}{dx_{\rm p}} \mathbf{A}(\mathbf{p}(x_p, y_{\rm p}))\Big|_{x_{\rm p}=0, y_{\rm p}=0}$ etc. are directly obtained by total derivative of Eq. (156) with respect to $x_{\rm p}$ and $y_{\rm p}$, evaluated for $x_{\rm p} = 0$ and $y_{\rm p} = 0$. For the orders $k = k_x + k_y \geq 2$ only the results $w_{\rm p}^{(k_x,k_y)}(0,0)$ for the propagated wavefront are interesting, therefore we directly provide those result. The resulting second-order law is (omitting the argument '(0)')

$$\begin{aligned} w_{\rm p}^{(2,0)} &= \gamma\left(\tau/_n \left(w_{\rm o}^{(1,1)}\right)^2 + \left(1-\tau/_n\, w_{\rm o}^{(0,2)}\right) w_{\rm o}^{(2,0)}\right) \\ w_{\rm p}^{(1,1)} &= \gamma\, w_{\rm o}^{(1,1)} \\ w_{\rm p}^{(0,2)} &= \gamma\left(\tau/_n \left(w_{\rm o}^{(1,1)}\right)^2 + \left(1-\tau/_n\, w_{\rm o}^{(2,0)}\right) w_{\rm o}^{(0,2)}\right) \end{aligned} \tag{159}$$

which is well-known as the propagation equation and reveals to be a special case of the results. If the coordinate axes coincide with the directions of principal curvature of the wavefront, which means that $w_{\rm o}^{(1,1)} = 0$, Eq. (159) can be simplified to

$$\begin{aligned} w_{\rm p}^{(2,0)} &= \frac{1}{1-\tau/_n\, w_{\rm o}^{(2,0)}}\, w_{\rm o}^{(2,0)} \\ w_{\rm p}^{(1,1)} &= 0 \\ w_{\rm p}^{(0,2)} &= \frac{1}{1-\tau/_n\, w_{\rm o}^{(0,2)}}\, w_{\rm o}^{(0,2)} \end{aligned} \tag{160}$$

<u>The resulting higher-order laws can be written in a similar fashion</u>

$$w_p^{(3,0)} = \gamma^3 \Big((1 - \tfrac{\tau}{n} w_o^{(0,2)})^3 w_o^{(3,0)} + \tfrac{\tau}{n} w_o^{(1,1)} \Big(3(1 - \tfrac{\tau}{n} w_o^{(0,2)})^2 w_o^{(2,1)} + \tfrac{\tau}{n} w_o^{(1,1)} (\tfrac{\tau}{n} w_o^{(0,3)} w_o^{(1,1)}) + 3(1 - \tfrac{\tau}{n} w_o^{(0,2)})^2 w_o^{(1,2)} \Big) \Big)$$

$$\begin{aligned} w_p^{(2,1)} = \gamma^3 \Big(& w_o^{(2,1)} + \tfrac{\tau}{n} \Big(w_o^{(1,1)} (2 w_o^{(1,2)} + w_o^{(3,0)}) - (2 w_o^{(0,2)} + w_o^{(2,0)}) w_o^{(2,1)} \Big) + \\ & (\tfrac{\tau}{n})^2 \Big(w_o^{(2,1)} w_o^{(0,2)^2} - 2(w_o^{(1,1)} (w_o^{(1,2)} + w_o^{(3,0)}) - w_o^{(2,0)} w_o^{(2,1)}) w_o^{(0,2)} + \\ & w_o^{(0,3)} w_o^{(1,1)^2} + 2 w_o^{(1,1)} (w_o^{(1,1)} w_o^{(2,1)} - w_o^{(1,2)} w_o^{(2,0)}) \Big) + \\ & (\tfrac{\tau}{n})^3 \Big(w_o^{(1,2)} w_o^{(1,1)^3} - (w_o^{(0,3)} w_o^{(2,0)} + 2 w_o^{(0,2)} w_o^{(2,1)}) w_o^{(1,1)^2} + \\ & w_o^{(0,2)} (2 w_o^{(1,2)} w_o^{(2,0)} + w_o^{(0,2)} w_o^{(3,0)}) w_o^{(1,1)} - w_o^{(0,2)^2} w_o^{(2,0)} w_o^{(2,1)} \Big) \Big) \end{aligned}$$

$$\begin{aligned} w_p^{(1,2)} = \gamma^3 \Big(& w_o^{(1,2)} + \tfrac{\tau}{n} \Big(w_o^{(1,1)} (2 w_o^{(2,1)} + w_o^{(0,3)}) - (2 w_o^{(2,0)} + w_o^{(0,2)}) w_o^{(1,2)} \Big) + \\ & (\tfrac{\tau}{n})^2 \Big(w_o^{(1,2)} w_o^{(2,0)^2} - 2(w_o^{(1,1)} (w_o^{(2,1)} + w_o^{(0,3)}) - w_o^{(0,2)} w_o^{(1,2)}) w_o^{(2,0)} + \\ & w_o^{(3,0)} w_o^{(1,1)^2} + 2 w_o^{(1,1)} (w_o^{(1,1)} w_o^{(1,2)} - w_o^{(2,1)} w_o^{(0,2)}) \Big) + \\ & (\tfrac{\tau}{n})^3 \Big(w_o^{(2,1)} w_o^{(1,1)^3} - (w_o^{(3,0)} w_o^{(0,2)} + 2 w_o^{(2,0)} w_o^{(1,2)}) w_o^{(1,1)^2} + \\ & w_o^{(2,0)} (2 w_o^{(2,1)} w_o^{(0,2)} + w_o^{(2,0)} w_o^{(0,3)}) w_o^{(1,1)} - w_o^{(2,0)^2} w_o^{(0,2)} w_o^{(1,2)} \Big) \Big) \end{aligned}$$

(161)

$$w_p^{(0,3)} = \gamma^3 \Big((1 - \tfrac{\tau}{n} w_o^{(2,0)})^3 w_o^{(0,3)} + \tfrac{\tau}{n} w_o^{(1,1)} \Big(3(1 - \tfrac{\tau}{n} w_o^{(2,0)})^2 w_o^{(1,2)} + \tfrac{\tau}{n} w_o^{(1,1)} (\tfrac{\tau}{n} w_o^{(3,0)} w_o^{(1,1)}) + 3(1 - \tfrac{\tau}{n} w_o^{(2,0)})^2 w_o^{(2,1)} \Big) \Big)$$

Eqs. (159)-(161) show that the result for $w_p^{(i,j)}$ can be derived from the result of $w_p^{(j,i)}$ by interchanging i and j.

5.2.4. Special Case

Analogously to the special situation that leads to Eq. (149) in the 2D case, it is possible to find a corresponding special case in the 3D case. By a similar reasoning as in the 2D case and as in chapter 3, it is found that if all lower order aberrations for $j_x + j_y < k_x + k_y$ vanish, then Eq. (78) will reduce to the lowest term, yielding

$$
\begin{aligned}
\mathbf{p}^{(k_x,0)} &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,0)}\mathbf{A}^{-1}\mathbf{b}_x &&, \quad k_x \neq 3, k_y = 0 \\
\mathbf{p}^{(3,0)} &= \mathbf{A}^{-1}(2\mathbf{A}^{(1,0)}\mathbf{A}^{-1}\mathbf{A}^{(1,0)} - \mathbf{A}^{(2,0)})\mathbf{A}^{-1}\mathbf{b}_x &&, \quad k_x = 3, k_y = 0 \\
\mathbf{p}^{(2,1)} &= \mathbf{A}^{-1}(\mathbf{A}^{(1,0)}\mathbf{A}^{-1}\mathbf{A}^{(0,1)} + \mathbf{A}^{(0,1)}\mathbf{A}^{-1}\mathbf{A}^{(1,0)} - \mathbf{A}^{(2,0)})\mathbf{A}^{-1}\mathbf{b}_x &&, \quad k_x = 2, k_y = 1 \\
\mathbf{p}^{(k_x,k_y)} &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,k_y)}\mathbf{A}^{-1}\mathbf{b}_x &&, \quad k_x \neq 0, k_y \neq 0, k_x + k_y \neq 3 \\
&= -\mathbf{A}^{-1}\mathbf{A}^{(k_x,k_y-1)}\mathbf{A}^{-1}\mathbf{b}_y && \\
\mathbf{p}^{(1,2)} &= \mathbf{A}^{-1}(\mathbf{A}^{(0,1)}\mathbf{A}^{-1}\mathbf{A}^{(1,0)} + \mathbf{A}^{(1,0)}\mathbf{A}^{-1}\mathbf{A}^{(0,1)} - \mathbf{A}^{(0,2)})\mathbf{A}^{-1}\mathbf{b}_y &&, \quad k_x = 1, k_y = 2 \\
\mathbf{p}^{(0,3)} &= \mathbf{A}^{-1}(2\mathbf{A}^{(0,1)}\mathbf{A}^{-1}\mathbf{A}^{(0,1)} - \mathbf{A}^{(0,2)})\mathbf{A}^{-1}\mathbf{b}_y &&, \quad k_x = 0, k_y = 3 \\
\mathbf{p}^{(0,k_y)} &= -\mathbf{A}^{-1}\mathbf{A}^{(0,k_y-1)}\mathbf{A}^{-1}\mathbf{b}_y &&, \quad k_x = 0, k_y \neq 3
\end{aligned}
\tag{162}
$$

The result in Eqs. (162) is similar as Eq. (73) in chapter 3, but it differs due to different conditions under which the matrix $\mathbf{A}$ or one of its derivatives vanish. For finally evaluating Eqs. (162) 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 is given as

$$
\mathbf{A}^{(m_x,m_y)} = \begin{cases}
\begin{pmatrix} \mathbf{A}_{m_x,m_y} & & \begin{matrix} 0 \\ 0 \end{matrix} \\ w_o^{(m_x+1,m_y+1)} & w_o^{(m_x,m_y)} & 0 \end{pmatrix} & , \quad m_x + m_y = 2 \\
\begin{pmatrix} -\tfrac{\tau}{n} w_o^{(m_x+2,m_y)} & -\tfrac{\tau}{n} w_o^{(m_x+1,m_y+1)} & 0 \\ -\tfrac{\tau}{n} w_o^{(m_x+1,m_y+1)} & -\tfrac{\tau}{n} w_o^{(m_x,m_y+2)} & 0 \\ w_o^{(m_x+1,m_y)} & w_o^{(m_x,m_y+1)} & 0 \end{pmatrix} & , \quad m_x + m_y > 2
\end{cases}
\tag{163}
$$

with

$$
\mathbf{A}_{m_x,m_y} = -\tfrac{\tau}{n} \begin{pmatrix} \tfrac{\tau}{n} \mathbf{v} \begin{pmatrix} w_o^{(3,0)} \\ w_o^{(2,1)} \end{pmatrix} + w_o^{(m_x+2,m_y)} & \tfrac{\tau}{n} \mathbf{v} \begin{pmatrix} w_o^{(2,1)} \\ w_o^{(1,2)} \end{pmatrix} + w_o^{(m_x+1,m_y+1)} \\ \tfrac{\tau}{n} \mathbf{v} \begin{pmatrix} w_o^{(2,1)} \\ w_o^{(1,2)} \end{pmatrix} + w_o^{(m_x+1,m_y+1)} & \tfrac{\tau}{n} \mathbf{v} \begin{pmatrix} w_o^{(1,2)} \\ w_o^{(0,3)} \end{pmatrix} + w_o^{(m_x,m_y+2)} \end{pmatrix}
$$

$$
\mathbf{v} = \begin{pmatrix} w_o^{(m_x+1,m_y)} \\ w_o^{(m_x,m_y+1)} \end{pmatrix}
$$

where $x_{\mathrm{o}}^{(1,0)}$, $x_{\mathrm{o}}^{(0,1)}$, $y_{\mathrm{o}}^{(1,0)}$, $y_{\mathrm{o}}^{(0,1)}$, etc. have been substituted by their solutions according to Eq. (158). Inserting $\mathbf{A}^{(m_x,m_y)}$ from Eqs. (163) and $\mathbf{A}(\mathbf{0})^{-1}$ from Eq. (157) into Eqs. (162) yields one common relation for $w_{\mathrm{p}}^{(k_x,k_y)}$ for the various subcases in Eqs. (162) (omitting the argument '$(0,0)$'):

$$w_{\mathrm{p}}^{(k_x,k_y)} = w_{\mathrm{o}}^{(k_x,k_y)} \tag{164}$$

for all orders $k = k_x + k_y > 2$.

5.3. Results

5.3.1. 2D Case

Eq. (141) holds likewise for the derivatives and for the coefficients $a_{\mathrm{o},k}$, and $a_{\mathrm{p},k}$ due to Eqs. (124),(125). In terms of local aberrations and substituting $d = \tau / n$ and $\beta = \dfrac{1}{1-\tau/_n w_{\mathrm{o}}^{(2)}} = \dfrac{1}{1-\frac{d}{n}S_o}$, Eq. (141) reads

$$\begin{aligned}
S_p &= \beta S_o \\
E_{p,3} &= \beta^3 E_{o,3} \\
E_{p,4} &= \beta^4\left(E_{o,4} + 3\tfrac{d}{n}\left(\beta E_{o,3}^2 - \frac{S_o^4}{n^2}\right)\right) \\
E_{p,5} &= \beta^5\left(E_{o,5} + 5\beta\tfrac{d}{n}E_{o,3}\left(2E_{o,4} + 3\beta\tfrac{d}{n}E_{o,3}^2 - 6\frac{S_o^3}{n^2}\right)\right) \\
E_{p,6} &= \beta^6\left(E_{o,6} + 5\beta\tfrac{d}{n}\left(3E_{o,3}E_{o,5} + 21\beta\tfrac{d}{n}E_{o,3}^2E_{o,4} - 12\frac{S_o^3E_{o,4}}{n^2}\right.\right. \\
&\quad \left.\left. + 2E_{o,4}^2 - 9\beta S_0^2E_{o,3}^2\frac{3+4\frac{d}{n}S_o}{n^2} + 21(\beta\tfrac{d}{n})^2E_{o,3}^4 + 9S_o^6\frac{1+\frac{d}{n}S_o}{n^4}\right)\right)
\end{aligned} \quad , \tag{165}$$

Eq. (165) can be generalized for $2 < k \leq 6$ to

$$E_{p,k} = \beta^k(E_{o,k} + R_k) \tag{166}$$

where in R_k all wavefront derivatives $E_{\mathrm{o},j}$ of lower order ($j < k$) are expressed in terms of local aberrations.

If only aberrations for one single given order k are present while for all lower orders $j < k$ we have $E_{o,j} = 0$, then $\beta = 1$ and $R_k = 0$, which means for fixed order k that Eq. (166) will be valid for vanishing remainder term and the aberration of the propagated wavefront will be equal to the aberration of the original wavefront independent of the propagation distance d.

$$E_{p,k} = E_{o,k} \tag{167}$$

Although the primary interest is to describe the relation between the aberrations of the original and propagated wavefront, our approach also delivers simultaneously the relation between the coordinates of the original and propagated wavefront as described in Eq. (128) (see Figure 26).
The relation between the coordinates is very interesting for example to calculate the changing boundary of the wavefront by propagation as done approximately in [44].
The function $y_o(y_p)$ describing the relation between the coordinate of the original and the propagated wavefront can be described by power series expansion with

$$y_o(y_p) = \sum_{k=0}^{\infty} \frac{y_o^{(k)}(0)}{k!} y_p^{\,k} \,. \tag{168}$$

The solutions for the derivatives of $y_o^{(k)}$ are given by the Eqs. (136) with

$$\begin{aligned}
&y_o(0) = 0 \\
&y_o^{(1)}(0) = \beta \\
&y_o^{(2)}(0) = \tau\!/\!_n\, \beta^3 w_o^{(3)} \\
&y_o^{(3)}(0) = \tau\!/\!_n\, \beta^4 \left(w_o^{(4)} + 3\left(\tau\!/\!_n\, \beta w_o^{(3)^2} - w_o^{(2)^3} \right)\right) \\
&y_o^{(4)}(0) = \tau\!/\!_n\, \beta^5 \left(w_o^{(5)} + \beta w_o^{(3)} \left(5\, \tau\!/\!_n (2 w_o^{(4)} + 3\, \tau\!/\!_n\, \beta\, w_o^{(3)^2}) - 6 w_o^{(2)^2} (3 + 2\, \tau\!/\!_n\, w_o^{(2)}) \right)\right) \\
&\ldots
\end{aligned} \tag{169}$$

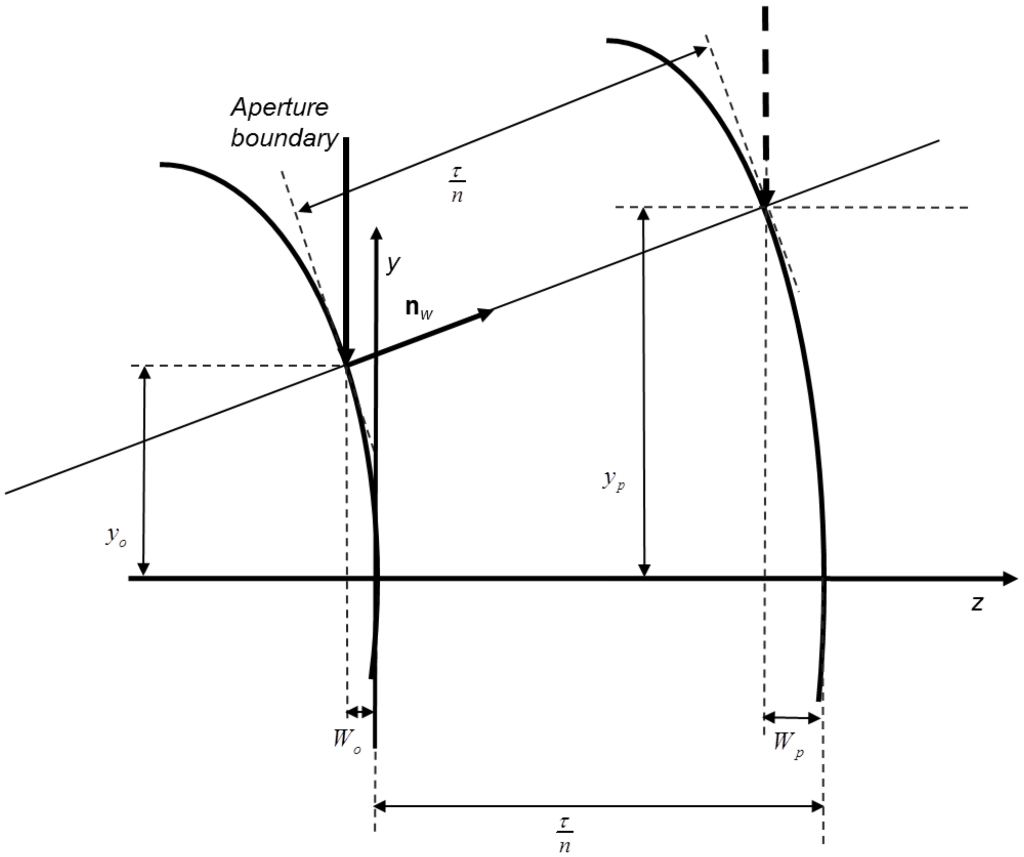

Figure 26: Propagation of a wavefront $\mathbf{w_o}$ about the distance $d = \tau/n$ to the propagated wavefront $\mathbf{w_p}$

Although the primary interest is to describe the relation between the aberrations of the original and propagated wavefront, our approach also delivers simultaneously the relation between the coordinates of the original and propagated wavefront. The relation between the coordinates is very interesting for example to calculate the changing boundary of the wavefront by propagation

5.3.2. 3D Case

Eq. (159) can be summarized to a vector equation in terms of local aberrations and substituting $d = \tau / n$

$$\mathbf{s}_p = \gamma \left(\mathbf{s}_o + \frac{d}{n} \begin{pmatrix} S_{o,xy}^2 - S_{o,xx} S_{o,yy} \\ 0 \\ S_{o,xy}^2 - S_{o,xx} S_{o,yy} \end{pmatrix} \right) \tag{170}$$

with

$$\gamma = \frac{1}{1 - d/n\, S_{o,xx} - (d/n\, S_{o,xy})^2 - d/n\, S_{o,yy} + (d/n)^2 S_{o,xx} S_{o,yy})}$$

also shown in terms of local aberrations.

The vector equation (170) is identical with the well-known propagation matrix equation (19) Equivalently Eq. (161) can be transformed to a vector equation in terms of local aberrations

$$\mathbf{e}_{p,3} = \begin{pmatrix} \beta_{xx}^3 & 3\beta_{xx}^2\beta_{xy} & 3\beta_{xx}\beta_{xy}^2 & \beta_{xy}^3 \\ \beta_{xx}^2\beta_{xy} & \beta_{xx}(\beta_{xx}\beta_{yy} + 2\beta_{xy}^2) & \beta_{xy}(2\beta_{xx}\beta_{yy} + \beta_{xy}^2) & \beta_{xy}^2\beta_{yy} \\ \beta_{xx}\beta_{xy}^2 & \beta_{xy}(2\beta_{xx}\beta_{yy} + \beta_{xy}^2) & \beta_{yy}(\beta_{xx}\beta_{yy} + 2\beta_{xy}^2) & \beta_{xy}\beta_{yy}^2 \\ \beta_{xy}^3 & 3\beta_{xy}^2\beta_{yy} & 3\beta_{xy}\beta_{yy}^2 & \beta_{yy}^3 \end{pmatrix} \mathbf{e}_{o,3} \tag{171}$$

with

$$\begin{pmatrix} \beta_{xx} & \beta_{xy} \\ \beta_{xy} & \beta_{yy} \end{pmatrix} = \left(\mathbf{1} - \frac{\tau}{n}\begin{pmatrix} w_{\mathrm{o}}^{(2,0)} & w_{\mathrm{o}}^{(1,1)} \\ w_{\mathrm{o}}^{(1,1)} & w_{\mathrm{o}}^{(0,2)} \end{pmatrix}\right)^{-1} = \left(\mathbf{1} - \frac{d}{n}\begin{pmatrix} S_{\mathrm{o},xx} & S_{\mathrm{o},xy} \\ S_{\mathrm{o},xy} & S_{\mathrm{o},yy} \end{pmatrix}\right)^{-1}$$

If the coordinate system is chosen in such a way that the *x*- and *y*- axis coincide with the directions of principal curvature of the wavefront, then the equations can be simplified. For doing so, the coefficients a of the original wavefront have to be rotated around the axis α of the wavefront (the direction of one principal curvature) with

$$\alpha = \frac{1}{2}\arctan\left(\frac{-2S_{o,xy}}{S_{o,yy} - S_{o,xx}}\right) \tag{172}$$

Then Eqs. (170) and (171) can be simplified to

$$\mathbf{s}_p = \begin{pmatrix} \beta_{xx} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \beta_{yy} \end{pmatrix} \mathbf{s}_o \tag{173}$$

$$\mathbf{e}_{p,3} = \begin{pmatrix} \beta_{xx}^3 & 0 & 0 & 0 \\ 0 & \beta_{xx}^2\beta_{yy} & 0 & 0 \\ 0 & 0 & \beta_{xx}\beta_{yy}^2 & 0 \\ 0 & 0 & 0 & \beta_{yy}^3 \end{pmatrix} \mathbf{e}_{o,3} \tag{174}$$

and also for the radial order $k = 4$ an appealing equation can be derived

$$\mathbf{e}_{p,4}=\begin{pmatrix}\beta_{xx}^{4} & \cdots & & \cdots & 0\\ \vdots & \beta_{xx}^{3}\beta_{yy}^{1} & & & \vdots\\ & & \beta_{xx}^{2}\beta_{yy}^{2} & & \\ \vdots & & & \beta_{xx}^{1}\beta_{yy}^{3} & \vdots\\ 0 & & & \cdots & \beta_{yy}^{4}\end{pmatrix} \left(\mathbf{e}_{o,4}+\frac{d}{n}\begin{pmatrix} 3\left(\beta_{xx}E_{o,xxx}^{2}+\beta_{yy}E_{o,xxy}^{2}-\frac{S_{o,xx}^{4}}{n^{2}}\right)\\ 3E_{o,xxy}\left(\beta_{xx}E_{o,xxx}+\beta_{yy}E_{o,xxy}\right)\\ \beta_{xx}(2E_{o,xxy}^{2}+E_{o,xxx}E_{o,xyy})+\beta_{yy}(2E_{o,xyy}^{2}+E_{o,xxy}E_{o,yyy})-\left(\frac{S_{o,xx}S_{o,yy}}{n}\right)^{2}\\ 3E_{o,xyy}\left(\beta_{xx}E_{o,xxy}+\beta_{yy}E_{o,yyy}\right)\\ 3\left(\beta_{xx}E_{o,xyy}^{2}+\beta_{yy}E_{o,yyy}^{2}-\frac{S_{o,yy}^{4}}{n^{2}}\right)\end{pmatrix}\right) \tag{175}$$

Afterwards the coefficients of the propagated wavefront have to be re-rotated to the original coordinate system. The resulting coefficients are then of course identical to the coefficients calculated by Eqs. (170) and (171).

Eq. (174)-(175) can be generalized for $2<k\leq 6$ to the novel equation

$$\mathbf{e}_{p,k}=\mathbf{B}_{k}(\mathbf{e}_{o,k}+\mathbf{r}_{k}) \tag{176}$$

where $\mathbf{r}_k$ is a vector collecting the remainder terms R_{k_x,k_y} analogously to R_k in Eq. (166) and with

$$\mathbf{B}_{k}=\begin{pmatrix}\beta_{xx}^{k} & \cdots & & \cdots & 0\\ \vdots & \beta_{xx}^{k-1}\beta_{yy}^{1} & & & \vdots\\ & & \ddots & & \\ \vdots & & & \beta_{xx}^{1}\beta_{yy}^{k-1} & \vdots\\ 0 & & & \cdots & \beta_{yy}^{k}\end{pmatrix} \tag{177}$$

The result of the special case treated in Eqs. (162)-(164) can be summarized in a similar fashion as Eq. (176) to a vector equation in the very appealing form

$$\mathbf{e}_{p,k}=\mathbf{e}_{o,k} \tag{178}$$

which is Eq. (176) for $\mathbf{r}_k=\mathbf{0}$. Eq. (178), an interesting result of the present thesis, is the propagation equation for aberrations of fixed order $k\geq 3$ under the assumption that all aberrations with order lower than k vanish, which means that the aberration of the propagated wavefront will be equal to the aberration of the original wavefront independent of the propagation distance d.

As written in the 2D case our primary interest is to describe the relation between the aberrations of the original and propagated wavefront. Our approach also delivers simultaneously the relation between the coordinates of the original and propagated wavefront as described in Eq. (152) . The relation between the coordinates is very interesting for example to calculate the changing boundary of the wavefront by propagation as done approximately in [44].

The functions $x_{\mathrm{o}}(x_{\mathrm{p}}, y_{\mathrm{p}})$ and $y_{\mathrm{o}}(x_{\mathrm{p}}, y_{\mathrm{p}})$ describing the relation between the coordinates of the original and the propagated wavefront can be described by power series expansion with

$$\begin{aligned} x_{\mathrm{o}}(x_p, y_{\mathrm{p}}) &= \sum_{k=0}^{\infty}\sum_{m=0}^{k} \frac{x_{\mathrm{o}}{}^{(m,k-m)}(0,0)}{m!(k-m)!} x_{\mathrm{p}}{}^{m} y_{\mathrm{p}}{}^{k-m} \\ y_{\mathrm{o}}(x_p, y_{\mathrm{p}}) &= \sum_{k=0}^{\infty}\sum_{m=0}^{k} \frac{y_{\mathrm{o}}{}^{(m,k-m)}(0,0)}{m!(k-m)!} x_{\mathrm{p}}{}^{m} y_{\mathrm{p}}{}^{k-m} \end{aligned} \tag{179}$$

Analogously to the definition of the vectors for aberrations in Eq. (26), similar vectors $\mathbf{x}_k$ and $\mathbf{y}_k$ of dimension $k+1$ can be defined (omitting the argument (0,0)).

$$\mathbf{x}_{o,k} = \begin{pmatrix} x_{\mathrm{o}}^{(k,0)} \\ x_{\mathrm{o}}^{(k-1,1)} \\ \vdots \\ x_{\mathrm{o}}^{(0,k)} \end{pmatrix}, \quad \mathbf{y}_{o,k} = \begin{pmatrix} y_{\mathrm{o}}^{(k,0)} \\ y_{\mathrm{o}}^{(k-1,1)} \\ \vdots \\ y_{\mathrm{o}}^{(0,k)} \end{pmatrix} \tag{180}$$

The solutions for the derivatives of $y_{\mathrm{o}}{}^{(k)}$ are given by the Eqs. (329) and reads for the special case that the coordinate system is chosen in such a way, that the *x*- and *y*- axis coincide with the directions of principal curvature of the wavefront.

$$\begin{aligned} \mathbf{x}_{\mathrm{o},0} &= 0 \\ \mathbf{y}_{\mathrm{o},0} &= 0 \\ \mathbf{x}_{\mathrm{o},1} &= \begin{pmatrix} \beta_{xx} \\ 0 \end{pmatrix} \\ \mathbf{y}_{\mathrm{o},1} &= \begin{pmatrix} 0 \\ \beta_{yy} \end{pmatrix} \\ \mathbf{x}_{\mathrm{o},2} &= \tau/n \begin{pmatrix} \beta_{xx}{}^3 & 0 & 0 \\ 0 & \beta_{xx}{}^2\beta_{yy} & 0 \\ 0 & 0 & \beta_{xx}\beta_{yy}{}^2 \end{pmatrix} \begin{pmatrix} w_{\mathrm{o}}^{(3,0)} \\ w_{\mathrm{o}}^{(2,1)} \\ w_{\mathrm{o}}^{(1,2)} \end{pmatrix} \\ \mathbf{y}_{\mathrm{o},2} &= \tau/n \begin{pmatrix} \beta_{xx}{}^2\beta_{yy} & 0 & 0 \\ 0 & \beta_{xx}\beta_{yy}{}^2 & 0 \\ 0 & 0 & \beta_{yy}{}^3 \end{pmatrix} \begin{pmatrix} w_{\mathrm{o}}^{(2,1)} \\ w_{\mathrm{o}}^{(1,2)} \\ w_{\mathrm{o}}^{(0,3)} \end{pmatrix} \end{aligned} \tag{181}$$

$$\mathbf{x}_{o,3} = \tau\!/\!n \begin{pmatrix} \beta_{xx}{}^{4} & 0 & 0 & 0 \\ 0 & \beta_{xx}{}^{3}\beta_{yy} & 0 & 0 \\ 0 & 0 & \beta_{xx}{}^{2}\beta_{yy}{}^{2} & 0 \\ 0 & 0 & 0 & \beta_{xx}\beta_{yy}{}^{3} \end{pmatrix} \left(\begin{pmatrix} w_o^{(4,0)} \\ w_o^{(3,1)} \\ w_o^{(2,2)} \\ w_o^{(1,3)} \end{pmatrix} + \begin{pmatrix} 3\,{}^{\tau}\!/_{n}\,(\beta_{xx} w_o^{(3,0)^2} + \beta_{yy} w_o^{(2,1)^2}) - 3 w_o^{(2,0)^3} \\ 3\,{}^{\tau}\!/_{n}\, w_o^{(2,1)} (\beta_{xx} w_o^{(3,0)} + \beta_{yy} w_o^{(1,2)}) \\ 2\,{}^{\tau}\!/_{n}\,\beta_{yy} w_o^{(1,2)^2} - w_o^{(0,2)} w_o^{(2,0)^2} + {}^{\tau}\!/_{n}\, w_o^{(2,1)} (2\beta_{xx} w_o^{(2,1)} + \beta_{yy} w_o^{(0,3)}) + {}^{\tau}\!/_{n}\,\beta_{xx} w_o^{(1,2)} w_o^{(3,0)} \\ 3\,{}^{\tau}\!/_{n}\, w_o^{(1,2)} (\beta_{xx} w_o^{(2,1)} + \beta_{yy} w_o^{(0,3)}) \end{pmatrix} \right)$$

$$\mathbf{y}_{o,3} = \tau\!/\!n \begin{pmatrix} \beta_{xx}{}^{3}\beta_{yy} & 0 & 0 & 0 \\ 0 & \beta_{xx}{}^{2}\beta_{yy}{}^{2} & 0 & 0 \\ 0 & 0 & \beta_{xx}\beta_{yy}{}^{3} & 0 \\ 0 & 0 & 0 & \beta_{yy}{}^{4} \end{pmatrix} \left(\begin{pmatrix} w_o^{(3,1)} \\ w_o^{(2,2)} \\ w_o^{(1,3)} \\ w_o^{(0,4)} \end{pmatrix} + \begin{pmatrix} 3\,{}^{\tau}\!/_{n}\, w_o^{(2,1)} (\beta_{xx} w_o^{(3,0)} + \beta_{yy} w_o^{(1,2)}) \\ 2\,{}^{\tau}\!/_{n}\,\beta_{yy} w_o^{(1,2)^2} - w_o^{(0,2)} w_o^{(2,0)^2} + {}^{\tau}\!/_{n}\, w_o^{(2,1)} (2\beta_{xx} w_o^{(2,1)} + \beta_{y} w_o^{(0,3)}) + {}^{\tau}\!/_{n}\,\beta_{xx} w_o^{(1,2)} w_o^{(3,0)} \\ 3\,{}^{\tau}\!/_{n}\, w_o^{(1,2)} (\beta_{xx} w_o^{(2,1)} + \beta_{yy} w_o^{(0,3)}) \\ 3\,{}^{\tau}\!/_{n}\,(\beta_{xx} w_o^{(1,2)^2} + \beta_{yy} w_o^{(0,3)^2}) - 3 w_o^{(0,2)^3} \end{pmatrix} \right)$$

$$\ldots \qquad (182)$$

5.4. Examples and Applications

One important application of the derived equations is that they allow determining the aberrations of a wavefront by propagation, which not only has a defined Power S_o, but also shows aberrations of higher aberrations. Because of the analytical nature of the equations it is not necessary to use an iterative numerical method.

We use the derived equations (173)-(175) to determine the aberrations of the propagated wavefront up to the radial order $k = 6$ and compare them firstly with the results calculated by the analytical wavefront approach described by Dai et al in [36,44]. One approximation with significant influence of the analytical wavefront approach described by Dai et al is that the transformation of the coefficients was solved without solving simultaneously the coordinate dependence. As we show in the examples, and as is also stated in [44], it is absolutely necessary to solve both dependencies simultaneously if wavefronts are containing both low-order and high-order aberrations.

Secondly we compare our results with the results calculated by a numerical ray-tracing approach using the optical design package ZEMAX® followed by a Zernike analysis.

We would like to stress again that our local aberration values are obtained by an analytical method and therefore by definition are exact. The transformation of our local Taylor coefficients to

Zernike coefficients, on the other hand, yields only an (however very good) approximation for their numerical values based on the assumption that the truncated subspaces of order $k \leq 6$ 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 by its nature resulting in small deviations from zero (see Table 4 to Table 7).

The necessary transformation between Zernike and Taylor coefficients, itself being state of the art, is in our case also accompanied by the transformation from an OPD wave aberration to a wavefront aberration referring to the sagitta, which is in detail discussed in chapter 3. The logical flow of the transformations is illustrated in Figure 38 in Appendix C.

The examples A1 and A2 are characterized by the specific feature that the first and second derivatives are zero which means that the coefficients of Taylor monomials of first and second order are also zero (see Table 11 in Appendix C). This implies that the low-order aberrations LOA (radial order $k<3$) expressed as Taylor monomials are zero while in the examples B1 and B2 low-order and high-order aberrations do occur (see Table 12 in Appendix C). In the examples A1 and B1 only rotationally symmetric aberrations are present while in the examples A2 and B2 also non rotational-symmetric aberrations like coma, trefoil, secondary astigmatism etc. occur.

The value of the propagation distance d is 20 mm, of the pupil diameter d_0 is 6 mm and of the refractive index n is 1 in all four examples.

For giving some more insight how the resulting values are obtained within our framework, we provide explicit formulas for the Taylor coefficients in the case of the rotationally symmetric examples A1 and B1. In this case all the odd order coefficients vanish, and we obtain directly for order $n = 2$ from Eq. (170)

$$\mathbf{s}_p = \begin{pmatrix} \beta_{xx} S_{o,xx} \\ 0 \\ \beta_{yy} S_{o,xx} \end{pmatrix} \tag{183}$$

For order $n = 4$ it follows from Eq. (175) that

$$\mathbf{e}_{p,4} = \begin{pmatrix} \beta_{xx}^4 E_{o,xxxx} \\ 0 \\ \beta_{xx}^2 \beta_{yy}^2 E_{o,xxyy} \\ 0 \\ \beta_{yy}^4 E_{o,yyyy} \end{pmatrix} - \frac{d}{n^3} \begin{pmatrix} 3\beta_{xx}^4 S_{o,xx}^4 \\ 0 \\ \beta_{xx}^2 \beta_{yy}^2 \left(S_{o,xx} S_{o,yy}\right)^2 \\ 0 \\ 3\beta_{yy}^4 S_{o,yy}^4 \end{pmatrix}, \tag{184}$$

and for order $n = 6$ it follows from the general solution in Eq. (176) after some algebra that

$$E_{p,xxxxxx} = \beta_{xx}^6 \left(E_{o,xxxxxx} + 5\frac{d}{n^5}\left(2\beta_{xx}\left(n^2 E_{o,xxxx} - 3S_{o,xx}^3\right) - 9S_{o,xx}^6\right)\right)$$

$$E_{p,xxxxyy} = \beta_{xx}^4 \beta_{yy}^2 \left(E_{o,xxxxyy} + \frac{d}{n^6} \begin{pmatrix} 6\beta_{yy} n^5 E_{o,xxxx}^2 \\ + \beta_{xx} S_{o,xx} S_{o,yy}^2 \left(3S_{o,xx}^3\left(n + d(3-2\beta_{yy})S_{o,xx} + 2n\beta_{yy}\right) - 4n^3 E_{o,xxxx}\right) \\ + 4n^3 \beta_{xx} E_{o,xxyy}\left(n^2 E_{o,xxxx} + 3S_{o,xx}^3\left((\beta_{yy}-2)S_{o,xx} - \beta_{yy}S_{o,yy}\right)\right) \end{pmatrix} \right),$$

$$E_{p,xxyyyy} = E_{p,xxxxyy}(x \leftrightarrow y)$$

$$E_{p,yyyyyy} = E_{p,xxxxxx}(x \leftrightarrow y)$$

(185)

Example A1:

Given is the original wavefront expressed with Zernike polynomials. The coefficients of the Zernike polynomials are zero except defocus c_2^0, spherical aberration c_4^0 and secondary spherical aberration c_6^0, their values being chosen such that the second-order local aberrations vanish, which means that the coefficients of Taylor monomials of first and second order are also zero (see Table 11 in Appendix C). In this example only rotationally symmetric aberrations are present.

In this case the equations derived by Dai et al [44] are a very good approximation as also stated in the conclusion by Dai et al [44]. The approximation made by Dai et al [44] is solving the transformation of the coefficients without solving simultaneously the coordinate dependence. This approximation will be in first order correct if the local second order wavefront aberrations are zero. As shown in Eq. (169) in the 2D case and Eq. (181) in the 3D case, the coordinates (x_o, y_o) of the original wavefront and the coordinates (x_p, y_p) of the propagated wavefront are then in first order equal because $\beta_{xx} = 1$ and $\beta_{yy} = 1$.

The values of the original wavefront and the resulting values of the propagated wavefront derived by all three methods are provided in Table 4. The consistency between the results of all three methods is obvious. The local aberration values are obtained by an analytical method and therefore by definition are exact. The transformation of our local Taylor coefficients to Zernike coefficients, on the other hand, yields only an (however very good) approximation for their numerical values based on the assumption that the truncated subspaces of order $k \le 6$ 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 by its nature resulting in small deviations from zero (see Table 4).

The logical flow of the transformations is illustrated in Figure 38 in Appendix C, which includes the steps transformation of the Zernike OPD representation of the original wavefront to Taylor OPD representation, then transforming the Taylor OPD representation to Taylor wavefront sagitta representation, then propagation of the Taylor wavefront sagitta representation using the derived equations and transforming back to Taylor OPD representation and Zernike OPD representation of the propagated wavefront. Additionally, the values of the local aberrations before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) are provided in Table 11 (see Appendix C)

Zernike coefficients					
		Original wavefront	Propagated wavefront		
Radial order	Symbol (OSA standard)		Numerical Ray-Tracing	Analytical Wavefront-Tracing	
			ZEMAX®	Dai [44]	Our method
k		$value/\mu m$	$value/\mu m$	$value/\mu m$	$value/\mu m$
0	c_0^0	-1.46532	-1.38629	-1.37962	-1.37911
1	c_1^{-1}	0	0	0	0
	c_1^1	0	0	0	0
2	c_2^{-2}	0	0	0	0
	c_2^0	-1.26853	-1.18718	-1.17953	-1.17894
	c_2^2	0	0	0	0
3	c_3^{-3}	0	0	0	0
	c_3^{-1}	0	0	0	0
	c_3^1	0	0	0	0
	c_3^3	0	0	0	0
4	c_4^{-4}	0	0	0	0
	c_4^{-2}	0	0	0	0
	c_4^0	-0.327046	-0.292971	-0.28882	-0.288494
	c_4^2	0	0	0	0
	c_4^4	0	$-6.46*10^{-8}$	0	0
5	c_5^{-5}	0	0	0	0
	c_5^{-3}	0	0	0	0
	c_5^{-1}	0	0	0	0
	c_5^1	0	0	0	0
	c_5^3	0	0	0	0
	c_5^5	0	0	0	0
6	c_6^{-6}	0	0	0	0
	c_6^{-4}	0	0	0	0
	c_6^{-2}	0	0	0	0
	c_6^0	0.000205909	0.00545139	0.00662599	0.00672247
	c_6^2	0	0	0	0
	c_6^4	0	$-7.05*10^{-8}$	0	0
	c_6^6	0	0	0	0

Table 4: Zernike coefficients of the original and propagated wavefront in example A1: Propagated wavefront. Left column: values based on the ray-tracing package (ZEMAX®). Middle column: values based on method on the method derived by Dai et al [36,44]. Right column: values based on our analytical method. The consistency between the results of all three methods is obvious.

Example A2:

In example A2 the original wavefront shows defocus, astigmatism, coma, trefoil, spherical aberration, secondary astigmatism, quadrafoil, secondary coma, secondary trefoil, secondary spherical aberration, secondary quadrafoil and tertiary astigmatism. Also in this example their values being chosen such that the second-order local aberrations vanish, which means that the coefficients of Taylor monomials of first and second order are also zero (see Table 11 in Appendix C).

Also in this more complex example containing also non-symmetric aberrations the equations derived by Dai et al [44] are a very good approximation, because the coordinates (x_o, y_o) of the original wavefront and the coordinates (x_p, y_p) of the propagated wavefront are in first order identical based on the fact that $\beta_{xx} = 1$ and $\beta_{yy} = 1$ (see Eq. (169) and Eq. (181)).

The values of the original wavefront and the resulting values of the propagated wavefront derived by all three methods are provided in Table 5. Also in this complex case the consistency between the results of all three methods is obvious.

The logical flow of the transformations is illustrated in Figure 38 in Appendix C. Again, values of the local aberrations before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) are provided in Table 11 (see Appendix C).

Zernike coefficients					
		Original wavefront	Propagated wavefront		
Radial order	Symbol (OSA standard)		Numerical Ray-Tracing	Analytical Wavefront-Tracing	
			ZEMAX®	Dai [44]	Our method
k		$value/\mu m$	$value/\mu m$	$value/\mu m$	$value/\mu m$
0	c_0^0	0.0675296	0.0716304	0.071439	0.0714675
1	c_1^{-1}	-0.469074	-0.471531	-0.471178	-0.471169
	c_1^1	0	0	0	0
2	c_2^{-2}	0	0	0	0
	c_2^0	0.0586014	0.0621846	0.0620453	0.062074
	c_2^2	-0.00939598	-0.0122335	-0.0122895	-0.0123183
3	c_3^{-3}	0.00510456	0.0053063	0.00526967	0.00527765
	c_3^{-1}	-0.167062	-0.1684	-0.168264	-0.168248
	c_3^1	0	0	0	0
	c_3^3	0	0	0	0
4	c_4^{-4}	0	0	0	0
	c_4^{-2}	0	0	0	0
	c_4^0	0.0152538	0.016233	0.0162035	0.0162148
	c_4^2	-0.0024714	-0.00327439	-0.00325126	-0.00326303
	c_4^4	0.0000898562	0.000141849	0.000138134	0.000140068
5	c_5^{-5}	$-2.28*10^{-6}$	$-5.3*10^{-6}$	$-4.36*10^{-6}$	$-4.32*10^{-6}$
	c_5^{-3}	0.0000541121	0.000100209	0.0000896324	0.0000894449
	c_5^{-1}	-0.000663872	-0.000959765	-0.000917853	-0.000905828
	c_5^1	0	0	0	0
	c_5^3	0	0	0	0
	c_5^5	0	0	0	0
6	c_6^{-6}	0	0	0	0
	c_6^{-4}	0	0	0	0
	c_6^{-2}	0	0	0	0
	c_6^0	0.000051976	0.000084556	0.0000778738	0.0000791508
	c_6^2	-0.000019171	-0.00003832	-0.0000332	-0.000034846
	c_6^4	$1.45*10^{-6}$	$3.71*10^{-6}$	$2.88*10^{-6}$	$3.16*10^{-6}$
	c_6^6	$-6.65*10^{-8}$	$-2.00*10^{-7}$	$-1.49*10^{-7}$	$-1.69*10^{-7}$

Table 5: Zernike coefficients of the original and propagated wavefront in example A2: Propagated wavefront. Left column: values based on the ray-tracing package (ZEMAX®). Middle column: values based on the method derived by Dai et al [36,44]. Right column: values based on our analytical method. The consistency between the results of all three methods is obvious.

Example B1:

Example B1 is similar to example A1. Also in this example the coefficients of the Zernike polynomials are zero expect defocus c_2^0, spherical aberration c_4^0 and secondary spherical aberration c_6^0, which means only rotationally symmetric aberrations are present. But now the original wavefront is characterized by the specific feature that low order aberrations LOA (radial order k=2) expressed as Taylor monomials are non-zero (see Table 12). In this case the equations derived by Dai et al [44] are not a good approximation as also stated in the conclusion by Dai et al [44].

The values of the original wavefront and the resulting values of the propagated wavefront derived by all three methods are provided in Table 6. The consistency between the results derived by the optical design package ZEMAX® and our analytical method is obvious while the results derived by the analytical method of Dai et al [44] differ strongly. The wrong results derived by the analytical method of Dai et al are based on the fact that in this method the coordinate change by propagation is not considered. This approximation will lead to wrong results, also in this simple case containing only rotationally symmetric aberrations, because low order and high aberrations order occur as stated by Dai et al [44] in their conclusion. As shown in Eq. (169) in the 2D case and Eq. (181) in the 3D case, the coordinates (x_o, y_o) of the original wavefront and the coordinates (x_p, y_p) of the propagated wavefront are then in first order not equal because $\beta_{xx} \neq 1$ and $\beta_{yy} \neq 1$.

The logical flow of the transformations is illustrated in Figure 38 in Appendix C. Again, values of the local aberrations before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) are provided in Table 12 (see Appendix C).

Zernike coefficients						
		Original wavefront	Propagated wavefront			
Radial order	Symbol (OSA standard)		Numerical Ray-Tracing	Analytical Wavefront-Tracing		
			ZEMAX®	Dai [44]	Our method	
k		$value/\mu m$	$value/\mu m$	$value/\mu m$	$value/\mu m$	
0	c_0^0	-50.1362	-34.3311	-26.5342	-34.3309	
1	c_1^{-1}	0	$1.18*10^{-8}$	0	0	
	c_1^1	0	$1.18*10^{-8}$	0	0	
2	c_2^{-2}	0	$-1.76*10^{-8}$	0	0	
	c_2^0	-29.3453	-19.9117	-14.9908	-19.9115	
	c_2^2	0	0	0	0	
3	c_3^{-3}	0	$5.88*10^{-9}$	0	0	
	c_3^{-1}	0	0	0	0	
	c_3^1	0	0	0	0	
	c_3^3	0	$-5.88*10^{-9}$	0	0	
4	c_4^{-4}	0	0	0	0	
	c_4^{-2}	0	0	0	0	
	c_4^0	-0.309331	-0.069658	0.261713	-0.0695334	
	c_4^2	0	0	0	0	
	c_4^4	0	$-1.76*10^{-8}$	0	0	
5	c_5^{-5}	0	$1.76*10^{-8}$	0	0	
	c_5^{-3}	0	0	0	0	
	c_5^{-1}	0	0	0	0	
	c_5^1	0	0	0	0	
	c_5^3	0	0	0	0	
	c_5^5	0	$1.76*10^{-8}$	0	0	
6	c_6^{-6}	0	$2.94*10^{-8}$	0	0	
	c_6^{-4}	0	$-1.18*10^{-8}$	0	0	
	c_6^{-2}	0	0	0	0	
	c_6^0	-0.000110975	0.000437634	0.00598868	0.000473857	
	c_6^2	0	0	0	0	
	c_6^4	0	$1.18*10^{-8}$	0	0	
	c_6^6	0	0	0	0	

Table 6: Zernike coefficients of the original and propagated wavefront in example B1: Propagated wavefront. Left column: values based on the ray-tracing package (ZEMAX®). Middle column: values based on the method derived by Dai et al [36,44]. Right column: values based on our analytical method. The consistency between the results derived by the optical design package ZEMAX® and our analytical method is obvious while the results derived by the analytical method of Dai et al [44] differ strongly.

Example B2:

Example B2 is similar to example A2 but here the original wavefront is also as in example B1 characterized by the specific feature that the low order aberrations LOA (radial order *k*=2) expressed as Taylor monomials are non-zero (see Table 12). In this case the equations derived by Dai et al [44] are also not a good approximation.

In contrast to example B1, in example B2 also non rotationally symmetric aberrations as coma, trefoil, secondary astigmatism etc. occur.

The values of the original wavefront and the resulting values of the propagated wavefront derived by all three methods are provided in Table 7. Also this complex example shows an obvious consistency between the results derived by the optical design package ZEMAX® and our analytical method. In contrast, the results derived by the analytical method of Dai et al [44] differ significantly. The wrong results derived by the analytical method of Dai et al are based on the fact that in this method the coordinate change by propagation is not considered. Also in this case the coordinates (x_o, y_o) of the original wavefront and the coordinates (x_p, y_p) of the propagated wavefront are in first order not equal because $\beta_{xx} \neq 1$ and $\beta_{yy} \neq 1$.

The logical flow of the transformations is illustrated in Figure 38 in Appendix C. Again, values of the local aberrations before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) are provided in Table 12 (see Appendix C).

Zernike coefficients					
		Original wavefront	Propagated wavefront		
Radial order	Symbol (OSA standard)		Numerical Ray-Tracing	Analytical Wavefront-Tracing	
			ZEMAX®	Dai [44]	Our method
k		$value/\mu m$	$value/\mu m$	$value/\mu m$	$value/\mu m$
0	c_0^0	-104.73	-53.8326	-3.35952	-53.8326
1	c_1^{-1}	-4.9774	-0.595659	10.947	-0.595597
	c_1^1	0	$-2.35*10^{-8}$	0	0
2	c_2^{-2}	0	0	0	0
	c_2^0	-60.791	-31.0906	-0.77533	-31.0906
	c_2^2	9.48371	2.41668	-10.2031	2.41668
3	c_3^{-3}	0.541095	0.0328263	-1.80039	0.0328297
	c_3^{-1}	-1.82051	-0.210901	4.23289	-0.210908
	c_3^1	0	0	0	0
	c_3^3	0	$-3.53*10^{-8}$	0	0
4	c_4^{-4}	0	$-4.70*10^{-8}$	0	0
	c_4^{-2}	0	$1.76*10^{-8}$	0	0
	c_4^0	-0.25745	-0.00801529	0.943405	-0.00801618
	c_4^2	0.175173	0.00367726	-0.794462	0.003678
	c_4^4	-0.0561936	-0.000561498	0.318015	-0.000561742
5	c_5^{-5}	-0.00501814	$-4.44*10^{-6}$	0.042954	$-4.81*10^{-6}$
	c_5^{-3}	0.0152086	0.00004036	-0.109211	0.000041581
	c_5^{-1}	-0.0330566	-0.000178401	0.202975	-0.000180914
	c_5^1	0	$-1.18*10^{-8}$	0	0
	c_5^3	0	$-1.18*10^{-8}$	0	0
	c_5^5	0	$3.53*10^{-8}$	0	0
6	c_6^{-6}	0	$2.35*10^{-8}$	0	0
	c_6^{-4}	0	0	0	0
	c_6^{-2}	0	$-1.76*10^{-8}$	0	0
	c_6^0	-0.00467708	$-1.28*10^{-6}$	0.033557188	$-1.57*10^{-6}$
	c_6^2	0.00439538	$-2.12*10^{-7}$	-0.0364403	$1.95*10^{-8}$
	c_6^4	-0.00191776	$4.47*10^{-7}$ 0	0.0179451	$3.70*10^{-7}$
	c_6^6	0.000655743	$-1.70*10^{-7}$	-0.00696252	$-1.6*10^{-7}$

Table 7: Zernike coefficients of the original and propagated wavefront in example B1: Propagated wavefront. Left column: values based on the ray-tracing package (ZEMAX®). Middle column: values based on the method derived by Dai et al [36,44]. Right column: values based on our analytical method. Also this complex example shows an obvious consistency between the results derived by the optical design package ZEMAX® and our analytical method. In contrast, the results derived by the analytical method of Dai et al [44] differ significantly.

6. Derivation of the Reflection Equations

6.1. Mathematical Approach in the 2D Case

6.1.1. Coordinates in the 2D case

For giving insight into the method with smallest possible effort, we first treat in detail a fictitious two-dimensional problem in which the third space dimension does not exist. Later we will transfer the corresponding approach to the three-dimensional case, i.e. the case of interest, but now we will for an instant 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 reflective 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, shall still be called ‘surface’). All rays and normal vectors then lie in that plane, too. We summarize this situation in 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 x-direction, but this is by no means necessary since it is inherent to the mathematics of the two-component system that any ray deflection in a direction other that in the given plane cannot occur.

The two-dimensional version of the rotation matrix takes the form

$$\mathbf{R}(\varepsilon)=\begin{pmatrix}\cos\varepsilon & -\sin\varepsilon\\ \sin\varepsilon & \cos\varepsilon\end{pmatrix}. \qquad (186)$$

6.1.2. 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

$$\mathbf{w}_{\mathrm{In}}(y)=\begin{pmatrix}y\\ w_{\mathrm{In}}(y)\end{pmatrix} \qquad (187)$$

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

$$w_{\mathrm{In}}(y)=\sum_{k=0}^{\infty}\frac{a_{\mathrm{In},k}}{k!}y^k \qquad (188)$$

Equivalently, we represent the reflected wavefront and the reflective surface in their preferred frames by the vectors

$$\mathbf{w'}_{\text{Out}}(y') = \begin{pmatrix} y' \\ w'_{\text{Out}}(y') \end{pmatrix}, \qquad \overline{\mathbf{w}}_{\text{S}}(\bar{y}) = \begin{pmatrix} \bar{y} \\ \overline{w}_{\text{S}}(\bar{y}) \end{pmatrix} \tag{189}$$

where

$$w'_{\text{Out}}(y') = \sum_{k=0}^{\infty} \frac{a'_{\text{Out},k}}{k!} y'^k, \qquad \overline{w}_{\text{S}}(\bar{y}) = \sum_{k=0}^{\infty} \frac{\bar{a}_{\text{S},k}}{k!} \bar{y}^k, \tag{190}$$

As in Eq. (4), again the normalization factor $k!$ is chosen such that the coefficients $a_{\text{In},k}$ are given by the derivatives of the wavefront at $y = 0$,

$$a_{\text{In},k} = \left. \frac{\partial^k}{\partial y^k} w_{\text{In}}(y) \right|_{y=0} = w_{\text{In}}^{(k)}(0) \tag{191}$$

In the 2D case the vector $\mathbf{e}_k$ in Eq. (26) reduces to a scalar $E_k = n w_{\text{In}}^{(k)} = n a_{\text{In},k}$, e.g. for second and third-order aberrations, we have $E_2 = n w_{\text{In}}^{(2)} = n a_2$, $E_3 = n w_{\text{In}}^{(3)} = n a_3$, etc.. A similar reasoning applies for the vectors $\mathbf{e'}_k$, $\bar{\mathbf{e}}_k$ and yields the local aberrations E'_k, $\overline{E}_k$, connected to the coefficients $a'_{\text{Out},k}$, $\bar{a}_{\text{S},k}$ by multiplication with the refractive index $-n$ for the reflected wavefront and with the factor $-2n$ for the reflective surface, respectively.

Each surface has zero slope at its coordinate origin because by construction the z axis points along the normal of its corresponding surface. Additionally, 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. $a_{\text{In},k} = 0$, $a'_{\text{Out},k} = 0$, $\bar{a}_{\text{S},k} = 0$ for $k < 2$.

The normal vectors and their derivatives are described as in chapter 3 and obey the same relations as. (36)-(38). Since the normal vector of the original wavefront and the normal vector of the propagated wavefront are equal, the normal vector will be labeled generally with $\mathbf{n}_w$.

In application on the functions of interest, $\mathbf{n}_w(y) = \mathbf{n}(w_{\text{o}}^{(1)}(y))$, this means that $\mathbf{n}_w(0) = (0,1)^T$. Further, the first derivatives are given by

$$\left. \frac{\partial}{\partial y} \mathbf{n}_w(y) \right|_{y=0} \equiv \mathbf{n}_{\text{w}}^{(1)}(0) = \mathbf{n}^{(1)}(0) w_{\text{o}}^{(2)}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix} w_{\text{o}}^{(2)}(0) \tag{192}$$

and similarly for the higher derivatives.

6.1.3. Ansatz for Determining the Reflection 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. (187)-(191)) are determined for all orders $2 \le k \le k_0$ for the order k_0 of interest, and to assign values to its corresponding local aberrations.

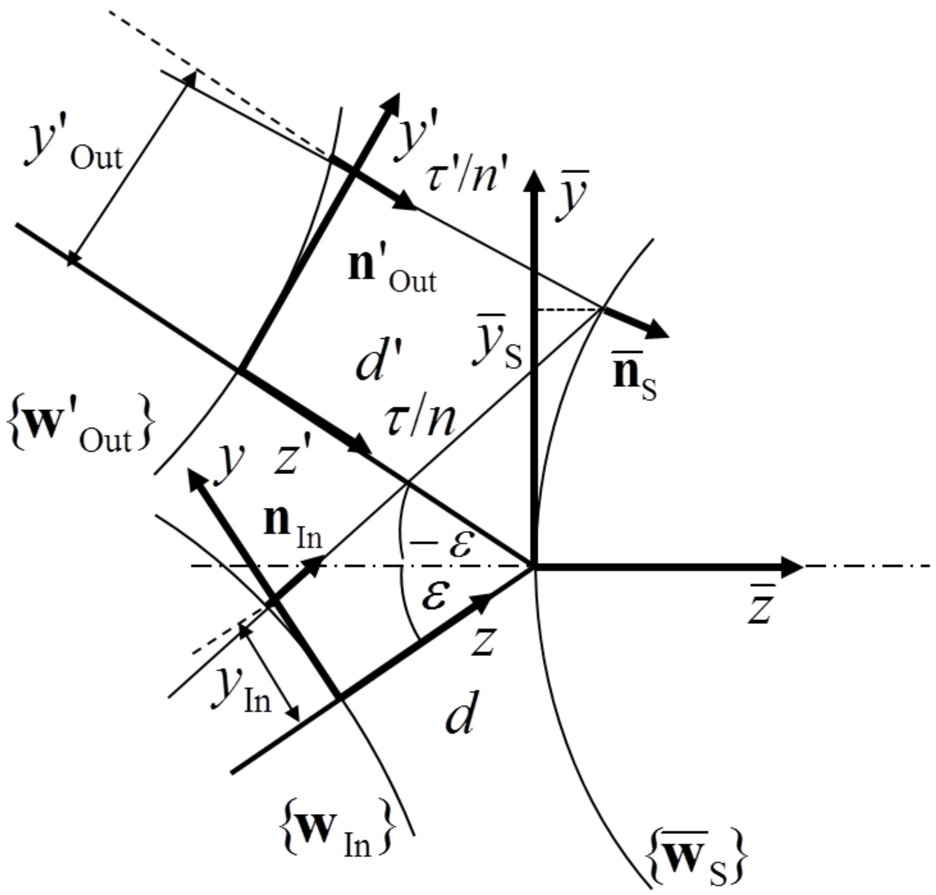

Figure 27: Local coordinates systems of the reflective surface, of the incoming wavefront and of the reflected wavefront. The true situation is that the origins of all coordinate systems coincide. Shown is the fictitious situation of separated origins by *d* and *d’* for a better understanding of nomenclature. The surface normal vectors along the neighboring ray are also drawn, referred to as $\bar{\mathbf{n}}_{\text{In}}$, $\bar{\mathbf{n}}_{\text{S}}$, $\bar{\mathbf{n}}_{\text{Out}}$ in the common global system $(\bar{x}, \bar{y}, \bar{z})$. 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.

Our starting point is the following situation. While the chief ray and the coordinate systems are fixed, a neighboring ray scans the incoming wavefront $\{\mathbf{w}_{\text{In}}\}$ and hits it at an intercept $y_{\text{In}} \neq 0$, then hits the reflective surface $\{\bar{\mathbf{w}}_{\text{S}}\}$, and finally propagates to the reflected wavefront $\{\mathbf{w}'_{\text{Out}}\}$, where the brackets

$\{.\}$ shall denote the entity of vectors described by Eq. (187), (see Figure 27). Except for the limiting case $y_{\text{In}} \to 0$, the three points in space, $\mathbf{w}_{\text{In}}, \mathbf{w}'_{\text{Out}}, \overline{\mathbf{w}}_{\text{S}}$, do in general not coincide. As shown in Figure 27, and consistently with our notation, we denote as y_{In} the projection of the neighboring ray's intersection with $\{\mathbf{w}_{\text{In}}\}$ onto the y axis. Analogously, the projection of the intersection with $\{\mathbf{w}'_{\text{Out}}\}$ onto the y' axis is denoted as y'_{Out}, and the projection of the intersection with $\{\overline{\mathbf{w}}_{\text{S}}\}$ onto the $\overline{y}$ axis is called $\overline{y}_{\text{S}}$.

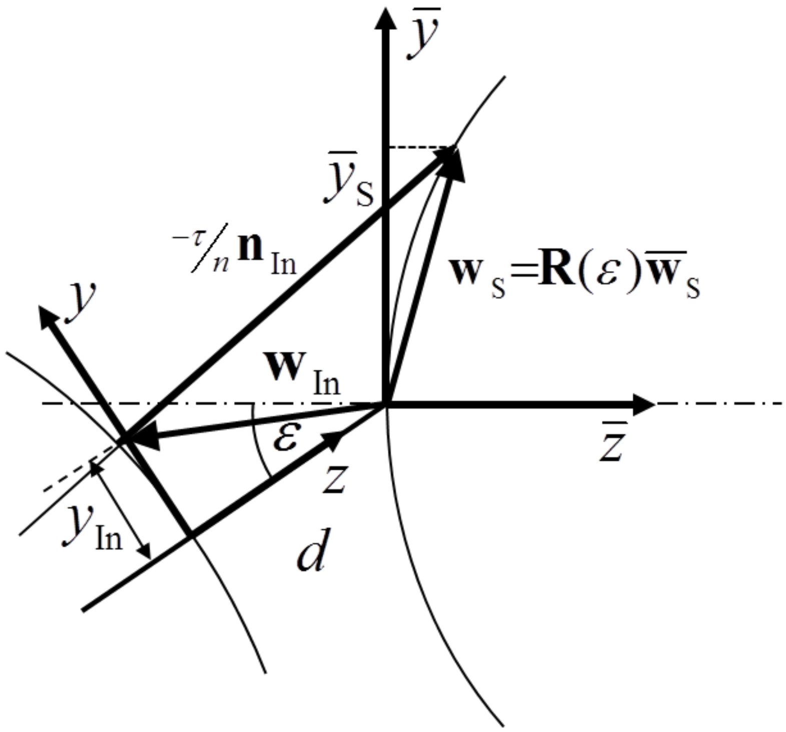

Figure 28: Shown is the fictitious situation of separated origins for a better understanding of the nomenclature. The vector $\mathbf{w}_{\text{In}} = \mathbf{w}_{\text{In}}(y_{\text{In}})$ (see Eq. (187)) points to the neighboring ray's intersection point with the incoming wavefront, and the wavefront's OPD referred to the reflective surface along the ray is denoted by τ, correspondingly the vector from the wavefront to the surface is $-\tau/n\,\mathbf{n}_{\text{In}}$. Hence, the vector to the point on the surface itself, $\mathbf{w}_{\text{S}}$, must be equal to the vector sum $\mathbf{w}_{\text{S}} = \mathbf{w}_{\text{In}} - \tau/n\,\mathbf{n}_{\text{In}}$. Transforming $\mathbf{w}_{\text{S}}$ to its preferred frame by $\mathbf{w}_{\text{S}} = \mathbf{R}(\varepsilon)\overline{\mathbf{w}}_{\text{S}}$ (see Eq. (1)) yields the first one of the fundamental equations in Eq. (193).

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 reflection, and that the reflected wavefront is evaluated at a distance $d' > 0$ after the reflection, 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 Figure 27, Figure 28 and Figure 29. The true situation is $d = d' = 0$, which is relevant throughout the thesis.

While in Figure 27 all quantities are drawn in their preferred frames, Figure 28 shows the quantities concerning the incoming wavefront and the reflective surface in the common frame (y, z). The vector $\mathbf{w}_{\mathrm{In}} = \mathbf{w}_{\mathrm{In}}(y_{\mathrm{In}})$ (see Eq. (187)) points to the neighboring ray's intersection point with the incoming wavefront, and the wavefront's OPD referred to the reflective surface along the ray is denoted by τ, whereas the absolute value τ is determined by the optical path distance between the neighboring ray's intersection point with the incoming wavefront and the reflective surface and the sign of τ is determined by the relative position of the these intersection points. If the intersection point of the ray with the wavefront is before the intersection point of the ray with the reflective surface the OPD will be negative $(\tau < 0)$, and if the ray first intersects the reflective surface the OPD will be positive $(\tau > 0)$. Therefore the vector from the wavefront to the surface is $-\tau/n\mathbf{n}_{\mathrm{In}}$, determined by the product of the OPD and the normal unit vector of the incoming wavefront. 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 $\mathbf{w}_{\mathrm{S}} = \mathbf{R}(\varepsilon)\overline{\mathbf{w}}_{\mathrm{S}}$ (see Eq. (1)) yields the first one of the fundamental equations in Eq. (193).

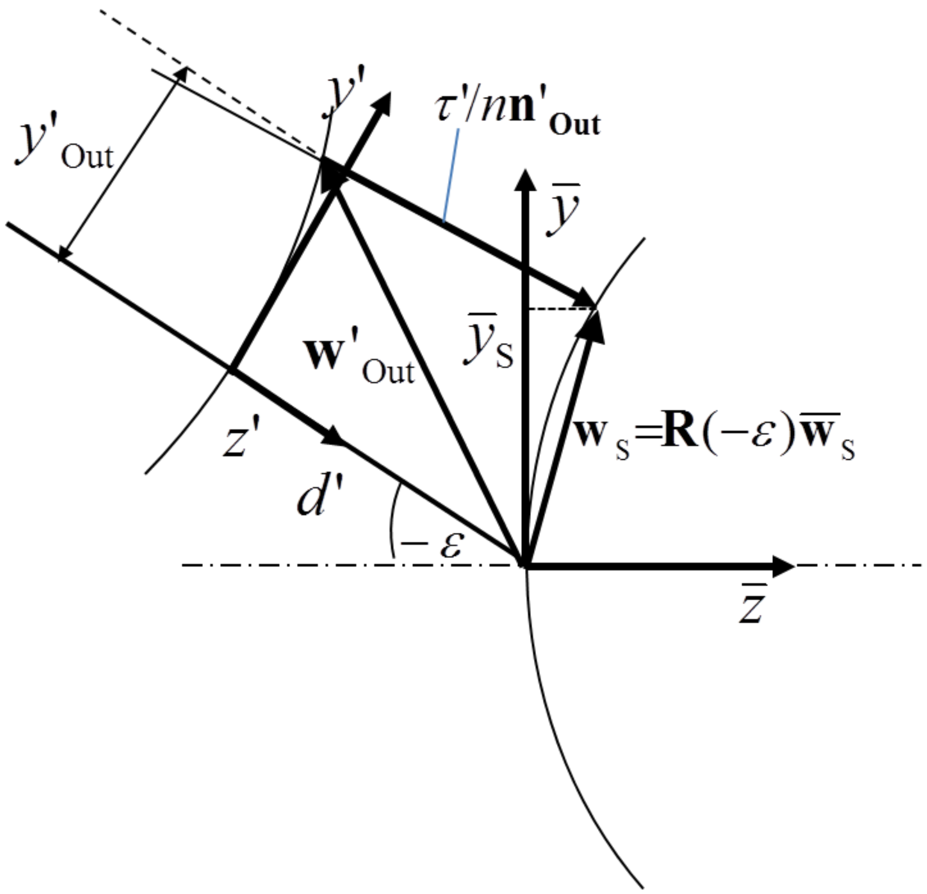

Figure 29: Shown is the fictitious situation of separated origins for a better understanding of the nomenclature. The vector $\mathbf{w}'_{\mathrm{Out}} = \mathbf{w}'_{\mathrm{Out}}(y'_{\mathrm{Out}})$ (see Eq. (189)) points to the neighboring ray's intersection point with the reflected wavefront, and the wavefront's OPD referred to the reflective surface along the ray is denoted by τ', correspondingly the vector from the wavefront to the surface is $-\tau'/n'\mathbf{n}'_{\mathrm{Out}} = \tau'/n\mathbf{n}'_{\mathrm{Out}}$. Hence, the vector to the point on the surface itself, $\mathbf{w}'_{\mathrm{S}}$, must be equal to the vector sum $\mathbf{w}'_{\mathrm{S}} = \mathbf{w}'_{\mathrm{Out}} + \tau'/n\,\mathbf{n}'_{\mathrm{Out}}$. Transforming $\mathbf{w}'_{\mathrm{S}}$ to its preferred frame by $\mathbf{w}_{\mathrm{S}} = \mathbf{R}(-\varepsilon)\overline{\mathbf{w}}_{\mathrm{S}}$ (see Eq. (1)) yields the second one of the fundamental equations in Eq. (193).

Analogously we have $\mathbf{w}'_{\mathrm{Out}} - \tau'/n'\,\mathbf{n}'_{\mathrm{Out}} = \mathbf{w}'_{\mathrm{S}}$ for the reflected wavefront in the frame (y', z'), yielding the second equation in Eq. (193) (see Figure 29). The sum of the OPD from the ray's intersection point with the incoming wavefront to the reflective surface $(-\tau)$ and the OPD from the reflective surface to the ray's intersection point with the outgoing wavefront (τ') has to be constant, and in the true situation with $d = d' = 0$ yields $-\tau + \tau' = 0$. Therefore the condition for the reflected wavefront to be the surface of constant OPD is that $\tau = \tau'$ for all neighboring rays. Inserting this condition and replacing n' by $-n$, we establish as starting point of our computations the fundamental equations

$$\begin{aligned} \begin{pmatrix} y_{\mathrm{In}} \\ w_{\mathrm{In}}(y_{\mathrm{In}}) \end{pmatrix} - \frac{\tau}{n}\mathbf{n}_{\mathrm{In}} &= \mathbf{R}(\varepsilon)\begin{pmatrix} \bar{y}_{\mathrm{S}} \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix} \\ \begin{pmatrix} y'_{\mathrm{Out}} \\ w'_{\mathrm{Out}}(y'_{\mathrm{Out}}) \end{pmatrix} + \frac{\tau}{n}\mathbf{n}'_{\mathrm{Out}} &= \mathbf{R}(-\varepsilon)\begin{pmatrix} \bar{y}_{\mathrm{S}} \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix} \end{aligned} \tag{193}$$

From Eq. (193), 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 reflective surface $\bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}})$ as the unknown function. Although only the surface is of interest, in Eq. (193) additionally the four quantities τ, y_{In}, y'_{Out}, $\bar{y}_{\mathrm{S}}$ are also unknown. However, they are not independent from each other: if any one of them is given, the other three ones can no longer be chosen independently. We use $\bar{y}_{\mathrm{S}}$ as independent variable and to consider the three other unknowns τ, y_{In}, y'_{Out} as functions of it.

We arrive at the conclusion that Eq. (193) 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 only interested in a solution 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

$$\mathbf{p}(\bar{y}_{\mathrm{S}}) = \begin{pmatrix} y_{\mathrm{In}}(\bar{y}_{\mathrm{S}}) \\ y'_{\mathrm{Out}}(\bar{y}_{\mathrm{S}}) \\ \tau(\bar{y}_{\mathrm{S}}) \\ \bar{w}_{\mathrm{S}}(\bar{y}_{\mathrm{S}}) \end{pmatrix} \tag{194}$$

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 these Eq. (193) up to some order, which yields relations between the curvatures, third derivatives etc. of the wavefronts and the reflective 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.

Rewriting Eq. (193) leads to

$$\begin{pmatrix}0\\0\\0\\0\end{pmatrix}=\begin{pmatrix} y_{\text{In}}-\frac{\tau}{n}n_y \quad -\left(\bar{y}_{\text{S}}\cos\varepsilon-\bar{w}_{\text{S}}\sin\varepsilon\right)\\ w_{\text{In}}(y_{\text{In}})-\frac{\tau}{n}n_z \quad -\left(\bar{y}_{\text{S}}\sin\varepsilon+\bar{w}_{\text{S}}\cos\varepsilon\right)\\ y'_{\text{Out}}+\frac{\tau}{n}n_y-\left(\bar{y}_{\text{S}}\cos\varepsilon+\bar{w}_{\text{S}}\sin\varepsilon\right)\\ w'_{\text{Out}}(y'_{\text{Out}})+\frac{\tau}{n}n_z-\left(-\bar{y}_{\text{S}}\sin\varepsilon+\bar{w}_{\text{S}}\cos\varepsilon\right)\end{pmatrix} \tag{195}$$

Before solving Eq. (193), we distinguish if the independent variable $\bar{y}_{\text{S}}$ enters into Eq. (193) explicitly like in the first component of the vector $(\bar{y}_{\text{S}},\bar{w}_{\text{S}}(\bar{y}_{\text{S}}))^T$, or implicitly via one of the components of Eq. (194). To this end, we follow the concept of chapter 3 and define the function $\left(\mathrm{IR}^4\times\mathrm{IR}\right)\mapsto\mathrm{IR}^4:(\mathbf{p},\bar{y}_{\text{S}})\mapsto\mathbf{f}$ by

$$\mathbf{f}(\mathbf{p},\bar{y}_{\text{S}})=\begin{pmatrix} y_{\text{In}}-\frac{\tau}{n}n_y\left(w_{\text{In}}^{(1)}(y_{\text{In}})\right) \quad -\left(\bar{y}_{\text{S}}\cos\varepsilon-\bar{w}_{\text{S}}\sin\varepsilon\right)\\ w_{\text{In}}(y_{\text{In}})-\frac{\tau}{n}n_z\left(w_{\text{In}}^{(1)}(y_{\text{In}})\right) \quad -\left(\bar{y}_{\text{S}}\sin\varepsilon+\bar{w}_{\text{S}}\cos\varepsilon\right)\\ y'_{\text{Out}}+\frac{\tau}{n}n_y\left(w'^{(1)}_{\text{Out}}(y'_{\text{Out}})\right)-\left(\bar{y}_{\text{S}}\cos\varepsilon+\bar{w}_{\text{S}}\sin\varepsilon\right)\\ w'_{\text{Out}}(y'_{\text{Out}})+\frac{\tau}{n}n_z\left(w'^{(1)}_{\text{Out}}(y'_{\text{Out}})\right)-\left(-\bar{y}_{\text{S}}\sin\varepsilon+\bar{w}_{\text{S}}\cos\varepsilon\right)\end{pmatrix}, \tag{196}$$

where $(p_1,p_2,p_3,p_4)=(y_{\text{In}},y'_{\text{Out}},\tau,\bar{w}_{\text{S}})$ are the components of $\mathbf{p}$. Setting now $\mathbf{p}=\mathbf{p}(\bar{y}_{\text{S}})$, Eq. (196) allows rewriting the fundamental system of Eq. (104) in a more compact way as

$$\mathbf{f}\left(\mathbf{p}(\bar{y}_{\text{S}}),\bar{y}_{\text{S}}\right)=\mathbf{0} \tag{197}$$

as can be verified explicitly by component wise comparison with Eq. (193).

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. (197) with respect to $\bar{y}_{\text{S}}$, evaluated in the origin. The advantage of the form of Eq. (197) using Eq. (196) is that the various terms can be tracked in a fairly compact manner.

The total derivative of $\mathbf{f}\left(\mathbf{p}(\bar{y}_{\text{S}}),\bar{y}_{\text{S}}\right)$ in Eq. (197) 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 $p_i(\bar{y}_{\text{S}})$, plus the partial derivative of $\mathbf{f}$ with respect to the explicit dependence on $\bar{y}_{\text{S}}$. This transforms the system of algebraic equations in Eq. (193) to the system of differential equations

$$\sum_{j=1}^{4} \frac{\partial f_i}{\partial p_j} p_j^{(1)}(\bar{y}_S) + \frac{\partial f_i}{\partial \bar{y}_S} = 0, \quad i = 1,...,4, \tag{198}$$

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

$$\mathbf{A} := \begin{pmatrix} \frac{\partial f_1}{\partial y_{\text{In}}} & \frac{\partial f_1}{\partial y'_{\text{Out}}} & \frac{\partial f_1}{\partial \tau} & \frac{\partial f_1}{\partial \overline{w}_S} \\ \frac{\partial f_2}{\partial y_{\text{In}}} & \frac{\partial f_2}{\partial y'_{\text{Out}}} & \frac{\partial f_2}{\partial \tau} & \frac{\partial f_2}{\partial \overline{w}_S} \\ \frac{\partial f_3}{\partial y_{\text{In}}} & \frac{\partial f_3}{\partial y'_{\text{Out}}} & \frac{\partial f_3}{\partial \tau} & \frac{\partial f_3}{\partial \overline{w}_S} \\ \frac{\partial f_4}{\partial y_{\text{In}}} & \frac{\partial f_4}{\partial y'_{\text{Out}}} & \frac{\partial f_4}{\partial \tau} & \frac{\partial f_4}{\partial \overline{w}_S} \end{pmatrix} = \begin{pmatrix} 1 - \frac{\tau}{n} n_{\text{In},y}^{(1)} w_{\text{In}}^{(2)} & 0 & -\frac{1}{n} n_{\text{In},y} & \sigma \\ w_{\text{In}}^{(1)} - \frac{\tau}{n} n_{\text{In},z}^{(1)} w_{\text{In}}^{(2)} & 0 & -\frac{1}{n} n_{\text{In},z} & -\chi \\ 0 & 1 + \frac{\tau}{n} n'^{(1)}_{\text{Out},y} w'^{(2)}_{\text{Out}} & \frac{1}{n} n'_{\text{Out},y} & -\sigma \\ 0 & w'^{(1)}_{\text{Out}} + \frac{\tau}{n} n'^{(1)}_{\text{Out},z} w'^{(2)}_{\text{Out}} & \frac{1}{n} n'_{\text{Out},z} & -\chi \end{pmatrix} \tag{199}$$

where for convenience we have introduced $\sigma = \sin \varepsilon$, $\chi = \cos \varepsilon$. In Eq. (199), the occurring expressions are understood as $w_{\text{In}}^{(1)} \equiv w_{\text{In}}^{(1)}(y_{\text{In}})$, $w_{\text{In}}^{(2)} \equiv w_{\text{In}}^{(2)}(y_{\text{In}})$, $n_{\text{In},y} \equiv n_{\text{In},y}(w_{\text{In}}^{(1)}(y_{\text{In}}))$, $n_{\text{In},y}^{(1)} \equiv n_{\text{In},y}^{(1)}(w_{\text{In}}^{(1)}(y_{\text{In}}))$, etc, and analogously for the ‘Out’ quantities, and additionally $y_{\text{In}}, y'_{\text{Out}}, \tau, \overline{w}_S$ are themselves functions of $\bar{y}_S$.

The derivative vector $\partial f_i / \partial \bar{y}_S$ in Eq. (198) shall be summarized as

$$\mathbf{b} := -\frac{\partial \mathbf{f}}{\partial \bar{y}_S} = \begin{pmatrix} \chi \\ \sigma \\ \chi \\ -\sigma \end{pmatrix}. \tag{200}$$

Similarly as in chapter 3 we conclude that we can write $\mathbf{A}$ with argument $\mathbf{A}(\mathbf{p}(y_p))$ only and $\mathbf{b}$ without argument at all because $\mathbf{b}$ is constant.. Eq. (198) can be written in the form

$$\mathbf{A}(\mathbf{p}(\bar{y}_S))\mathbf{p}^{(1)}(\bar{y}_S) = \mathbf{b}. \tag{201}$$

6.1.4. Solving techniques for the fundamental equation

Eq. (201) is the derivative of the fundamental equation in Eq. (197), and therefore it is itself a fundamental equation. But additionally, it allows a stepwise solution for the derivatives $\mathbf{p}^{(k)}(\bar{y}_S = 0)$ for increasing order k. Formally, Eq. (201) can be solved for $\mathbf{p}^{(1)}(\bar{y}_S)$ by

$$\mathbf{p}^{(1)}(\bar{y}_\mathrm{S}) = \mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\mathbf{b}. \tag{202}$$

Eq. (202) holds as a function of $\bar{y}_\mathrm{S}$, but of course for arbitrary $\bar{y}_\mathrm{S}$ both sides of Eq. (202) are unknown. However, evaluating Eq. (202) for $\bar{y}_\mathrm{S} = 0$ exploits that then the right-hand side (rhs) is known because $\mathbf{p}(0) = \mathbf{0}$ is known! In the same manner, Eq. (202) serves as starting point for a recursion scheme by repeated total derivative and evaluation for $\bar{y}_\mathrm{S} = 0$. Remembering that $\mathbf{b}$ is constant, we obtain

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \\
\mathbf{p}^{(2)}(0) &= \left(\mathbf{A}^{-1}\right)^{(1)}\mathbf{b} \\
&\cdots \\
\mathbf{p}^{(k)}(0) &= \left(\mathbf{A}^{-1}\right)^{(k-1)}\mathbf{b},
\end{aligned} \tag{203}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1)} = \left.\frac{d}{d\bar{y}_\mathrm{S}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\right|_{\bar{y}_\mathrm{S}=0}$, …, $\left(\mathbf{A}^{-1}\right)^{(k-1)} = \left.\frac{d^{k-1}}{d\bar{y}_\mathrm{S}^{k-1}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\right|_{\bar{y}_\mathrm{S}=0}$ are total derivatives of the function $\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}$. The reason why Eq. (203) really does provide solutions for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$ is that in any row of Eq. (203) the entries on the rhs are all known assuming that the equations above are already solved. Although on the rhs there occur implicit derivatives $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, … as well, they are always of an order less than on the left-hand side (lhs). For example, the second row in Eq. (203) reads in explicit form $\mathbf{p}^{(2)}(0) = \sum_{i=1}^{4}\left(\frac{\partial}{\partial p_i}\mathbf{A}(\mathbf{p})^{-1}\right)p_i^{(1)}\Big|_{\bar{y}_\mathrm{S}=0}\cdot\mathbf{b}$ where $\bar{y}_\mathrm{S} = 0$ 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 due to the first row in Eq. (203). Generally, the highest derivative of $\mathbf{p}$ occurring in $\left.\left(\frac{d^{k-1}}{d\bar{y}_\mathrm{S}^{k-1}}\mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))^{-1}\right)\right|_{\bar{y}_\mathrm{S}=0}$ is $\mathbf{p}^{(k-1)}(0)$, which is already known at the stage when $\mathbf{p}^{(k)}(0)$ is to be computed by Eq. (203).

Although looking attractive and formally simple, applying Eq. (203) in practice requires still 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 $\partial^2/\partial p_i \partial p_j$. Both tasks are straightforward to be executed by a computer algebra package but nevertheless lengthy and not the best way how 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! To this purpose, we start the recursion scheme from Eq. (201) instead of Eq. (202). The first $(k-1)$ total derivatives of Eq. (201) are

$$\begin{aligned}
\mathbf{A}\mathbf{p}^{(1)}(0) &= \mathbf{b} && \text{(a)}\\
\mathbf{A}^{(1)}\mathbf{p}^{(1)}(0) + \mathbf{A}\mathbf{p}^{(2)}(0) &= \mathbf{0} && \text{(b)}\\
\mathbf{A}^{(2)}\mathbf{p}^{(1)}(0) + 2\mathbf{A}^{(1)}\mathbf{p}^{(2)}(0) + \mathbf{A}\mathbf{p}^{(3)}(0) &= \mathbf{0} && \text{(c)}\\
&\dots\\
\sum_{j=1}^{k}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0) &= \mathbf{0}, \quad k \ge 2 && \text{(d)}
\end{aligned} \tag{204}$$

where $\mathbf{A} = \mathbf{A}(\mathbf{p}(0)) = \mathbf{A}(\mathbf{0})$, and $\mathbf{A}^{(1)} = \left.\frac{d}{d\bar{y}_{\mathrm{S}}}\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))\right|_{\bar{y}_{\mathrm{S}}=0}$, …, $\mathbf{A}^{(k-j)} = \left.\frac{d^{k-j}}{d\bar{y}_{\mathrm{S}}^{k-j}}\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))\right|_{\bar{y}_{\mathrm{S}}=0}$ are total derivatives of the function $\mathbf{A}(\mathbf{p}(\bar{y}_{\mathrm{S}}))$. For the last line of Eq. (204) we have applied the formula for the p-th derivative of a product, $(fg)^{(p)} = \sum_{j=0}^{p}\binom{p}{j}f^{(p-j)}g^{(j)}$. Eq. (204) represents a recursion scheme where in each equation containing $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$, only $\mathbf{p}^{(k)}(0)$ (in the last term for $j = k$) is unknown provided that all previous equations for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k-1)}(0)$ are already solved. A formal solution for $\mathbf{p}^{(k)}(0)$, expressed in terms of its predecessors, is

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b}, && k = 1\\
\mathbf{p}^{(k)}(0) &= -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), && k \ge 2.
\end{aligned} \tag{205}$$

Although quite different in appearance at first glance, Eq. (205) yields exactly the same solutions as Eq. (203).

6.1.5. Solutions for the General Reflection Equations

In the result for $\mathbf{p}^{(1)}(0)$, the first rows of both Eqs. (203),(205) involve $\mathbf{A}(\mathbf{0})^{-1}$. For obtaining $\mathbf{A}(\mathbf{0})^{-1}$, we evaluate Eq. (199) for $\mathbf{p} = \mathbf{0}$ and apply Eqs. (192), yielding

$$\mathbf{A(0)} = \begin{pmatrix} 1 & 0 & 0 & \sigma \\ 0 & 0 & -1/n & -\chi \\ 0 & 1 & 0 & -\sigma \\ 0 & 0 & 1/n & -\chi \end{pmatrix} \Rightarrow \mathbf{A(0)}^{-1} = \begin{pmatrix} 1 & \sigma/(2\chi) & 0 & \sigma/(2\chi) \\ 0 & -\sigma/(2\chi) & 1 & -\sigma/(2\chi) \\ 0 & -n/2 & 0 & n/2 \\ 0 & -1/(2\chi) & 0 & -1/(2\chi) \end{pmatrix} \tag{206}$$

The final result for $\mathbf{p}^{(1)}(0)$ is

$$\mathbf{p}^{(1)}(0) = \begin{pmatrix} \chi \\ \chi \\ -n\sigma \\ 0 \end{pmatrix} \tag{207}$$

For the orders $k \geq 2$ we apply Eqs. (205). The derivatives $\mathbf{A}^{(1)} = \frac{d}{d\bar{y}_\mathrm{S}} \mathbf{A}(\mathbf{p}(\bar{y}_\mathrm{S}))\Big|_{\bar{y}_\mathrm{S}=0}$, etc. are directly obtained by total derivative of Eq. (199) with respect to $\bar{y}_\mathrm{S}$, evaluating for $\bar{y}_\mathrm{S} = 0$ and again applying Eqs. (192). For the orders $k \geq 2$ only the results $\overline{w}_\mathrm{S}^{(k)}(0)$ for the reflective surface are interesting, therefore we directly provide those result. The resulting second-order law is (omitting the argument ‘ (0) ’)

$$\overline{w}_\mathrm{S}^{(2)} = \tfrac{1}{2}\chi(w'^{(2)}_\mathrm{Out} + w^{(2)}_\mathrm{In}) \tag{208}$$

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

$$\begin{aligned} \overline{w}_\mathrm{S}^{(3)} &= \tfrac{1}{2}\chi^2(w'^{(3)}_\mathrm{Out} + w^{(3)}_\mathrm{In} + R_3) \\ \overline{w}_\mathrm{S}^{(4)} &= \tfrac{1}{2}\chi^3(w'^{(4)}_\mathrm{Out} + w^{(4)}_\mathrm{In} + R_4) \\ &\dots \\ \overline{w}_\mathrm{S}^{(k)} &= \tfrac{1}{2}\chi^{k-1}(w'^{(k)}_\mathrm{Out} + w^{(k)}_\mathrm{In} + R_k) \end{aligned} \tag{209}$$

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

$$R_3 = \frac{3\sigma}{2\chi}\left(w^{(2)\,2}_\mathrm{In} - w'^{(2)\,2}_\mathrm{Out}\right) \tag{210}$$

$$\begin{aligned} R_4 = {} & \left(\alpha\, w'^{(2)}_\mathrm{Out} + \beta w^{(2)}_\mathrm{In}\right) w'^{(3)}_\mathrm{Out} - \left(\alpha\, w^{(2)}_\mathrm{In} + `\beta w'^{(2)}_\mathrm{Out}\right) w^{(3)}_\mathrm{In} \\ & + \gamma\left(w^{(2)\,3}_\mathrm{In} + w'^{(2)\,3}_\mathrm{Out}\right) + \delta\, w^{(2)}_\mathrm{In}\, w'^{(2)}_\mathrm{Out}\left(w^{(2)}_\mathrm{In} + w'^{(2)}_\mathrm{Out}\right) \end{aligned} \tag{211}$$

with

$$\begin{aligned} \alpha &= -7\frac{\sigma}{\chi} \\ \beta &= \frac{\sigma}{\chi} \\ \gamma &= \frac{3}{4\chi^2}\left(5\sigma^2 - 4\chi^2\right) \\ \delta &= \frac{3}{4\chi^2}\left(4\chi^2 - \sigma^2\right) \end{aligned} \tag{212}$$

Eq. (209) holds likewise for the derivatives and for the coefficients $a_{\text{In},k}$, $a'_{\text{Out},k}$, $\bar{a}_{\text{S},k}$ due to Eqs. (187)-(191). In terms of local aberrations, Eq. (209) reads (after substituting χ by the cosin)

$$\bar{E}_k = \cos^{k-1}\varepsilon(E'_k - E_k - \tilde{R}_k)\,, \tag{213}$$

where in $\tilde{R}_k = nR_k$ all wavefront derivatives are expressed in terms of local aberrations.

6.1.6. Generalization of the Coddington Equation

Although application of Eq. (203) or Eq. (205) provides a solution for $w_{\text{S}}^{(k)}(0)$ 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. (210),(211), for R_3 (or R_4) will vanish if we set $w_{\text{In}}^{(j)} = 0$ and $w'^{(j)}_{\text{Out}} = 0$ 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 only aberrations for one single given order k are present while for all lower orders $j < k$ we have $w_{\text{In}}^{(j)} = 0$ and $w'^{(j)}_{\text{Out}} = 0$, then $R_k = 0$, which means for fixed order k that Eq. (209) will be valid for vanishing remainder term. This assumption can in fact be shown to hold generally.
To this purpose, we start from the recursion scheme in Eq. (205) and show that only the term containing $\mathbf{p}^{(1)}$ can contribute to the sum if all aberrations vanish for order less than k. For doing so, it is necessary to exploit two basic properties of the derivatives $\mathbf{A}^{(m)} = \left.\frac{d^m}{d\bar{y}_{\text{S}}^m}\mathbf{A}(\mathbf{p}(\bar{y}_{\text{S}}))\right|_{\bar{y}_{\text{S}}=0}$ of the matrix $\mathbf{A}$ for the orders $1 \le m \le k-1$. As can be shown by element wise differentiation of the matrix $\mathbf{A}$, the highest wavefront derivatives present in $\mathbf{A}^{(m)}(\mathbf{p}(\bar{y}_{\text{S}}))$ (see Eq. (199)) occur in the terms proportional to τ, and those are proportional to either $w_{\text{In}}^{(m+2)}$ or $w'^{(m+2)}_{\text{Out}}$. Evaluating $\mathbf{A}^{(m)}(\mathbf{p}(\bar{y}_{\text{S}}))$ at the position $\bar{y}_{\text{S}} = 0$

implies $\tau = 0$, such that $\mathbf{A}^{(m)}$ cannot contain any higher wavefront derivatives than $w_{\text{In}}^{(m+1)}$ or $w'^{(m+1)}_{\text{Out}}$. It follows that

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

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. (205), we notice that the occurring derivatives of the matrix $\mathbf{A}$ are $\mathbf{A}^{(k-1)}$, $\mathbf{A}^{(k-2)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ for $j = 1,2,...,(k-1)$, respectively. It follows from property i) that the highest occurring wavefront derivatives in these terms are $k,(k-1),...,3,2$, respectively. Now, if all wavefront derivatives up to order $(k-1)$ vanish, it will follow from property ii) that all the matrix derivatives $\mathbf{A}^{(k-2)}$, … , $\mathbf{A}^{(2)}$, $\mathbf{A}^{(1)}$ must vanish, leaving only $\mathbf{A}^{(k-1)}$. Therefore all terms in Eq. (205) vanish, excluding only the contribution for $j = 1$. We directly conclude that

$$\begin{aligned}\mathbf{p}^{(k)} &= -\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{p}^{(1)} \\ &= -\left(\mathbf{A}^{-1}\mathbf{A}^{(k-1)}\mathbf{A}^{-1}\right)\cdot \mathbf{b}\end{aligned}, \qquad k \geq 2 \tag{214}$$

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

$$\mathbf{A}^{(m)} = \begin{pmatrix} -m\chi^{m-1}\sigma w_{\text{In}}^{(m+1)} & 0 & \frac{\chi^m}{n} w_{\text{In}}^{(m+1)} & 0 \\ \chi^m w_{\text{In}}^{(m+1)} & 0 & 0 & 0 \\ 0 & m\chi^{m-1}\sigma w'^{(m+1)}_{\text{Out}} & \frac{-\chi^m}{n} w_{\text{In}}^{(m+1)} & 0 \\ 0 & \chi^m w_{\text{In}}^{(m+1)} & 0 & 0 \end{pmatrix}, \tag{215}$$

where $y_{\text{In}}^{(1)}$, $y'^{(1)}_{\text{Out}}$ and $\tau^{(1)}$ have been substituted by their solutions χ, χ and ns wherever they occur, respectively (see Eq. (207)). Inserting $\mathbf{A}^{(m)}(0)$ for $m = k-1$ and $\mathbf{A}(0)^{-1}$ from Eq. (206) into Eq. (214) yields directly that

$$\bar{s}^{(k)}(0) = \frac{\chi^{k-1}}{2}\left(w'^{(k)}_{\text{Out}}(0) + w_{\text{In}}^{(k)}(0)\right) \tag{216}$$

for all orders $k \geq 2$.

The novel resulting reflection equation in the situation of Eq. (216) in terms of local aberrations reads

$$\overline{E}_k = \cos^{k-1}\varepsilon\left(E'_k{}' - E_k\right), \tag{217}$$

which is indeed Eq. (213) for $\widetilde{R}_k = 0$.

6.2. Mathematical Approach in the 3D Case

6.2.1. 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 only report the most important differences. Analogously to Eq. (187), the incoming wavefront is now represented by the 3D vector

$$\mathbf{w}_{\mathrm{In}}(x,y) = \begin{pmatrix} x \\ y \\ w_{\mathrm{In}}(x,y) \end{pmatrix} \tag{218}$$

where $w_{\mathrm{In}}(x,y)$ is given by Eq. (8), 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. (27) for $\mathbf{e}_k$). The reflected wavefront and the reflective surface are treated similarly.

For treating the normal vectors, we introduce the analogous functions to Eq. (36) as

$$\mathbf{n}(u,v) := \frac{1}{\sqrt{1+u^2+v^2}} \begin{pmatrix} -u \\ -v \\ 1 \end{pmatrix}, \tag{219}$$

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

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

In the intersection point we have now $\mathbf{n}_{\mathrm{In}}(0,0) = (0,0,1)^T$, $\mathbf{n}'_{\mathrm{Out}}(0,0) = (0,0,1)^T$, $\overline{\mathbf{n}}_{\mathrm{S}}(0,0) = (0,0,1)^T$, and the derivatives corresponding to Eq. (192) can directly be obtained from Eq. (219).

6.2.2. Ansatz for Determining the Reflection Equations

The starting point for establishing the relations between the wavefronts and the reflective surface is now given by equations analogous to Eq. (193), 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

$$\mathbf{p}(\bar{x}_S, \bar{y}_S) = \begin{pmatrix} x_{In}(\bar{x}_S, \bar{y}_S) \\ y_{In}(\bar{x}_S, \bar{y}_S) \\ x'_{Out}(\bar{x}_S, \bar{y}_S) \\ y'_{Out}(\bar{x}_S, \bar{y}_S) \\ \tau(\bar{x}_S, \bar{y}_S) \\ \bar{s}(\bar{x}_S, \bar{y}_S) \end{pmatrix} \tag{220}$$

and the 3D analogue to Eq. (193) leads now to

$$\mathbf{f}\big(\mathbf{p}(\bar{x}_S, \bar{y}_S), \bar{x}_S, \bar{y}_S\big) = \mathbf{0} \tag{221}$$

where $\mathbf{f}$ is the 3D analogue to Eq. (196).

One important difference compared to 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

$$\begin{aligned} \mathbf{A}\big(\mathbf{p}(\bar{x}_S, \bar{y}_S)\big)\mathbf{p}^{(1,0)}(\bar{x}_S, \bar{y}_S) = \mathbf{b}_x \\ \mathbf{A}\big(\mathbf{p}(\bar{x}_S, \bar{y}_S)\big)\mathbf{p}^{(0,1)}(\bar{x}_S, \bar{y}_S) = \mathbf{b}_y \end{aligned} \tag{222}$$

where the different inhomogeneities are given as column vectors

$$\mathbf{b}_x = -\frac{\partial \mathbf{f}}{\partial \bar{x}_S} = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}^T, \quad \mathbf{b}_y = -\frac{\partial \mathbf{f}}{\partial \bar{y}_S} = \begin{pmatrix} 0 & \chi & -\sigma & 0 & \chi & \sigma \end{pmatrix}^T. \tag{223}$$

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

The Jacobian matrix $\mathbf{A}(\mathbf{p}(\bar{x}_S, \bar{y}_S))$ with elements $A_{ij} := \partial f_i / \partial p_j$ is the same for both equations and analogous to Eq. (199) but now of size 6×6. It is practical to provide it in block structure notation

$$\mathbf{A}(\mathbf{p}(\bar{x}_\mathrm{S},\bar{y}_\mathrm{S})) = \left(\begin{array}{cc|cc} \mathbf{A}_\mathrm{In} & \mathbf{0} & \mathbf{A}_\tau & \overline{\mathbf{A}}_\mathrm{S} \\ \mathbf{0} & \mathbf{A}'_\mathrm{Out} & & \end{array}\right) \tag{224}$$

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

$$\mathbf{A}_\mathrm{In} = \begin{pmatrix} 1+\frac{\tau}{n}\left(n_{\mathrm{In},x}^{(0,1)}w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},x}^{(1,0)}w_\mathrm{In}^{(2,0)}\right) & \frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)}w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},z}^{(1,0)}w_\mathrm{In}^{(1,1)}\right) \\ \frac{\tau}{n}\left(n_{\mathrm{In},y}^{(0,1)}w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},y}^{(1,0)}w_\mathrm{In}^{(2,0)}\right) & 1+\frac{\tau}{n}\left(n_{\mathrm{In},y}^{(0,1)}w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},y}^{(1,0)}w_\mathrm{In}^{(1,1)}\right) \\ w_\mathrm{In}^{(1,0)} + \frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)}w_\mathrm{In}^{(1,1)} + n_{\mathrm{In},z}^{(1,0)}w_\mathrm{In}^{(2,0)}\right) & w_\mathrm{In}^{(0,1)} + \frac{\tau}{n}\left(n_{\mathrm{In},z}^{(0,1)}w_\mathrm{In}^{(0,2)} + n_{\mathrm{In},z}^{(1,0)}w_\mathrm{In}^{(1,1)}\right) \end{pmatrix} \tag{225}$$

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

$$\mathbf{A}_\tau = \begin{pmatrix} n_{\mathrm{In},x}/n \\ n_{\mathrm{In},y}/n \\ n_{\mathrm{In},z}/n \\ -n'_{\mathrm{Out},x}/n \\ -n'_{\mathrm{Out},y}/n \\ -n'_{\mathrm{Out},z}/n \end{pmatrix}, \quad \overline{\mathbf{A}}_\mathrm{S} = \begin{pmatrix} 0 \\ -\sigma \\ -\chi \\ 0 \\ \sigma \\ -\chi \end{pmatrix} \tag{226}$$

6.2.3. Solutions for the General Reflection Equations

The direct solutions analogously to Eq. (203) are now given by

$$\begin{aligned} \mathbf{p}^{(1,0)}(0,0) &= \mathbf{A}^{-1}\mathbf{b}_x \\ \mathbf{p}^{(0,1)}(0,0) &= \mathbf{A}^{-1}\mathbf{b}_y \\ \mathbf{p}^{(2,0)}(0,0) &= \left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_x \\ \mathbf{p}^{(1,1)}(0,0) &= \left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_x = \left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_y \\ \mathbf{p}^{(0,2)}(0,0) &= \left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_y \\ &\dots \\ \mathbf{p}^{(k_x,k_y)}(0,0) &= \begin{cases} \left(\mathbf{A}^{-1}\right)^{(k_x-1,0)}\mathbf{b}_x & , \quad k_x \neq 0, k_y = 0 \\ \left(\mathbf{A}^{-1}\right)^{(k_x-1,k_y)}\mathbf{b}_x = \left(\mathbf{A}^{-1}\right)^{(k_x,k_y-1)}\mathbf{b}_y & , \quad k_x \neq 0, k_y \neq 0 \\ \left(\mathbf{A}^{-1}\right)^{(0,k_y-1)}\mathbf{b}_y & , \quad k_x = 0, k_y \neq 0 \end{cases} \end{aligned} \tag{227}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0,0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1,0)} = \frac{d}{d\bar{x}_\mathrm{S}} \mathbf{A}\left(\mathbf{p}(\bar{x}_\mathrm{S}, \bar{y}_\mathrm{S})\right)^{-1}\Big|_{\bar{x}_\mathrm{S}=0,\bar{y}_\mathrm{S}=0}$,

$\left(\mathbf{A}^{-1}\right)^{(k_x,k_y)} = \frac{d^{k_x}}{d\bar{x}_\mathrm{S}^{k_x}} \frac{d^{k_y}}{d\bar{x}_\mathrm{S}^{k_y}} \mathbf{A}\left(\mathbf{p}(\bar{x}_\mathrm{S}, \bar{y}_\mathrm{S})\right)^{-1}\Big|_{\bar{x}_\mathrm{S}=0,\bar{y}_\mathrm{S}=0}$, etc. The fact that there are two starting equations (222) 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. (221), for each $\mathbf{p}^{(k_x,k_y)}$ both 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. (206),(207) for the 2D case, we provide here the explicit results

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -\sigma \\ 0 & 0 & 0 & 0 & 1/n & -\chi \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \sigma \\ 0 & 0 & 0 & 0 & -1/n & -\chi \end{pmatrix} \Rightarrow \mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -\sigma/(2\chi) & 0 & 0 & -\sigma/(2\chi) \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sigma/(2\chi) & 0 & 1 & \sigma/(2\chi) \\ 0 & 0 & n/2 & 0 & 0 & -n/2 \\ 0 & 0 & -1/(2\chi) & 0 & 0 & -1/(2\chi) \end{pmatrix} \quad (228)$$

and, after application of Eqs. (223),(227) the solutions

$$\mathbf{p}^{(1,0)}(0,0) = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \mathbf{p}^{(0,1)}(0,0) = \begin{pmatrix} 0 \\ \chi \\ 0 \\ \chi \\ -n\sigma \\ 0 \end{pmatrix} \quad (229)$$

The general result for the reflection equation can be written in the way

$$\bar{w}_\mathrm{S}^{(k_x,k_y)} = \frac{\chi^{k_y-1}}{2}\left(w'^{(k_x,k_y)}_\mathrm{Out} + w_\mathrm{In}^{(k_x,k_y)} + R_{k_x,k_y}\right), \quad (230)$$

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 reflection takes place in the $y-z$ plane whereas in x the direction no tilting cosines occur at all. Summarizing all components of Eq. (230) for a fixed value of $k = k_x + k_y$ and applying Eqs. (5),(27),(29) yields <u>the novel reflection equation in terms of local aberrations</u>,

$$\bar{\mathbf{e}}_k = \mathbf{C}_k\left(\mathbf{e}'_k - \mathbf{e}_k - \mathbf{r}_k\right), \quad (231)$$

where $\mathbf{r}_k$ is a vector collecting the remainder terms $n R_{k_x,k_y}$ in Eq. (230) analogously to R_k in Eq. (213) . Eq. (231) is the general reflection equation for aberrations of any order in the 3D case.

6.2.4. Generalization of the Coddington Equation

Although Eq. (227) 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 $w_{\text{In}}^{(j_x,j_y)}$, $w'^{(j_x,j_y)}_{\text{Out}}$ for all lower orders, i.e. for $j_x + j_y < k_x + k_y$. This works analogously to the treatment of Eqs. (204)-(216), with the only difference that the notation requires more effort.

Analogously to Eq. (205) we obtain as a result that

$$\begin{aligned}
\mathbf{p}^{(k_x,0)}(0,0) &= -\mathbf{A}^{-1}\sum_{j_x=1}^{k_x-1}\binom{k_x-1}{j_x-1}\mathbf{A}^{(k_x-j_x,0)}\mathbf{p}^{(j_x,0)}, && k_x \ge 2, k_y = 0 \quad (a)\\
\mathbf{p}^{(k_x,k_y)}(0,0) &= -\mathbf{A}^{-1}\sum_{\substack{j_x\ge 1, j_y \ge 0\\ j_x+j_y<k_x+k_y}}\binom{k_x-1}{j_x-1}\binom{k_y}{j_y}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)} && (b)\\
&= -\mathbf{A}^{-1}\sum_{\substack{j_x\ge 0, j_y \ge 1\\ j_x+j_y<k_x+k_y}}\binom{k_x}{j_x}\binom{k_y-1}{j_y-1}\mathbf{A}^{(k_x-j_x,k_y-j_y)}\mathbf{p}^{(j_x,j_y)}, && k_x \ne 0, k_y \ne 0 \quad (c)\\
\mathbf{p}^{(0,k_y)}(0,0) &= -\mathbf{A}^{-1}\sum_{j_y=1}^{k_y-1}\binom{k_y-1}{j_y-1}\mathbf{A}^{(0,k_y-j_y)}\mathbf{p}^{(0,j_y)}, && k_x = 0, k_y \ge 2 \quad (d)
\end{aligned} \tag{232}$$

where again for $\mathbf{p}^{(k_x,k_y)}$ two formally different solutions occur which are essentially identical. We recognize that Eq. (232) (a) is a special case of Eq. (232) (b) for $k_y = 0$, $j_y = 0$, and similarly Eq. (232) (d) is a special case of Eq. (232) (c) for $k_x = 0$, $j_x = 0$. By means of a similar reasoning as 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. (232) will reduce to the lowest term, yielding

$$\begin{aligned}
\mathbf{p}^{(k_x,0)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,0)}\mathbf{p}^{(1,0)}, && k_x \ge 2, k_y = 0 \quad (a)\\
\mathbf{p}^{(k_x,k_y)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(k_x-1,k_y)}\mathbf{p}^{(1,0)} && (b)\\
&= -\mathbf{A}^{-1}\mathbf{A}^{(k_x,k_y-1)}\mathbf{p}^{(0,1)}, && k_x \ne 0, k_y \ne 0 \quad (c)\\
\mathbf{p}^{(0,k_y)}(0,0) &= -\mathbf{A}^{-1}\mathbf{A}^{(0,k_y-1)}\mathbf{p}^{(0,1)}, && k_x = 0, k_y \ge 2 \quad (d)
\end{aligned} \tag{233}$$

For finally evaluating Eqs. (232) 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 is given as

$$\mathbf{A}^{(m_x,m_y)} = \left(\begin{matrix} \mathbf{A}_{\text{In}}^{(m_x,m_y)} & \mathbf{0} \\ \mathbf{0} & \mathbf{A'}_{\text{Out}}^{(m_x,m_y)} \end{matrix} \right| \begin{matrix} \mathbf{A}_{\tau}^{(m_x,m_y)} & \overline{\mathbf{A}}_{\text{S}}^{(m_x,m_y)} \end{matrix} \Bigg) \tag{234}$$

with the block

$$\mathbf{A}_{\text{In}}^{(m_x,m_y)} = \begin{pmatrix} -m_y \chi^{m_y-1} \sigma w_{\text{In}}^{(m_x+2,m_y-1)} & -m_y \chi^{m_y-1} \sigma w_{\text{In}}^{(m_x+1,m_y)} \\ -m_y \chi^{m_y-1} \sigma w_{\text{In}}^{(m_x+1,m_y)} & -m_y \chi^{m_y-1} \sigma w_{\text{In}}^{(m_x,m_y+1)} \\ \chi^{m_y} w_{\text{In}}^{(m_x+1,m_y)} & \chi^{m_y} w_{\text{In}}^{(m_x,m_y+1)} \end{pmatrix} \tag{235}$$

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

$$\mathbf{A}_{\tau} = \begin{pmatrix} \chi^{m_y} w_{\text{In}}^{(m_x+1,m_y)} / n \\ \chi^{m_y} w_{\text{In}}^{(m_x,m_y+1)} / n \\ 0 \\ -\chi^{m_y} w'^{(m_x+1,m_y)}_{\text{Out}} / n \\ -\chi^{m_y} w'^{(m_x,m_y+1)}_{\text{Out}} / n \\ 0 \end{pmatrix}, \qquad \overline{\mathbf{A}}_{\text{S}} = \mathbf{0}, \tag{236}$$

where $x_{\text{In}}^{(1,0)}$, $x_{\text{In}}^{(0,1)}$, $y_{\text{In}}^{(1,0)}$, $y_{\text{In}}^{(0,1)}$, etc. have been substituted by their solutions according to Eq. (229). Inserting $\mathbf{A}^{(m_x,m_y)}$ from Eqs. (234)-(236) and $\mathbf{A}(\mathbf{0})^{-1}$ from Eq. (228) into Eqs. (233) yields one common relation for $\overline{w}_{\text{S}}^{(k_x,k_y)}$ for the various subcases in Eqs. (233) (omitting the argument ‘ $(0,0)$ ’):

$$\overline{w}_{\text{S}}^{(k_x,k_y)} = \frac{\chi^{k_y-1}}{2} \left(w'^{(k_x,k_y)}_{\text{Out}} + w_{\text{In}}^{(k_x,k_y)} \right) \tag{237}$$

for all orders $k \geq 2$.

Eq. (237) can be summarized in a similar fashion as Eq. (230) to a vector equation in the very appealing form

$$\bar{\mathbf{e}}_k = \mathbf{C}_k (\mathbf{e'}_k - \mathbf{e}_k) \tag{238}$$

which is Eq. (231) for $\mathbf{r}_k = \mathbf{0}$. Eq. (238), an interesting result of the present thesis, is the reflection equation for aberrations of fixed order $k \geq 2$ under the assumption that all aberrations with order lower than k vanish.

6.3. Results and Discussion

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

6.3.1. 2D Case

Eq. (217) describes the special case that for given order k the aberrations of the incoming and reflected 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 reflected wavefront, Eq. (217) can be transformed to

$$E'_k = E_k + \cos^{-(k-1)} \varepsilon \; \overline{E}_k \; . \tag{239}$$

<u>we could generally show this statement to hold for all orders $k \geq 2$ including as a special case for $k = 2$ the well-known Coddington and Vergence equation.</u> Therefore Eq. (239) represents an interesting result of the present thesis.

Also Eq. (213) for the general case can be transformed in such a way that E'_k of the reflected wavefront is the unknown quantity to be determined

$$E'_k = E_k + \cos^{-(k-1)} \varepsilon \, \overline{E}_k + \widetilde{R}_k \; . \tag{240}$$

_ In R_k only aberrations E_j, E'_j of order $j < k$ occur. These aberrations can be determined by successively solving of Eq. (240) for lower orders.

E.g., assume that the aberrations E'_k of the reflected wavefront up to order $k = 3$ ($E'_2 \equiv S', E'_3$) are the unknown quantities, and the aberrations E_k of the incoming wavefront and $\overline{E}_k$ of the reflective surface are given. In a first step the aberrations of order $k = 2$ are calculated using Eq. (240), which is in this case identical with the well-known Coddington equation

$$S' = S + \cos^{-1} \varepsilon \; \overline{S} \; . \tag{241}$$

In a second step the aberrations of order k = 3 are calculated using Eq. (240) and the results of Eq. (241)

$$E'_3 = E_3 + \cos^{-2} \varepsilon \; \overline{E}_3 + \widetilde{R}_3 \tag{242}$$

with $$\tilde{R}_3 = \frac{3\sin\varepsilon}{2n\cos\varepsilon}\left(S^2 - S'^2\right).$$

6.3.2. 3D Case

Equivalently to the 2D case transforming Eq. (238) leads to $\mathbf{e}'_k = \mathbf{e}_k + \mathbf{C}_k^{-1}\bar{\mathbf{e}}_k$ for the case that $\mathbf{e}_j = \mathbf{0}; \mathbf{e}'_j = \mathbf{0}$ for $j < k$, a statement which we could generally show to hold for all orders $k \geq 2$ including the special case of the Coddington equation.

In the general case Eq. (231) can as well be transformed in such a way that the unknown aberration vector $\mathbf{e}'_k$ of the reflected wavefront is determined by the incoming wavefront and the reflective surface.

$$\mathbf{e}'_k = \mathbf{e}_k + \mathbf{C}_k^{-1} \cdot \bar{\mathbf{e}}_k + \mathbf{r}_k, \qquad (243)$$

where in $\mathbf{r}_k$ only aberrations of order $j < k$ occur. Therefore, $\mathbf{r}_k$ can be determined by successively solving of Eq. (243) for lower orders. Eq. (243) is the general reflection equation for aberrations of any order in the 3D case.

6.4. Examples and Applications

6.4.1. Aspherical Surface Correction up to Sixth Order

One important application of the derived equations is that they allow determining a reflective surface, which not only has a defined Power $\bar{S}$, but also generates a reflected wavefront which 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, which images an axial object point with the distance s to the reflective surface to an axial image point with the distance s' to the reflective surface (Figure 30).

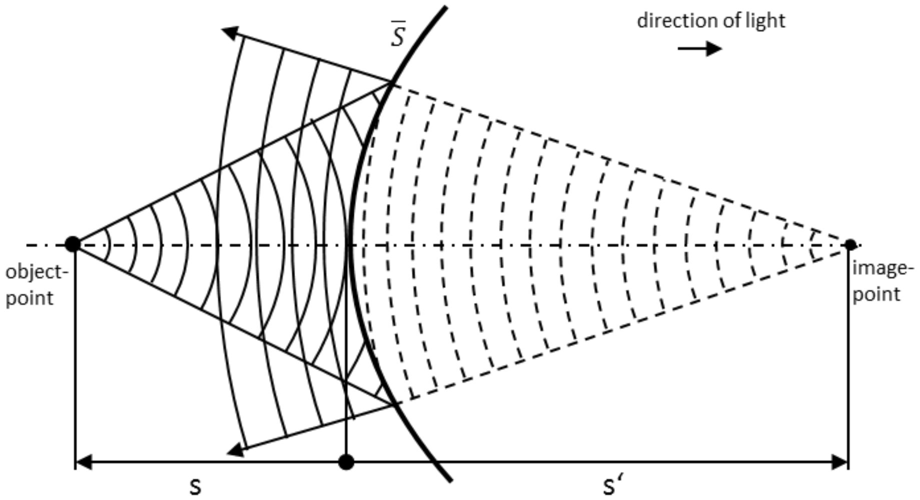

Figure 30: One important application of the derived equations is that they allow determining a reflective surface, which not only has a defined Power $\bar{S}$, but also generates a reflected wavefront which shows no deviation from an ideal sphere up to the order $k = 6$. The task is to determine a rotationally symmetric aspherical surface $\bar{S}$, which images an axial object point with the distance s to the reflective surface to an axial image point with the distance s' to the reflective surface.

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

$$f(y) = r\left(1 - \sqrt{1 - y^2/r^2}\right), \tag{244}$$

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

$$f(y) = \frac{1}{2r}y^2 + \frac{1}{8r^3}y^4 + \frac{1}{16r^5}y^6 + \ldots. \tag{245}$$

Applying Eq. (245) once on $f(y) = w_{\text{In}}(y)$, $r = s$ and secondly on $f(y') = w'_{\text{Out}}(y')$, $r = s'$ (including in both cases the sign of s or s') allows us to identify the wavefronts' coefficients in the sense of Eqs. (187)-(191):

$$\begin{aligned} a_{\text{In},2} &= \frac{1}{s} = \frac{S}{n}, \quad a_{\text{In},4} = 3\frac{1}{s^3} = 3\left(\frac{S}{n}\right)^3, \quad a_{\text{In},6} = 45\frac{1}{s^5} = 45\left(\frac{S}{n}\right)^5 \\ a'_{\text{Out},2} &= \frac{1}{s'} = -\frac{S'}{n}, \quad a'_{\text{Out},4} = 3\frac{1}{s'^3} = -3\left(\frac{S'}{n}\right)^3, \quad a'_{\text{Out},6} = 45\frac{1}{s'^5} = -45\left(\frac{S'}{n}\right)^5. \end{aligned} \tag{246}$$

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

$$\bar{s}(y) = \frac{\bar{a}_{S,2}}{2} y^2 + \frac{\bar{a}_{S,4}}{24} y^4 + \frac{\bar{a}_{S,6}}{720} y^6 + \ldots \tag{247}$$

as in Eq. (190), will be found up to the order $k = 6$ if we provide expression for the three coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$ (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 $\bar{a}_{S,2}$ can be directly determined by Eq. (208). In the present case of orthogonal incidence we exploit that $\sigma = 0, \chi = 1$, such that Eq. (208) reads as $\bar{a}_{S,2} = \frac{1}{2}(a'_{Out,2} + a_{In,2})$, yielding

$$\bar{a}_{S,2} = \frac{S - S'}{2n}. \tag{248}$$

For finding $\bar{a}_{S,4}$, we have to apply Eqs. (209)-(213). Due to the orthogonal incidence Eq. (212) simplifies to

$$\alpha = 0, \beta = 0, \gamma = -3, \delta = 3, \tag{249}$$

and consequently Eq. (211) simplifies to

$$R_4 = -3\left(w_{In}^{(2)} + w'^{(2)}_{Out}\right)\left(w_{In}^{(2)} - w'^{(2)}_{Out}\right)^2 \tag{250}$$

Inserting Eq. (250) into Eq. (209) and substituting $w_{In}^{(2)}$, $w'^{(2)}_{Out}$ by the coefficients in Eq. (246) yields

$$\begin{aligned} \bar{a}_{S,4} &= \bar{w}_S^{(4)} = \frac{1}{2}\left(w'^{(4)}_{Out} + w_{In}^{(4)} + R_4\right) \\ &= \frac{1}{2}\left(a'_{Out,4} + a_{In,4} - 3\left(a_{In,2} + a_{Out,2}\right)\left(a_{In,2} - a_{Out,2}\right)^2\right) \\ &= 3\frac{SS'}{2n^3}\left(S' - S\right) \end{aligned} \tag{251}$$

Similarly, we find that

$$\bar{a}_{S,6} = \bar{w}_S^{(6)} = 45\frac{S^2 S'^2}{2n^5}(S - S'). \tag{252}$$

Eqs. (251), (252) complete the demanded solution, i.e. the coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$ of the aspherical reflective 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 $k = 6$.

6.4.2. Special examples

The Eqs. (248). (251) and (252) are the solution for the coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$ of the aspherical reflective surface, 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 $k = 6$. Figure 31 shows the coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$, and $\bar{a}_{S,6}$ of the aspheric reflective surface as a function of the object vergence $S = n/s$. For simplicity the image vergence S' is chosen to be 1D. We will discuss three special examples in detail.

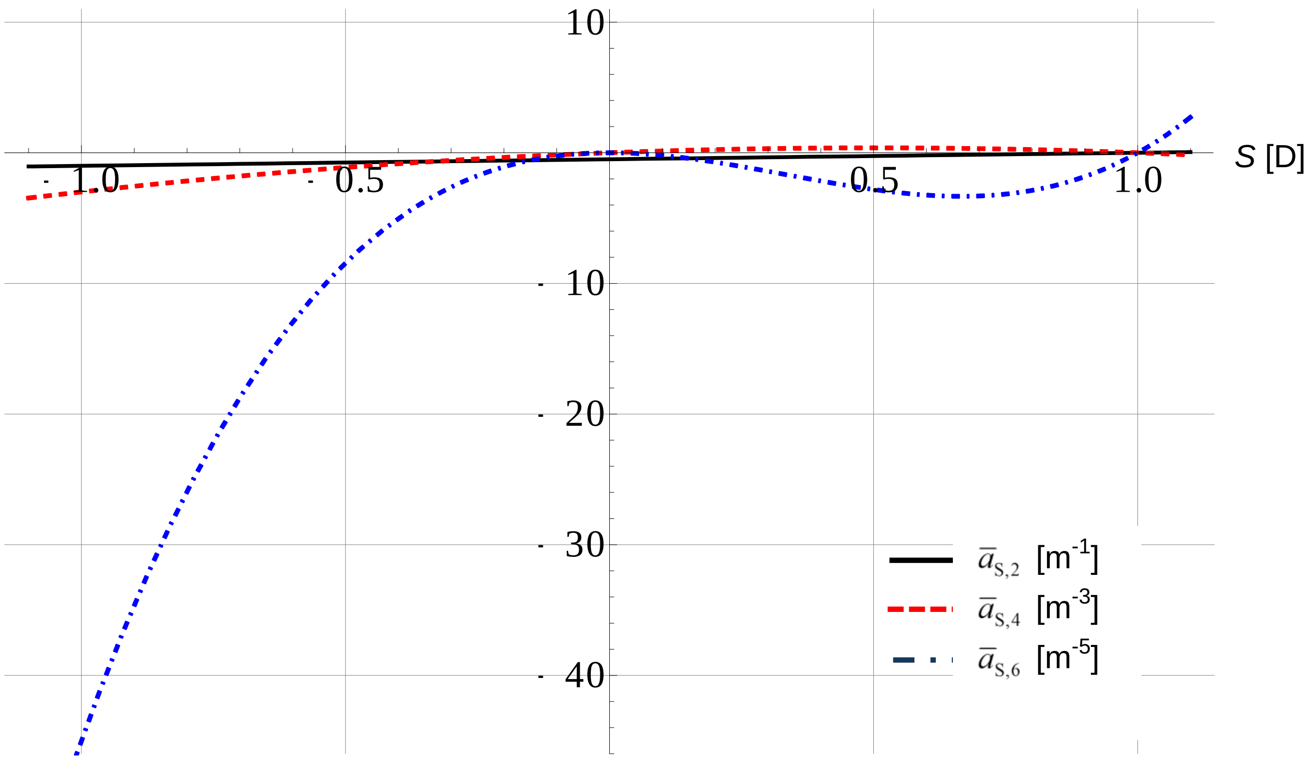

Figure 31: General overview: Solution for the coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$ of the aspherical reflective surface, such that an object point with the vergence S is imaged to a point with the vergence S' without aberrations with order less or equal to $k = 6$. For simplicity the image vergence S' is chosen by 1D. The solid black line shows the coefficient $\bar{a}_{S,2}$, the dashed red line the coefficient $\bar{a}_{S,4}$ and the dot-dashed blue line shows the coefficient $\bar{a}_{S,6}$.

A1. Spherical mirror

The spherical mirror has ideal imaging properties if the object is imaged exactly on itself ($s'=s \quad <=> \quad S'=-S$). In this case Eqs. (248), (251), (252) yield

$$\bar{a}_{S,2}=\frac{S-S'}{2n}=\frac{S}{n}=\frac{1}{s},$$

$$\bar{a}_{S,4}=3\frac{SS'}{2n^3}(S'-S)=3\frac{S^3}{n^3}=\frac{3}{s^3}$$

$$\bar{a}_{S,6}=45\frac{S^2S'^2}{2n^5}(S-S')=45\frac{S^5}{n^5}=\frac{45}{s^5}. \qquad (253)$$

From the graph in in Figure 31 and Figure 32 the coefficients of the reflective surface can be derived. If $S=-1\mathrm{D}$, which means $S=-S'$ because $S'=1\mathrm{D}$, then will be $\bar{a}_{S,2}=-1m^{-1}$, $\bar{a}_{S,4}=-3m^{-3}$ (Figure 32) and $\bar{a}_{S,6}=-45m^{-5}$ (Figure 31), which are the coefficients of a spherical surface, as shown in Eq. (246) ($\bar{a}_{S,2}=\frac{1}{s}$, $\bar{a}_{S,4}=\frac{3}{s^3}$ and $\bar{a}_{S,6}=\frac{45}{s^5}$).

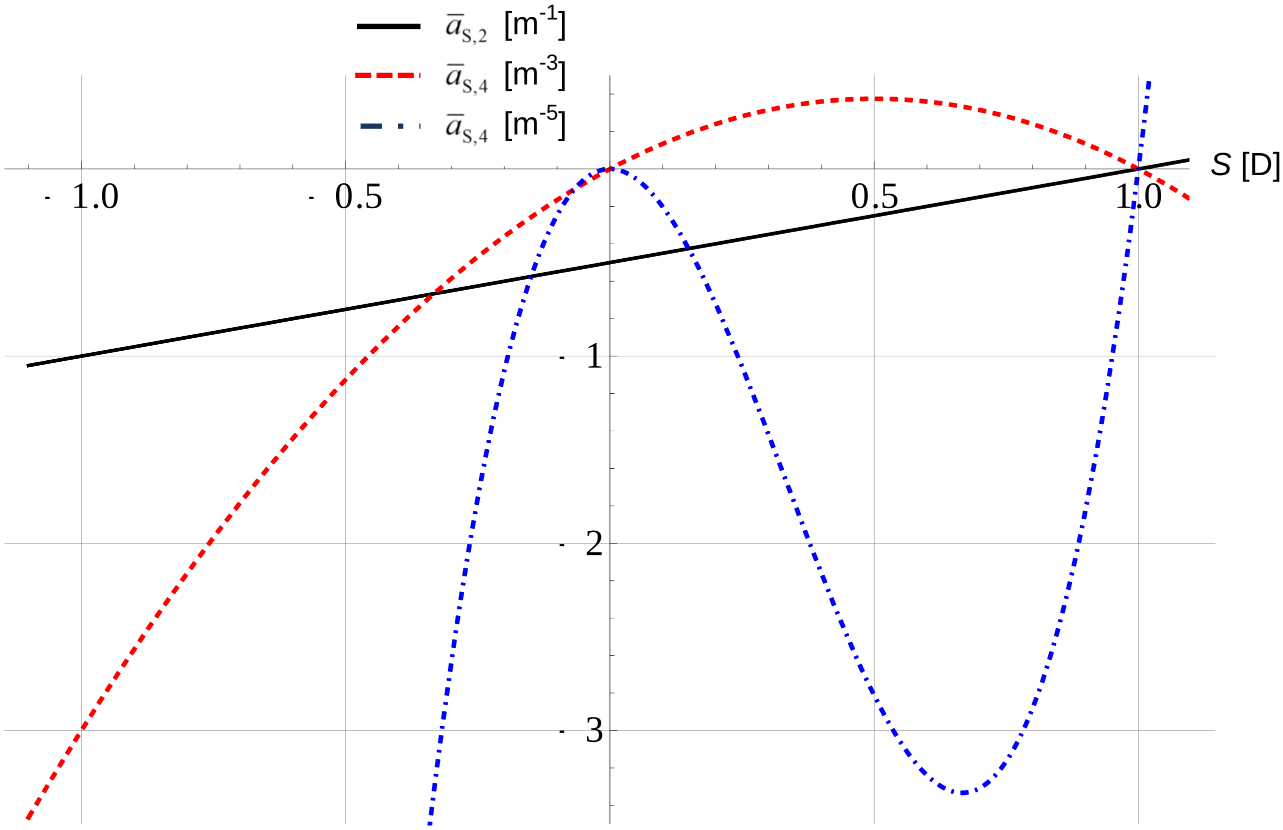

Figure 32: Detailed view: Solution for the coefficients $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$ of the aspherical reflective surface, such that an object point with the vergence S is imaged to a point with the vergence S' without aberrations with order less or equal to $k=6$.For simplicity the image vergence S' is chosen by 1D. The solid black line shows the coefficient $\bar{a}_{S,2}$, the dashed red line the coefficient $\bar{a}_{S,4}$ and the dot-dashed blue line shows the coefficient $\bar{a}_{S,6}$.

A2. Parabolic mirror

The parabolic mirror has ideal imaging properties if the object or equivalently the image is placed in infinity ($S=0$ or $S'=0$). In this case Eqs. (248), (251), (252) yield

$$\bar{a}_{\mathrm{S},2}=\frac{S-S'}{2n}=\frac{-S'}{2n}=\frac{1}{2s'}$$

$$\bar{a}_{\mathrm{S},4}=3\frac{SS'}{2n^3}\left(S'-S\right)=0$$

$$\bar{a}_{\mathrm{S},6}=45\frac{S^2S'^2}{2n^5}\left(S-S'\right)=0. \tag{254}$$

From the graph in Figure 31 and Figure 32 the coefficients of the reflective surface can be derived. If $S=0$, then will be $\bar{a}_{\mathrm{S},2}=-0.5m^{-1}$ and $\bar{a}_{\mathrm{S},4}=\bar{a}_{\mathrm{S},4}=0$. (Figure 32), which are the coefficients of a parabolic surface.

A3. Plane mirror

The plane mirror has ideal imaging properties if the object is imaged exactly behind the mirror with the same distance as the object is placed in front of the mirror ($s'=-s$ <=> $S'=S$). In this case Eqs. (248), (251), (252) yield

$$\bar{a}_{\mathrm{S},2}=\frac{S-S'}{2n}=0,$$

$$\bar{a}_{\mathrm{S},4}=3\frac{SS'}{2n^3}\left(S'-S\right)=0$$

$$\bar{a}_{\mathrm{S},6}=45\frac{S^2S'^2}{2n^5}\left(S-S'\right)=0. \tag{255}$$

From the graph in in Figure 31 and Figure 32 the coefficients of the reflective surface can be derived. If $S=1\mathrm{D}$, which means that $S=S'$ because $S'=1\mathrm{D}$, then all coefficients will be zero ($\bar{a}_{\mathrm{S},2}=\bar{a}_{\mathrm{S},4}=\bar{a}_{\mathrm{S},4}=0$,Figure 32), which are the coefficients of a plane surface.

6.4.3.Numerical example

The results of Eqs. (248), (251), (252) can be illustrated by a numerical example in which the refractive index of the first medium is $n=1$ and the object and image distance are given by $s=-30.0mm$ and $s'=-9.13043\,mm$, respectively. Eqs. (248), (251), (252) then yield $\bar{a}_{\mathrm{S},2}=-0.0714286\,mm^{-1}$, $\bar{a}_{\mathrm{S},4}=-0.000782314\,mm^{-3}$, $\bar{a}_{\mathrm{S},6}=-0.000042841\,mm^{-5}$. 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 $r=1/\bar{a}_{\mathrm{S},2}=-80.0mm$ and a stop with semi-diameter $r_{\mathrm{stop}}=16.0mm$ (see Figure 33).

Paraxial the imaging is perfect, but the peripheral rays introduce large errors. Next, we have considered a parabolic surface with the same paraxial curvature $\bar{a}_{S,2}$ (see Figure 34). Again, the peripheral rays introduce large errors.

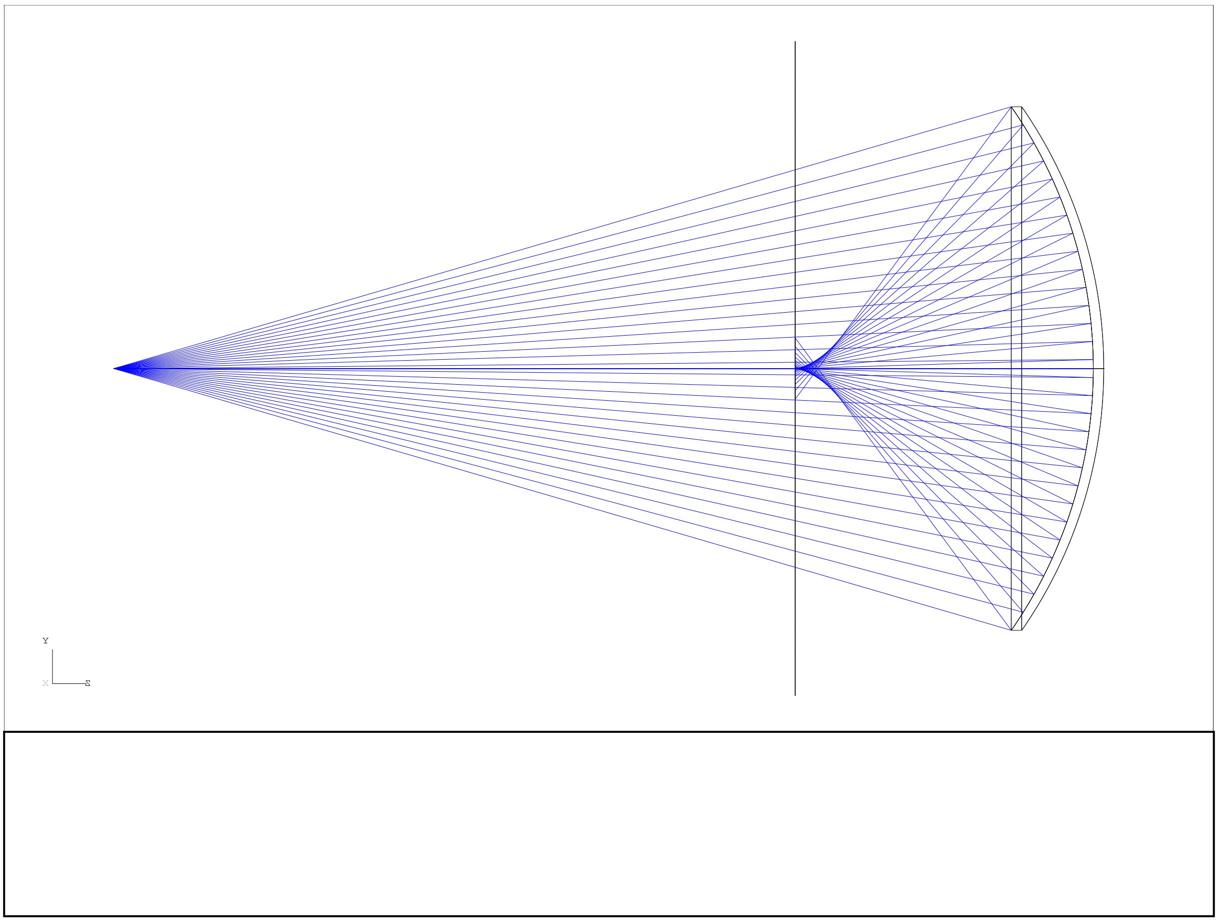

Figure 33: Numerical example in which the refractive index of the first medium is $n=1$ and the object and image distance are given by $s=-30.0mm$ and $s'=-9.13043\,mm$. Ray-tracing generated by the optical design package ZEMAX®: Spherical surface with radius $r=1/\bar{a}_{S,2}=-80.0mm$ and a aperture stop with a semi-diameter $r_{\text{stop}}=16.0mm$. Paraxial the imaging is perfect, but the peripheral rays introduce large errors. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context.

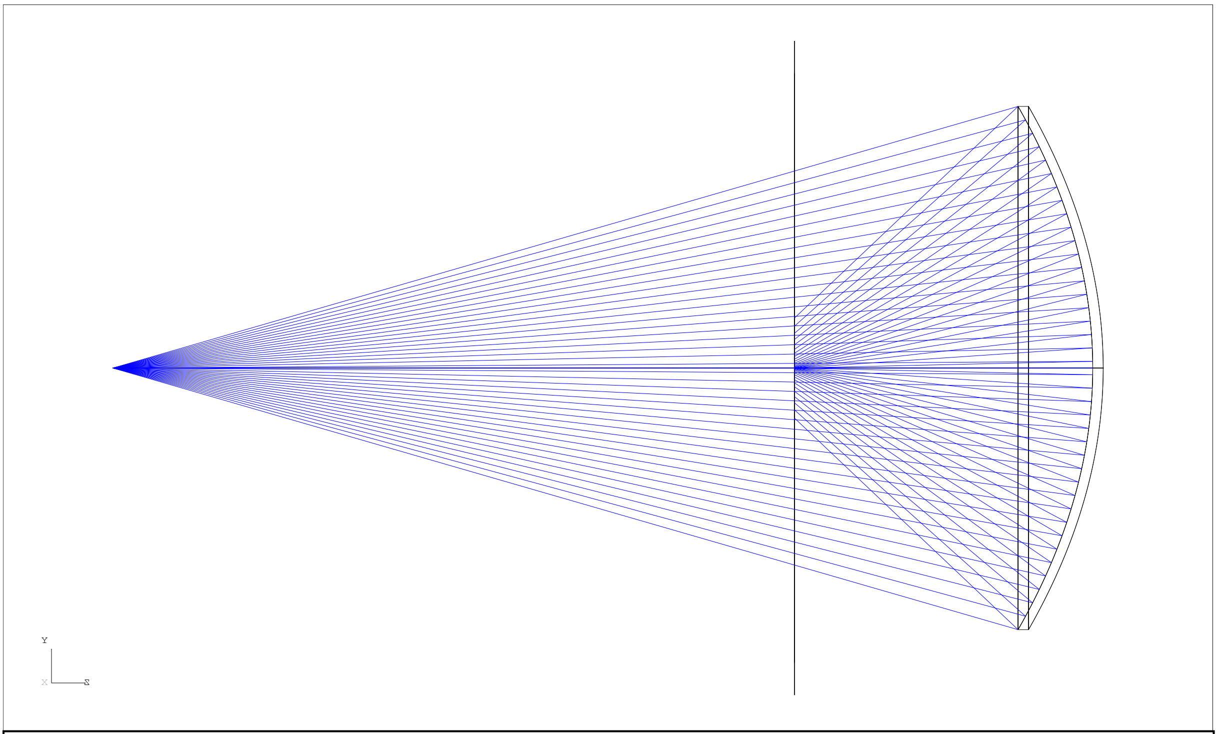

Figure 34: Numerical example in which the refractive index of the first medium is $n=1$ and the object and image distance are given by $s=-30.0mm$ and $s'=-9.13043\,mm$. Ray-tracing generated by the optical design package ZEMAX®: Parabolic surface with the same paraxial curvature $\bar{a}_{S,2}=-0.0714286\,mm^{-1}$ and a aperture stop with a semi-diameter $r_{stop}=16.0mm$. Paraxial the imaging is perfect, but the peripheral rays introduce large errors. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context.

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 $\bar{a}_{S,2}$, $\bar{a}_{S,4}$ and $\bar{a}_{S,6}$. Figure 35 shows that the errors are reduced to a level which is no longer visible on the scale of the plot.

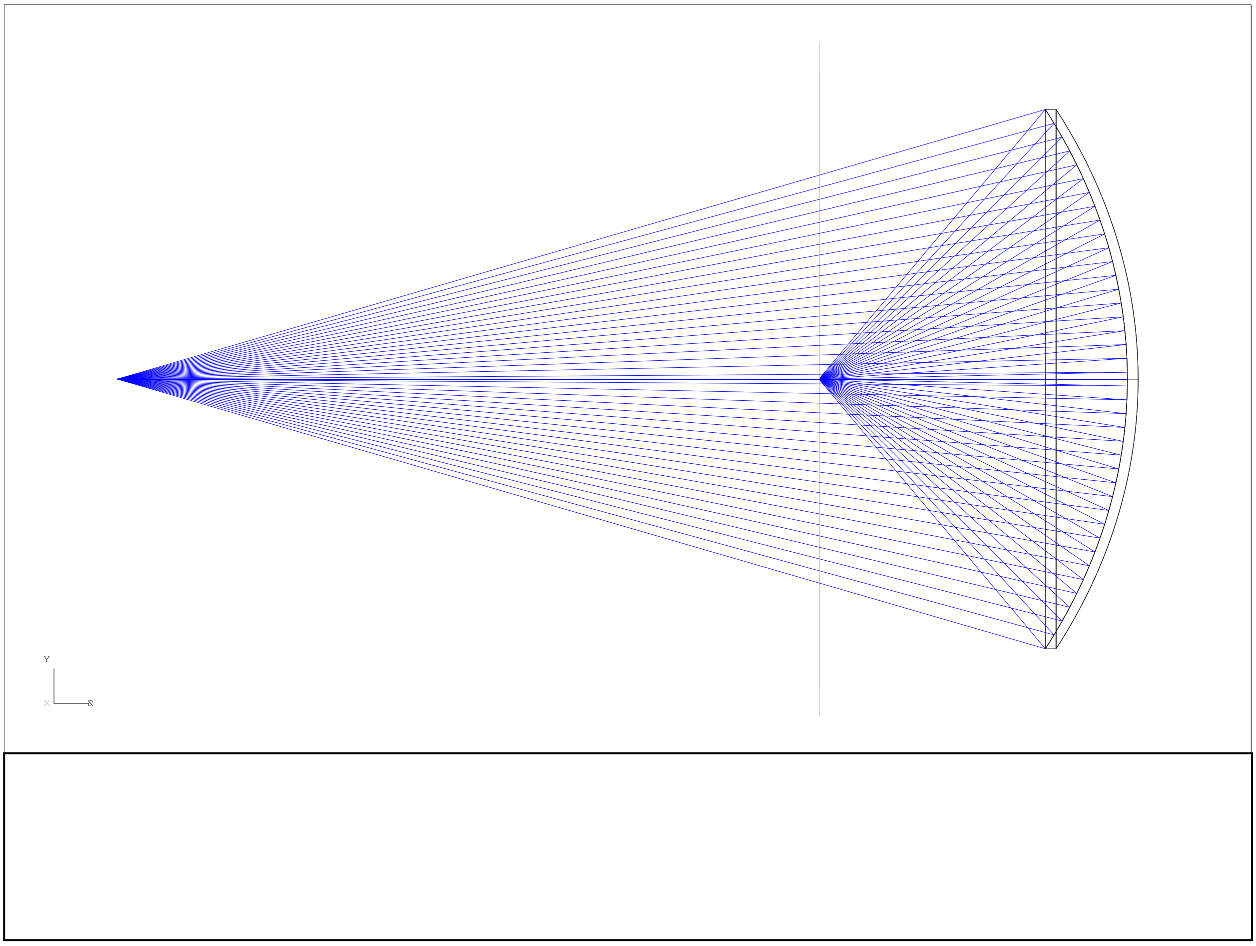

Figure 35: Numerical example in which the refractive index of the first medium is $n = 1$ and the object and image distance are given by $s = -30.0mm$ and $s' = -9.13043\,mm$. Ray-tracing generated by the optical design package ZEMAX®: Strongly reduced aberrations due to aspherical surface of 6th order with coefficients $\bar{a}_{S,2} = -0.0714286\,mm^{-1}$, $\bar{a}_{S,4} = -0.000782314\,mm^{-3}$ and $\bar{a}_{S,6} = -0.000042841\,mm^{-5}$ and a aperture stop with a semi-diameter $r_{stop} = 16.0mm$. The errors are reduced to a level which is no longer visible on the scale of the plot. The vertical lines in the drawings are construction lines of ZEMAX® and have no relevance in our context.

7. Propagation of OPD Aberrations

The propagation of OPD aberrations can also be derived directly by the algorithm described in chapter 3 and 5. Equivalently to Figure 25, the propagation of the OPD aberrations is shown in Figure 36.

7.1. Mathematical Approach in the 2D Case

7.1.1. Description of Wavefronts described by their OPD

Then the wavefronts themselves are each described by power series expansions. Any point on the original wavefront is given by the vector

$$\boldsymbol{\tau}_o(y_t) = \begin{pmatrix} y_t \\ \tau_{\mathrm{o}}(y_t) \end{pmatrix} \tag{256}$$

where in the 2D case $\tau_{\mathrm{o}}(y_t)$ is the curve defined by

$$\tau_{\mathrm{o}}(y_t) = \sum_{k=0}^{\infty} \frac{b_{\mathrm{o},k}}{k!} y_t^k \tag{257}$$

Equivalently, we represent the propagated wavefront by the vector

$$\boldsymbol{\tau}_p(y_t) = \begin{pmatrix} y_t \\ \tau_{\mathrm{p}}(y_t) \end{pmatrix} \tag{258}$$

where

$$\tau_{\mathrm{p}}(y_t) = \sum_{k=0}^{\infty} \frac{b_{\mathrm{p},k}}{k!} y_t^k \tag{259}$$

As in Eq. (4), again the normalization factor $k!$ is chosen such that the coefficients $b_{\mathrm{o},k}$ are given by the derivatives of the wavefront at $y_t = 0$,

$$b_{\mathrm{o},k} = \frac{\partial^k}{\partial y_t^k} \tau_{\mathrm{o}}(y_t)\bigg|_{y_t=0} = \tau_{\mathrm{o}}^{(k)}(0) \tag{260}$$

The relation between the derivatives of the OPD of the wavefront $\tau_o^{(k)}$ and the local OPD aberrations $E_{o,k}^{OPD}$ reads for the 2D case $E_{o,k}^{OPD} = \tau_o^{(k)} = b_{o,k}$, e.g. for second and third-order aberrations, we have $S_o^{OPD} = E_{o,2}^{OPD} = \tau_o^{(2)} = b_{o,2}$, $E_{o,3}^{OPD} = \tau_o^{(3)} = b_{o,3}$, etc., equivalent to Eqs. (26). A similar reasoning applies for the local OPD aberrations $E_{p,k}^{OPD}$ connected to the coefficients $b_{p,k}$ for the propagated wavefront.

7.1.2. Normal Vectors and their Derivatives

If the wavefront is described by their saggita as done in chapter 5, it will exist a relation between the normal of the wavefront $\mathbf{n}(w^{(1)}(y))$ and the first derivation of the saggita of the wavefront $w^{(1)}(y)$. This relation is shown in Eq. (36). It is necessary to derive also an equivalent relation between the normal of the wavefront $\mathbf{n}(\tau_w^{(1)}(y_t))$ and the first derivation of the OPD of the wavefront $\tau_w^{(1)}(y_t)$. The lower index w has to be understood as a synonym for the original wavefront with the index o or for the propagated wavefront with the index p.

The starting point for deriving this relation is Eq. (319), which describes the relation between the OPD $\tau_w(y_t(y))$ and the saggita $w(y)$ of the wavefront.

Derivation of Eq. (319) with respect to y reads

$$\frac{\partial \tau_w(y_t(y))}{\partial y_t}\frac{\partial y_t(y)}{\partial y} = \frac{d}{dy}\left(n w(y)\sqrt{1+w^{(1)}(y)^2}\right) \tag{261}$$

Inserting Eq. (320) and solving the derivatives leads to

$$\tau_w^{(1)}(y_t(y))\left(1+w(y)^{(1)^2}+w(y)w(y)^{(2)}\right) = n\frac{w^{(1)}(y)}{\sqrt{1+w^{(1)}(y)^2}}\left(1+w(y)^{(1)^2}+w(y)w(y)^{(2)}\right) \tag{262}$$

From Eq. (262) follows directly

$$w^{(1)}(y) = \frac{\dfrac{\tau_w^{(1)}(y_t(y))}{n}}{\sqrt{1-\left(\dfrac{\tau_w^{(1)}(y_t(y))}{n}\right)^2}} \tag{263}$$

Inserting Eq. (263) into Eq. (36) leads to requested relation between the normal vector $\mathbf{n}_w(y_t)$ of the wavefront and its OPD $\tau_w(y_t)$. This relation is given by $\mathbf{n}_w(y_t) = (-\frac{\tau_w^{(1)}(y_t)}{n}, \sqrt{1-\left(\frac{\tau_w^{(1)}(y_t)}{n}\right)^2})^T$

where $\tau_w^{(1)} = \partial \tau_w / \partial y_t$. In principle, we are interested in derivatives of $\mathbf{n}_w(y_t)$ with respect to y_t. Observing, however, that $\mathbf{n}_w(y_t)$ depends on y_t only via the slope $\tau_w^{(1)}(y_t)$, it is very practical to concentrate on this dependence $\mathbf{n}_w(\tau_w{}^{(1)})$ first and to deal with the inner dependence $\tau_w{}^{(1)}(y_t)$ later. To do this, we set $v \equiv \tau_w{}^{(1)}$ and to introduce the function

$$\mathbf{n}(v) := \begin{pmatrix} -\dfrac{v}{n} \\ \sqrt{1-\left(v/n\right)^2} \end{pmatrix} \tag{264}$$

Since at the intersection point of the chief ray with the original wavefront 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 $\mathbf{n}^{(1)}(0) \equiv \partial/\partial v\,\mathbf{n}(v)\big|_{v=0}$, $\mathbf{n}^{(2)}(0) \equiv \partial^2/\partial v^2\,\mathbf{n}(v)\big|_{v=0}$, etc.:

$$\mathbf{n}(0) := \begin{pmatrix} 0 \\ 1 \end{pmatrix},\ \mathbf{n}^{(1)}(0) := \frac{1}{n}\begin{pmatrix} -1 \\ 0 \end{pmatrix},\ \mathbf{n}^{(2)}(0) := \frac{1}{n^2}\begin{pmatrix} 0 \\ -1 \end{pmatrix},\ \mathbf{n}^{(3)}(0) := \begin{pmatrix} 0 \\ 0 \end{pmatrix},\ \mathbf{n}^{(4)}(0) := \frac{1}{n^4}\begin{pmatrix} 0 \\ -3 \end{pmatrix}, \text{ etc.,} \tag{265}$$

In application on the functions of interest, $\mathbf{n}_w(y) = \mathbf{n}(\tau_\mathrm{o}^{(1)}(y_t))$ and this means that $\mathbf{n}_w(0) = (0,1)^T$. Further, the first derivatives are given by

$$\frac{\partial}{\partial y_t}\mathbf{n}_w(y_t)\bigg|_{y_t=0} \equiv \mathbf{n}_\mathrm{w}^{(1)}(0) = \mathbf{n}^{(1)}(0)\tau_\mathrm{o}^{(2)}(0) = \begin{pmatrix} -1 \\ 0 \end{pmatrix}\frac{\tau_\mathrm{o}^{(2)}(0)}{n} \tag{266}$$

,

and similarly for the higher derivatives.

7.1.3. Ansatz for Determining the Propagation Equations

As shown in Figure 36 the vector $\mathbf{w}_o = \mathbf{w}_o(y_\mathrm{o})$ points to the neighboring ray's intersection point with the original wavefront, and the wavefront's OPD referred to the original wavefront along the ray is denoted by τ_o. Hence, the vector $\begin{pmatrix} y_{\mathrm{t}o} \\ 0 \end{pmatrix}$ pointing to the intersection point with the plane $z=0$, must be equal to the vector sum

$$\begin{pmatrix} y_o \\ w_o(y_o) \end{pmatrix} - \frac{\tau_o(y_{\mathrm{t}o})}{n}\mathbf{n}_w = \begin{pmatrix} y_{\mathrm{t}o} \\ 0 \end{pmatrix}. \tag{267}$$

Correspondingly the vector $\mathbf{w}_p = \mathbf{w}_p(y_\mathrm{p})$ points to the neighboring ray's intersection point with the propagated wavefront, and the wavefront's OPD referred to the propagated wavefront along the ray is denoted by τ_p. Hence, the vector $\begin{pmatrix} y_{\mathrm{tp}} \\ \frac{\tau}{n} \end{pmatrix}$ points to the intersection point with the plane $z = \frac{\tau}{n}$, must be equal to the vector sum

$$\begin{pmatrix} y_p \\ w_p(y_p) \end{pmatrix} - \frac{\tau_p(y_{\mathrm{tp}})}{n}\mathbf{n}_w = \begin{pmatrix} y_{\mathrm{tp}} \\ \frac{\tau}{n} \end{pmatrix}. \qquad (268)$$

The vector from the original wavefront to the propagated surface is $\tau/n\,\mathbf{n}_w$. Hence, the vector to the point on the propagated wavefront itself, $\mathbf{w}_p$, must be equal to the vector sum $\mathbf{w}_p = \mathbf{w}_o + \tau/n\,\mathbf{n}_w$. This yields the fundamental equation:

$$\begin{pmatrix} y_{\mathrm{t}p} - y_{\mathrm{to}} \\ \frac{\tau}{n} \end{pmatrix} = \frac{\tau + \tau_o(y_{\mathrm{to}}) - \tau_p(y_{\mathrm{t}p})}{n}\mathbf{n}_w \qquad (269)$$

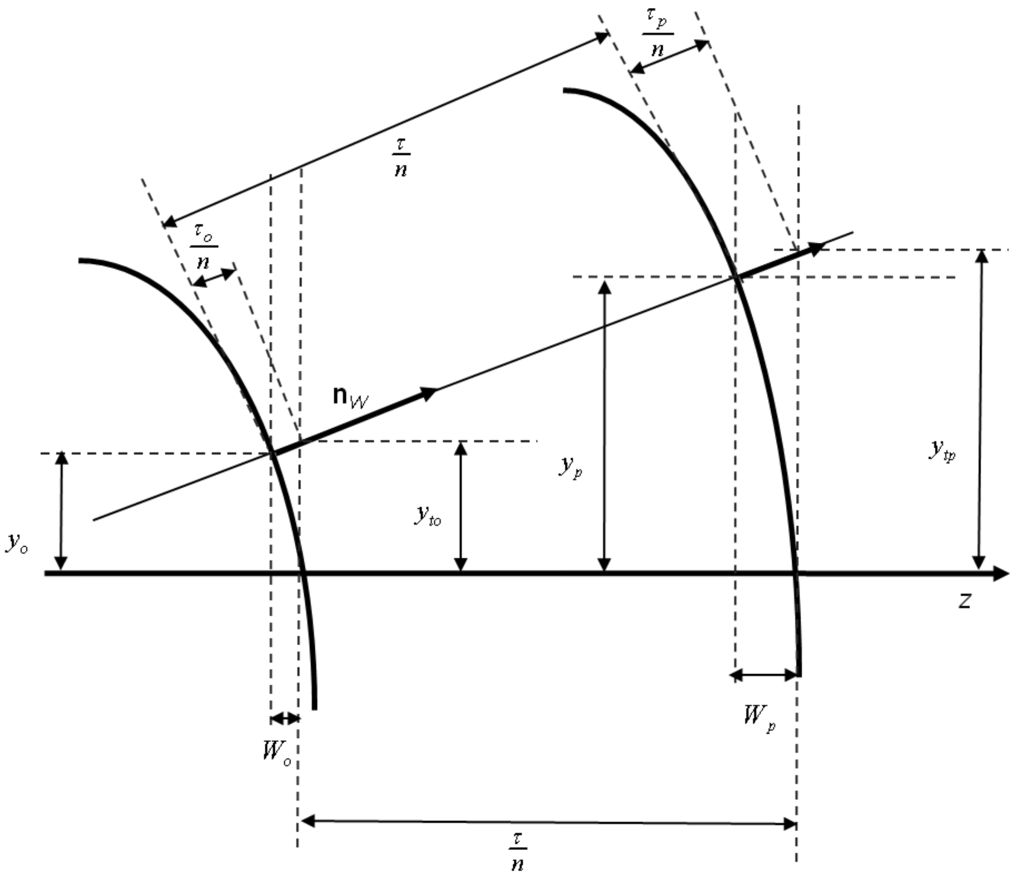

Figure 36: Propagation of a wavefront $\mathbf{w_0}$ about the distance τ/n to the propagated wavefront $\mathbf{w_p}$. The chief ray and the coordinate system are fixed, a neighboring ray scans the original wavefront $\{\mathbf{w}_o\}$ and hits it at an intercept $y_o \neq 0$, then propagates to the propagated wavefront $\{\mathbf{w}_p\}$, where the brackets $\{.\}$ shall denote the entity of vectors described by Eq. (124). Consistently with our notation, we denote as y_o the projection of the neighboring ray's intersection with $\{\mathbf{w}_o\}$ onto the y axis and analogously, the projection of the intersection with $\{\mathbf{w}_p\}$ onto the y axis is denoted as y_p. The wavefronts are described by their OPD τ_o .and τ_p

From Eq. (269), it is now possible to derive the desired relations order by order. Although only the OPD of the propagated wavefront is of interest, in Eq. (269) additionally the quantities y_{to} and y_{tp} are also unknown. However, those are not independent from each other: if any one of them is given, the other one can no longer be chosen independently. y_{tp} is used as independent variable and to consider y_{to} as function of it.

Eq. (269) represents a nonlinear system of two algebraic equations for the two unknown functions $\tau_p(y_{tp})$ and $y_{to}(y_{tp})$. Even if we are only interested in a solution for the function $\tau_p(y_{tp})$, we cannot obtain it without simultaneously solving the equations for both unknowns order by order. Introducing the vector of unknown functions as

$$\mathbf{p}(y_{\text{tp}}) = \begin{pmatrix} y_{\text{to}}(y_{\text{tp}}) \\ \tau_{\text{p}}(y_{\text{tp}}) \end{pmatrix} \tag{270}$$

and observing that the initial condition $\mathbf{p}(0) = \begin{pmatrix} 0 \\ \tau/n \end{pmatrix}$ has to be fulfilled, it is now straightforward to compute all the derivatives of these Eq. (269) up to some order, which yields relations between the curvatures, third derivatives etc. of the OPD of the original and propagated wavefront. Rewriting these relations in terms of series coefficients $b_{\text{o},k}$ and solving them for the desired coefficients $b_{\text{p},k}$ yields the desired result.

Before solving Eq. (269), we distinguish if the independent variable y_{tp} enters into Eq. (269) explicitly like in the first component of the vector $(y_{\text{tp}}, \tau_{\text{p}}(y_{\text{tp}}))^T$, or implicitly via one of the components of Eq. (270). To this end, we define the function $\left(\mathrm{IR}^2 \times \mathrm{IR}\right) \mapsto \mathrm{IR}^2 : (\mathbf{p}, y_{\text{tp}}) \mapsto \mathbf{f}$ by

$$\mathbf{f}\left(\mathbf{p}, y_{\text{tp}}\right) = \begin{pmatrix} y_{\text{to}} + \dfrac{\tau + \tau_o(y_{\text{to}}) - \tau_p}{n} n_{w,y}\left(\tau_{\text{o}}^{(1)}(y_{\text{to}})\right) & - y_{\text{tp}} \\ \dfrac{\tau + \tau_o(y_{\text{to}}) - \tau_p}{n} n_{w,z}\left(\tau_{\text{o}}^{(1)}(y_{\text{to}})\right) & - \dfrac{\tau}{n} \end{pmatrix}, \tag{271}$$

where $(p_1, p_2) = (y_{\text{to}}, \tau_{\text{p}})$ are the components of $\mathbf{p}$. Setting now $\mathbf{p} = \mathbf{p}(y_{\text{tp}})$, Eq. (271) allows rewriting the fundamental system of Eq. (269) in a more compact way as

$$\mathbf{f}\left(\mathbf{p}(y_{\text{tp}}), y_{\text{tp}}\right) = \mathbf{0} \tag{272}$$

as can be verified explicitly by component wise comparison with Eq. (269).

The key ingredient of the method is that the relations between the derivatives of the OPD of the original and propagated wavefront can be obtained by the first, second, etc. total derivative of Eq. (272) with respect to y_{tp}, evaluated in the origin. The advantage of the form of Eq. (272) using Eq. (271) is that the various terms can be tracked in a fairly compact manner.

The total derivative of $\mathbf{f}\left(\mathbf{p}(y_{\text{tp}}), y_{\text{tp}}\right)$ in Eq. (272) 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 $p_i(y_{\text{tp}})$, plus the partial derivative of $\mathbf{f}$ with respect to the explicit dependence on y_{tp}. This transforms the system of algebraic equations in Eq. (269) to the system of differential equations

$$\sum_{j=1}^{2} \frac{\partial f_i}{\partial p_j} p_j^{(1)}(y_{\text{tp}}) + \frac{\partial f_i}{\partial y_{\text{tp}}} = 0, \quad i = 1,2, \tag{273}$$

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 $\mathbf{p} = \mathbf{p}(y_{\text{tp}})$. The Jacobian $\mathbf{A}$ reads

$$\mathbf{A} := \begin{pmatrix} \frac{\partial f_1}{\partial y_{\text{to}}} & \frac{\partial f_1}{\partial \tau_{\text{p}}} \\ \frac{\partial f_2}{\partial y_{\text{to}}} & \frac{\partial f_2}{\partial \tau_{\text{p}}} \end{pmatrix} = \begin{pmatrix} -1 - \frac{\tau_{\text{o}}^{(1)}}{n} n_{w,y} - \frac{\tau + \tau_o - \tau_p}{n} n_{w,y}^{(1)} & \frac{n_{w,y}}{n} \\ -\frac{\tau_{\text{o}}^{(1)}}{n} n_{w,z} - \frac{\tau + \tau_o - \tau_p}{n} n_{w,z}^{(1)} & \frac{n_{w,z}}{n} \end{pmatrix} \tag{274}$$

In Eq.(274), the occurring expressions are understood as $\tau_{\text{o}}^{(1)} \equiv \tau_{\text{o}}^{(1)}(y_{\text{to}})$, $\tau_{\text{o}}^{(2)} \equiv w_{\text{o}}^{(2)}(y_{\text{to}})$, $n_{\text{w},y} \equiv n_{\text{w},y}(\tau_{\text{o}}^{(1)}(y_{\text{to}}))$, $n_{\text{w},y}^{(1)} \equiv n_{\text{w},y}^{(1)}(\tau_0^{(1)}(y_{\text{to}}))$, etc., and additionally $y_{\text{to}}, \tau_{\text{p}}$ are themselves functions of y_{tp}.

The derivative vector $\partial f_i / \partial y_{tp}$ in Eq. (273) shall be summarized as

$$\mathbf{b} := -\frac{\partial \mathbf{f}}{\partial y_{\text{tp}}} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \tag{275}$$

Both $\mathbf{A}$ and $\mathbf{b}$ are deduced from $\mathbf{f}\left(\mathbf{p}(y_{\text{tp}}), y_{\text{tp}}\right)$ and must in general themselves have the same kind of dependence, i.e. $\mathbf{A}\left(\mathbf{p}(y_{\text{tp}}), y_{\text{tp}}\right)$ and $\mathbf{b}\left(\mathbf{p}(y_{\text{tp}}), y_{\text{tp}}\right)$. However, due to the special property of $\mathbf{f}$ to be linear in y_{tp}, $\mathbf{b}$ is constant. Additionally, $\mathbf{A}$ has no explicit dependence on y_{tp} besides the implicit dependence via $\mathbf{p}(y_{\text{tp}})$. Hence we write $\mathbf{b}$ without argument and $\mathbf{A} = \mathbf{A}(\mathbf{p}(y_{\text{tp}}))$, and Eq. (43) can be written in the form

$$\mathbf{A}(\mathbf{p}(y_{\text{tp}}))\mathbf{p}^{(1)}(y_{\text{tp}}) = \mathbf{b}. \tag{276}$$

7.1.4. Solving techniques for the fundamental equation

Eq. (276) is the derivative of the fundamental equation in Eq. (272), and therefore it is itself a fundamental equation. But additionally, it allows a stepwise solution for the derivatives $\mathbf{p}^{(k)}(y_{\text{tp}} = 0)$ for increasing order k. Formally, Eq. (276) can be solved for $\mathbf{p}^{(1)}(y_{\text{tp}})$ by

$$\mathbf{p}^{(1)}(y_{\text{tp}}) = \mathbf{A}(\mathbf{p}(y_{\text{tp}}))^{-1}\mathbf{b}. \tag{277}$$

Eq. (277) holds as a function of y_{tp}, but of course for arbitrary y_{tp} both sides of Eq. (277) are unknown. However, evaluating Eq. (277) for $y_{\text{tp}} = 0$ exploits that then the right-hand side (rhs) is known because $\mathbf{p}(0) = \begin{pmatrix} 0 \\ \tau/n \end{pmatrix}$ is known! In the same manner, Eq. (277) serves as starting point for a recursion scheme by repeated total derivative and evaluation for $y_{\text{tp}} = 0$. Remembering that $\mathbf{b}$ is constant, we obtain

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \\
\mathbf{p}^{(2)}(0) &= \left(\mathbf{A}^{-1}\right)^{(1)}\mathbf{b} \\
&\dots \\
\mathbf{p}^{(k)}(0) &= \left(\mathbf{A}^{-1}\right)^{(k-1)}\mathbf{b},
\end{aligned} \tag{278}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1)} = \left.\frac{d}{dy_{\text{tp}}}\mathbf{A}\left(\mathbf{p}(y_{\text{tp}})\right)^{-1}\right|_{y_{\text{tp}}=0}$, …, $\left(\mathbf{A}^{-1}\right)^{(k-1)} = \left.\frac{d^{k-1}}{dy_{\text{tp}}^{k-1}}\mathbf{A}\left(\mathbf{p}(y_{\text{tp}})\right)^{-1}\right|_{y_{\text{tp}}=0}$ are total derivatives of the function $\mathbf{A}\left(\mathbf{p}(y_{\text{tp}})\right)^{-1}$. The reason why Eq. (278) really does provide solutions for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$ is that in any row of Eq. (278) the entries on the rhs are all known assuming that the equations above are already solved. Although on the rhs there occur implicit derivatives $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, … as well, they are always of an order less than on the left-hand side (lhs). For example, the second row in Eq. (278) reads in explicit form $\mathbf{p}^{(2)}(0) = \sum_{i=1}^{2}\left(\frac{\partial}{\partial p_i}\mathbf{A}(\mathbf{p})^{-1}\right)p_i^{(1)}\Big|_{y_{\text{tp}}=0} \cdot \mathbf{b}$ where $y_{\text{tp}} = 0$ implies $\mathbf{p} = \begin{pmatrix} 0 \\ \tau/n \end{pmatrix}$, and where on the rhs the highest occurring derivative of $\mathbf{p}$ is $\mathbf{p}^{(1)}(0)$ which is already known due to the first row in Eq. (278). Generally, the highest derivative of $\mathbf{p}$ occurring in $\left.\left(\frac{d^{k-1}}{dy_{\text{tp}}^{k-1}}\mathbf{A}\left(\mathbf{p}(y_{\text{tp}})\right)^{-1}\right)\right|_{y_{\text{tp}}=0}$ is $\mathbf{p}^{(k-1)}(0)$, which is already known at the stage when $\mathbf{p}^{(k)}(0)$ is to be computed by Eq. (278).

Although looking attractive and formally simple, applying Eq. (278) in practice requires still 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 $\partial^2/\partial p_i \partial p_j$. Both tasks are straightforward to be executed by a computer algebra package but nevertheless lengthy and not the best way how 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! To this purpose, we start the recursion scheme from Eq. (276) instead of Eq. (277). The first $(k-1)$ total derivatives of Eq. (276) are

$$\begin{aligned} \mathbf{A}\mathbf{p}^{(1)}(0) &= \mathbf{b} && \text{(a)} \\ \mathbf{A}^{(1)}\mathbf{p}^{(1)}(0) + \mathbf{A}\mathbf{p}^{(2)}(0) &= \mathbf{0} && \text{(b)} \\ \mathbf{A}^{(2)}\mathbf{p}^{(1)}(0) + 2\mathbf{A}^{(1)}\mathbf{p}^{(2)}(0) + \mathbf{A}\mathbf{p}^{(3)}(0) &= \mathbf{0} && \text{(c)} \\ &\ldots \\ \sum_{j=1}^{k}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0) &= \mathbf{0}, \quad k \geq 2 && \text{(d)} \end{aligned} \tag{279}$$

where $\mathbf{A} = \mathbf{A}(\mathbf{p}(0)) = \mathbf{A}(\mathbf{0})$, and $\mathbf{A}^{(1)} = \left.\frac{d}{dy_{\text{tp}}}\mathbf{A}(\mathbf{p}(y_{\text{tp}}))\right|_{y_{\text{tp}}=0}$, …, $\mathbf{A}^{(k-j)} = \left.\frac{d^{k-j}}{dy_{\text{tp}}^{k-j}}\mathbf{A}(\mathbf{p}(y_{\text{tp}}))\right|_{y_{\text{tp}}=0}$ are total derivatives of the function $\mathbf{A}(\mathbf{p}(y_{\text{tp}}))$. For the last line of Eq. (279) we have applied the formula for the p-th derivative of a product, $(fg)^{(l)} = \sum_{j=0}^{l}\binom{l}{j} f^{(l-j)} g^{(j)}$. Eq. (279) represents a recursion scheme where in each equation containing $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k)}(0)$, only $\mathbf{p}^{(k)}(0)$ (in the last term for $j = k$) is unknown provided that all previous equations for $\mathbf{p}^{(1)}(0)$, $\mathbf{p}^{(2)}(0)$, …, $\mathbf{p}^{(k-1)}(0)$ are already solved. A formal solution for $\mathbf{p}^{(k)}(0)$, expressed in terms of its predecessors, is

$$\begin{aligned} \mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \qquad , \quad k = 1 \\ \mathbf{p}^{(k)}(0) &= -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), \quad k \geq 2. \end{aligned} \tag{280}$$

Although quite different in appearance at first glance, Eq. (280) yields exactly the same solutions as Eq. (278).

7.1.5. Solutions for the General Propagation Equations

In the result for $\mathbf{p}^{(1)}(0)$, the first rows of both Eqs. (278),(280) involve $\mathbf{A}(\mathbf{0})^{-1}$. For obtaining $\mathbf{A}(\mathbf{0})^{-1}$, we evaluate Eq. (274) for $\mathbf{p} = \mathbf{0}$ and apply Eqs. (265), yielding

$$\mathbf{A}(\mathbf{0}) = \begin{pmatrix} -1 + \frac{\tau}{n^2}\tau_{\text{o}}^{(2)} & 0 \\ 0 & \frac{1}{n} \end{pmatrix} \Rightarrow \mathbf{A}(\mathbf{0})^{-1} = \begin{pmatrix} \frac{-1}{1 - \tau/_{n^2}\,\tau_{\text{o}}^{(2)}} & 0 \\ 0 & n \end{pmatrix} \tag{281}$$

The final result for $\mathbf{p}^{(1)}(0)$ is

$$\mathbf{p}^{(1)}(0)=\mathbf{A}^{-1}\mathbf{b}=\begin{pmatrix}\dfrac{-1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\\ 0\end{pmatrix} \tag{282}$$

The first derivative of the y_{to}-coordinate is a dilation depending on the curvature of the OPD of the original wavefront and the propagated optical path length τ, such that $y_{to}^{(1)}(0)=\dfrac{-1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}$. The slope of the OPD of the propagated wavefront vanishes, $\tau_p^{(1)}(0)=0$, as does the slope of the OPD of the original wavefront due to $\tau_o^{(1)}(0)=0$.

For the orders $k\geq 2$ we apply Eqs. (280). The derivatives $\mathbf{A}^{(1)}=\dfrac{d}{dy_{\mathrm{tp}}}\mathbf{A}(\mathbf{p}(y_{\mathrm{tp}}))\bigg|_{y_{\mathrm{tp}}=0}$, etc. are directly obtained by total derivative of Eq. (274) with respect to y_{tp}, evaluating for $y_{\mathrm{tp}}=0$ and again applying Eqs. (265). For the orders $k\geq 2$ only the results $\tau_{\mathrm{p}}^{(k)}(0)$ for the propagated wavefront are of interest, therefore we directly provide those result. The resulting second-order law is (omitting the argument '(0)')

$$\tau_{\mathrm{p}}^{(2)}=\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\tau_{\mathrm{o}}^{(2)} \tag{283}$$

which is well-known as the propagation equation and reveals to be a special case of the results. The resulting higher-order laws can be written in a similar fashion

$$\begin{aligned}
\tau_{\mathrm{p}}^{(3)}&=\left(\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\right)^3\tau_{\mathrm{o}}^{(3)}\\
\tau_{\mathrm{p}}^{(4)}&=\left(\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\right)^4\left(\tau_{\mathrm{o}}^{(4)}+3\frac{1}{1-\tau/_{n^2}\tau_{\mathrm{o}}^{(2)}}\frac{\tau}{n^2}\tau_{\mathrm{o}}^{(3)2}+3\frac{\tau}{n^4}\tau_{\mathrm{o}}^{(2)4}\right)\\
\tau_{\mathrm{p}}^{(5)}&=\left(\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\right)^5\\
&\quad\left(\tau_{\mathrm{o}}^{(5)}+5\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\frac{\tau}{n^2}\tau_{\mathrm{o}}^{(3)}\left(2\tau_{\mathrm{o}}^{(4)}+3\frac{1}{1-\tau/_{n^2}\,\tau_{\mathrm{o}}^{(2)}}\frac{\tau}{n^2}\tau_{\mathrm{o}}^{(3)2}+6\frac{1}{n^2}\tau_{\mathrm{o}}^{(2)3}\right)\right)\\
&\quad\ldots
\end{aligned} \tag{284}$$

Eq. (284) holds likewise for the derivatives and for the coefficients $b_{\mathrm{o},k}$, and $b_{\mathrm{p},k}$ due to Eqs. (257)-(260). In terms of local aberrations and substituting $d=\tau/n$ and $\beta=\frac{1}{1-\frac{d}{n}S_o^{OPD}}$, Eq. (284) reads

$$\begin{aligned}
S_p^{OPD} &= \beta S_o^{OPD}\\
E_{p,3}^{OPD} &= \beta^3 E_{o,3}^{OPD}\\
E_{p,4}^{OPD} &= \beta^4\left(E_{o,4}^{OPD}+3\tfrac{d}{n}\left(\beta E_{o,3}^{OPD\,2}+\frac{S_o^{OPD\,4}}{n^2}\right)\right)\\
E_{p,5}^{OPD} &= \beta^5\left(E_{o,5}^{OPD}+5\beta\tfrac{d}{n}E_{o,3}^{OPD}\left(2E_{o,4}^{OPD}+3\beta\tfrac{d}{n}E_{o,3}^{OPD\,2}+6\frac{S_o^{OPD\,3}}{n^2}\right)\right)\\
E_{p,6}^{OPD} &= \beta^6\left(E_{o,6}^{OPD}+5\beta\tfrac{d}{n}\left(3E_{o,3}^{OPD}E_{o,5}^{OPD}+21\beta\tfrac{d}{n}E_{o,3}^{OPD\,2}E_{o,4}^{OPD}+12\frac{S_o^{OPD\,3}E_{o,4}^{OPD}}{n^2}\right.\right.\\
&\left.\left.+2E_{o,4}^{OPD\,2}+9\beta S_o^{OPD\,2}E_{o,3}^{OPD\,2}\frac{3+4\tfrac{d}{n}S_o^{OPD}}{n^2}+21(\beta\tfrac{d}{n})^2E_{o,3}^{OPD\,4}+9S_o^{OPD\,6}\frac{1+\tfrac{d}{n}S_o^{OPD}}{n^4}\right)\right)
\end{aligned} \quad , \qquad (285)$$

Eq. (285) can be generalized to

$$E_{p,k}^{OPD}=\beta^{k-\max(3-k,0)}(E_{o,k}^{OPD}+\tilde{R}_k^{OPD}) \qquad (286)$$

where in $\tilde{R}_k^{OPD}$ all wavefront derivatives of lower order (<*k*) are expressed in terms of local aberrations. Table 8 shows the propagation equation for OPD aberrations up to order $k=6$ and the propagation equations for wavefront (saggita) aberrations are shown for comparison in Table 9.

Propagation OPD aberration:	
$\beta = \frac{1}{1-\frac{d}{n}S_o^{OPD}}, \quad d = \tau/n$	
S_p^{OPD}	$\beta\, S_o^{OPD}$
$E_{p,3}^{OPD}$	$\beta^3\, E_{o,3}^{OPD}$
$E_{p,4}^{OPD}$	$\beta^4 \left(E_{o,4}^{OPD} + 3\frac{d}{n}\left(\beta\; {E_{o,3}^{OPD}}^2 + \frac{{S_o^{OPD}}^4}{n^2} \right) \right)$
$E_{p,5}^{OPD}$	$\beta^5 \left(E_{o,5}^{OPD} + 5\,\beta\frac{d}{n}\, E_{o,3}^{OPD} \left(2\; E_{o,4}^{OPD} + 3\beta\frac{d}{n}\, {E_{o,3}^{OPD}}^2 + 6\frac{{S_o^{OPD}}^3}{n^2} \right) \right)$
$E_{p,6}^{OPD}$	$\beta^6 \left(E_{o,6}^{OPD} + 5\beta\frac{d}{n}\left(3\, E_{o,3}^{OPD}\, E_{o,5}^{OPD} + 21\beta\frac{d}{n}\, {E_{o,3}^{OPD}}^2\, E_{o,4}^{OPD} + 12\frac{{S_o^{OPD}}^3\, E_{o,4}^{OPD}}{n^2} + 2\, {E_{o,4}^{OPD}}^2 + 9\,\beta\, {S_o^{OPD}}^2\, {E_{o,3}^{OPD}}^2\, \frac{3\; + 4\,\frac{d}{n}\, S_o^{OPD}}{n^2}\, {E_{o,3}^{OPD}}^2 + 21\beta^2\frac{d^2}{n^2}\, {E_{o,3}^{OPD}}^4 + 9\, {S_o^{OPD}}^6\, \frac{1 + \frac{d}{n}\;\, S_o^{OPD}}{n^4} \right) \right)$

Table 8: Equations to calculate the OPD aberrations up to order *k* = 6 of the propagated wavefront as a function of the OPD aberrations of the original wavefront

Propagation Wavefront aberration:	
$\beta = \dfrac{1}{1 - \frac{d}{n} D} \qquad d = \tau / n$	
S_p	βS_o
$E_{p,3}$	$\beta^3 E_{o,3}$
$E_{p,4}$	$\beta^4 \left(E_{o,4} + 3 \tfrac{d}{n} \left(\beta E_{o,3}^2 - \dfrac{S_o^4}{n^2} \right) \right)$
$E_{p,5}$	$\beta^5 \left(E_{o,5} + 5 \beta \tfrac{d}{n} E_{o,3} \left(2 E_{o,4} + 3 \beta \tfrac{d}{n} E_{o,3}^2 - 6 \dfrac{S_o^3}{n^2} \right) \right)$
$E_{p,6}$	$\beta^6 \left(E_{o,6} + 5 \beta \tfrac{d}{n} \left(3 E_{o,3} E_{o,5} + 21 \beta \tfrac{d}{n} E_{o,3}^2 E_{o,4} - 12 \dfrac{S_o^3 E_{o,4}}{n^2} \right. \right.$ $\left. \left. + 2 E_{o,4}^2 - 9 \beta S_1^2 E_{o,3}^2 \dfrac{3 + 4 \frac{d}{n} S_o}{n^2} + 21 (\beta \tfrac{d}{n})^2 E_{o,3}^4 + 9 S_o^6 \dfrac{1 + \frac{d}{n} S_o}{n^4} \right) \right)$

Table 9: Equations to calculate the wavefront (saggita) aberrations up to order k = 6 of the propagated wavefront as a function of the wavefront aberrations of the original wavefront

7.2. Mathematical Approach in the 3D Case

7.2.1. Description of Wavefronts described by their OPD

Although more lengthy to demonstrate than the 2D case, conceptually the 3D case can be treated analogously to the 2D case. Therefore, we will only report the most important differences. Analogously to Eq. (256), the original wavefront is now represented by the 3D vector

$$\boldsymbol{\tau}_o(x_t, y_t) = \begin{pmatrix} x_t \\ y_t \\ \tau_o(x_t, y_t) \end{pmatrix} \tag{287}$$

where in the 3D case $\tau_o(x_t, y_t)$ is the surface defined by

$$\tau_o(x_t, y_t) = \sum_{k=0}^{\infty} \sum_{m=0}^{k} \frac{b_{o,m,k-m}}{m!(k-m)!} x_t^m y_t^{k-m} \tag{288}$$

As in Eq. (4), again the normalization factors $k!$ and $m!$ are chosen such that the coefficients $b_{o,m,k-m}$ are given by the derivatives of the wavefront at $x_t = 0, y_t = 0$,

$$b_{\mathrm{o,m},k-m} = \frac{\partial^k}{\partial x_t^m \partial y_t^{k-m}} \tau_{\mathrm{o}}(x_t, y_t)\Big|_{x_t=0, y_t=0} \tag{289}$$

Equivalently, we represent the propagated wavefront by the vector

$$\boldsymbol{\tau}_p(x_t, y_t) = \begin{pmatrix} x_t \\ y_t \\ \tau_{\mathrm{p}}(x_t, y_t) \end{pmatrix} \tag{290}$$

with

$$\tau_{\mathrm{p}}(x_t, y_t) = \sum_{k=0}^{\infty} \sum_{m=0}^{k} \frac{b_{p,m,k-m}}{m!(k-m)!} x_t^m y_t^{k-m} \tag{291}$$

7.2.2. Normal Vectors and their Derivatives

If the wavefront is described by their saggita as done in chapter 5, it will exist a relation between the normal of the wavefront $\mathbf{n}(w^{(1)}(x,y))$ and the first derivation of the saggita of the wavefront $w^{(1)}(x,y)$. This relation is shown in Eq. (65). It is necessary to derive also an equivalent relation between the normal of the wavefront $\mathbf{n}(\tau_w^{(1)}(x_t, y_t))$ and the first derivation of the OPD of the wavefront $\tau_w^{(1)}(x_t, y_t)$. The lower index w has to be understood as synonym for the original wavefront with the index o or for the propagated wavefront with the index p.

The starting point for deriving this relation is Eq. (318). Equivalently the fundamental equation in the 3D case takes the form

$$\begin{pmatrix} x \\ y \\ w(x,y) \end{pmatrix} - \frac{\tau_w}{n} \mathbf{n}_w = \begin{pmatrix} x_t \\ y_t \\ 0 \end{pmatrix}. \tag{292}$$

Our question is now posed such that $\tau_w(x_{\mathrm{t}}, y_{\mathrm{t}})$ is the unknown function of interest while $w(x,y)$ is given. In this case it is most practical to use x and y as the independent variable, such that the functions $x_{\mathrm{t}}(x,y), y_{\mathrm{t}}(x,y)$ and consequently $\tau_w(x_{\mathrm{t}}(x,y), y_{\mathrm{t}}(x,y))$ enter into Eq.(292).

Inserting $\mathbf{n}_w(x,y) = (-w^{(1,0)}(x,y), -w^{(0,1)}(x,y), 1)^T / \sqrt{1 + w^{(1,0)}(x,y)^2 + w^{(0,1)}(x,y)^2}$, the third row of Eq. (292) can be solved for $\tau_w(x_{\mathrm{t}}(x,y), y_{\mathrm{t}}(x,y))$, yielding

$$\tau_w(x_t(x,y),y_t(x,y)) = n\,w(x,y)\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}\,. \tag{293}$$

Inserting then Eq. (293) into the first and second row of Eq. (292) leads to

$$\begin{aligned} x_t(x,y) &= x + w(x,y)w^{(1,0)}(x,y) \\ y_t(x,y) &= y + w(x,y)w^{(0,1)}(x,y) \end{aligned}\,. \tag{294}$$

Inserting Eqs. (294) into the arguments of τ_w in Eq. (293), yields

$$\tau_w(x+w(x,y)w^{(1,0)}(x,y),y+w(x,y)w^{(0,1)}(x,y)) = n\,w(x,y)\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}\,. \tag{295}$$

Derivation of Eq. (293) with respects to x and y reads

$$\begin{aligned} &\frac{\partial\tau_w(x_t(x,y),y_t(x,y))}{\partial x_t}\frac{\partial x_t(x,y)}{\partial x}+\frac{\partial\tau_w(x_t(x,y),y_t(x,y))}{\partial y_t}\frac{\partial y_t(x,y)}{\partial x} \\ &= \frac{d}{dx}\left(n\,w(x,y)\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}\right) \\ &\frac{\partial\tau_w(x_t(x,y),y_t(x,y))}{\partial x_t}\frac{\partial x_t(x,y)}{\partial y}+\frac{\partial\tau_w(x_t(x,y),y_t(x,y))}{\partial y_t}\frac{\partial y_t(x,y)}{\partial y} \\ &= \frac{d}{dy}\left(n\,w(x,y)\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}\right) \end{aligned} \tag{296}$$

Inserting Eqs. (294) and solving the derivatives leads to

$$\begin{aligned} &\tau_w^{(1,0)}(x_t(x,y),y_t(x,y))\left(1+w(x,y)^{(1,0)^2}+w(x,y)w(x,y)^{(2,0)}\right)+ \\ &\tau_w^{(0,1)}(x_t(x,y),y_t(x,y))\left(w(x,y)^{(1,0)}w(x,y)^{(0,1)}+w(x,y)^{(1,1)}\right) \\ &= n\frac{w(x,y)^{(1,0)^3}+w(x,y)^{(0,1)}w(x,y)^{(1,1)}+w(x,y)^{(1,0)}(1+w(x,y)^{(0,1)^2}+w(x,y)^{(2,0)})}{\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}} \\ &\tau_w^{(0,1)}(x_t(x,y),y_t(x,y))\left(1+w(x,y)^{(0,1)^2}+w(x,y)w(x,y)^{(0,2)}\right)+ \\ &\tau_w^{(1,0)}(x_t(x,y),y_t(x,y))\left(w(x,y)^{(1,0)}w(x,y)^{(0,1)}+w(x,y)^{(1,1)}\right) \\ &= n\frac{w(x,y)^{(0,1)^3}+w(x,y)^{(1,0)}w(x,y)^{(1,1)}+w(x,y)^{(0,1)}(1+w(x,y)^{(1,0)^2}+w(x,y)^{(0,2)})}{\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}} \end{aligned} \tag{297}$$

The Eqs. (297) define a system of linear equations regarding $\tau_w^{(1,0)}$ and $\tau_w^{(0,1)}$. Solving this system of linear equations leads to

$$\tau_w^{(1,0)}(x_t(x,y),y_t(x,y)) = n\frac{w(x,y)^{(1,0)}}{\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}}$$
$$\tau_w^{(0,1)}(x_t(x,y),y_t(x,y)) = n\frac{w(x,y)^{(0,1)}}{\sqrt{1+w^{(1,0)}(x,y)^2+w^{(0,1)}(x,y)^2}} \tag{298}$$

From Eqs. (298) follows directly

$$w^{(1,0)}(x,y) = \frac{\dfrac{\tau_w^{(1,0)}(x_t(x,y),y_t(x,y))}{n}}{\sqrt{1-\left(\dfrac{\tau_w^{(1,0)}(x_t(x,y),y_t(x,y))}{n}\right)^2-\left(\dfrac{\tau_w^{(0,1)}(x_t(x,y),y_t(x,y))}{n}\right)^2}}$$
$$w^{(0,1)}(x,y) = \frac{\dfrac{\tau_w^{(0,1)}(x_t(x,y),y_t(x,y))}{n}}{\sqrt{1-\left(\dfrac{\tau_w^{(1,0)}(x_t(x,y),y_t(x,y))}{n}\right)^2-\left(\dfrac{\tau_w^{(0,1)}(x_t(x,y),y_t(x,y))}{n}\right)^2}} \tag{299}$$

Inserting Eqs. (299) into Eq. (65) leads to the requested relation between the normal vector $\mathbf{n}_w(x_t,y_t)$ of the wavefront and its OPD $\tau_w(x_t,y_t)$. This relation is given by

$$\mathbf{n}_w(x_t,y_t) = \left(-\frac{\tau_w{}^{(1,0)}(x_t,y_t)}{n},-\frac{\tau_w{}^{(0,1)}(x_t,y_t)}{n},\sqrt{1-\left(\frac{\tau_w{}^{(1,0)}(x_t,y_t)}{n}\right)^2-\left(\frac{\tau_w{}^{(0,1)}(x_t,y_t)}{n}\right)^2}\right)^T \tag{300}$$

where $\tau_w{}^{(1,0)} = \partial\tau_w/\partial x_t$ and $\tau_w{}^{(0,1)} = \partial\tau_w/\partial y_t$.

In principle, we are interested in derivatives of $\mathbf{n}_w(x_t,y_t)$ with respect to x_t and y_t. Observing, however, that $\mathbf{n}_w(x_t,y_t)$ depends on x_t and y_t only via the slopes $\tau_w{}^{(1,0)}(x_t,y_t)$ and $\tau_w{}^{(0,1)}(x_t,y_t)$, it is very practical to concentrate on this dependence $\mathbf{n}_w(\tau_w{}^{(1,0)},\tau_w{}^{(0,1)})$ first and to deal with the inner dependence $\tau_w{}^{(1,0)}(x_t,y_t)$ and $\tau_w{}^{(0,1)}(x_t,y_t)$ later. To do this, we set $u \equiv \tau_w{}^{(1,0)}$ and $v \equiv \tau_w{}^{(0,1)}$ and to introduce the function

$$\mathbf{n}(u,v) := \begin{pmatrix} -\dfrac{u}{n} \\ -\dfrac{v}{n} \\ \sqrt{1-\left(u/n\right)^2-\left(v/n\right)^2} \end{pmatrix} \tag{301}$$

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

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

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

$$\mathbf{n}^{(3,0)}(0,0)=\mathbf{n}^{(2,1)}(0,0)=\mathbf{n}^{(1,2)}(0,0)=\mathbf{n}^{(0,3)}(0,0):=\mathbf{0},\ \mathbf{n}^{(4,0)}(0):=\frac{1}{n^4}\begin{pmatrix}0\\0\\-3\end{pmatrix},\ \text{etc.,} \tag{302}$$

In application on the functions of interest, $\mathbf{n}_w(x,y)=\mathbf{n}(\tau_{\rm o}^{(1,0)}(x_t,y_t))$ and this means that $\mathbf{n}_w(0,0)=(0,0,1)^T$. Further, the first derivatives are given by

$$\frac{\partial}{\partial x_t}\mathbf{n}_w(x_t,y_t)\bigg|_{x_t=0,y_t=0}\equiv\mathbf{n}_{\rm w}^{(1,0)}(0,0)=\mathbf{n}^{(1,0)}(0,0)\tau_{\rm o}^{(2,0)}(0,0)=\begin{pmatrix}-1\\0\\0\end{pmatrix}\frac{\tau_{\rm o}^{(2,0)}(0,0)}{n} \tag{303}$$

,

and similarly for the higher derivatives.

7.2.3. Ansatz for Determining the Propagation Equation

As shown in Figure 36 the vector $\mathbf{w}_o=\mathbf{w}_o(x_{\rm o},y_{\rm o})$ points to the neighboring ray's intersection point with the original wavefront, and the wavefront's OPD referred to the original wavefront along the ray is denoted by τ_o. Hence, the vector $\begin{pmatrix}x_{{\rm t}o}\\y_{{\rm t}o}\\0\end{pmatrix}$ pointing to the intersection point with the plane $z=0$, must be equal to the vector sum

$$\begin{pmatrix} x_o \\ y_o \\ w_o(y_o) \end{pmatrix} - \frac{\tau_o(x_{to}, y_{to})}{n}\mathbf{n}_w = \begin{pmatrix} x_{to} \\ y_{to} \\ 0 \end{pmatrix}. \tag{304}$$

Correspondingly the vector $\mathbf{w}_p = \mathbf{w}_p(y_{\mathrm{p}})$ points to the neighboring ray's intersection point with the propagated wavefront, and the wavefront's OPD referred to the propagated wavefront along the ray is denoted by τ_p. Hence, the vector $\begin{pmatrix} x_{\mathrm{tp}} \\ y_{\mathrm{tp}} \\ \frac{\tau}{n} \end{pmatrix}$ points to the intersection point with the plane $z = \frac{\tau}{n}$, must be equal to the vector sum

$$\begin{pmatrix} x_p \\ y_p \\ w_p(y_p) \end{pmatrix} - \frac{\tau_p(x_{\mathrm{tp}}, y_{\mathrm{tp}})}{n}\mathbf{n}_w = \begin{pmatrix} x_{\mathrm{tp}} \\ y_{\mathrm{tp}} \\ \frac{\tau}{n} \end{pmatrix}. \tag{305}$$

The vector from the original wavefront to the propagated surface is $\tau/n\,\mathbf{n}_w$. Hence, the vector to the point on the propagated wavefront itself, $\mathbf{w}_p$, must be equal to the vector sum $\mathbf{w}_p = \mathbf{w}_o + \tau/n\,\mathbf{n}_w$. This yields the fundamental equation:

$$\begin{pmatrix} x_{\mathrm{t}p} - x_{\mathrm{to}} \\ y_{\mathrm{t}p} - y_{\mathrm{to}} \\ \frac{\tau}{n} \end{pmatrix} = \frac{\tau + \tau_o(x_{\mathrm{to}}, y_{\mathrm{to}}) - \tau_p(x_{\mathrm{t}p}, y_{\mathrm{t}p})}{n}\mathbf{n}_w \tag{306}$$

The starting point for establishing the relations between the original and the propagated wavefront is now given by Eq. (306). This equation is analogous to Eq. (269), with the only difference that x and y components are simultaneously present.

The vector of unknown functions is now given by

$$\mathbf{p}(x_{\mathrm{tp}}, y_{\mathrm{tp}}) = \begin{pmatrix} x_{\mathrm{to}}(x_{\mathrm{tp}}, y_{\mathrm{tp}}) \\ y_{\mathrm{to}}(x_{\mathrm{tp}}, y_{\mathrm{tp}}) \\ w_p(x_{\mathrm{tp}}, y_{\mathrm{tp}}) \end{pmatrix} \tag{307}$$

and observing that the initial condition $\mathbf{p}(0,0) = \begin{pmatrix} 0 \\ 0 \\ \tau/n \end{pmatrix}$ has to be fulfilled.

Eq. (306), the 3D analogue to Eq. (269), leads now to

$$\mathbf{f}\left(\mathbf{p}(x_{\mathrm{tp}}, y_{\mathrm{tp}}), x_{\mathrm{tp}}, y_{\mathrm{tp}}\right) = \mathbf{0} \tag{308}$$

where $\mathbf{f}$ is the 3D analogue to Eq.(271).

The key ingredient of the method is that the relations between the derivatives of the OPD of the original and propagated wavefront can be obtained by the first, second, etc. total derivative of Eq. (308) with respect to x_{tp} and y_{tp}, evaluated in the origin. The advantage of the form of Eq. (308) is that the various terms can be tracked in a fairly compact manner.

The total derivative of $\mathbf{f}\left(\mathbf{p}(y_{\mathrm{tp}}), y_{\mathrm{tp}}\right)$ in Eq. (308) 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 $p_i(x_{\mathrm{tp}}, y_{\mathrm{tp}})$, plus the partial derivative of $\mathbf{f}$ with respect to the explicit dependence on x_{tp} and y_{tp}. This transforms the system of algebraic equations in Eq. (306) to the system of differential equations

One important difference compared to the 2D case is that there are two arguments with respect to which the derivatives have to be taken. This implies that the dimension of the linear problems to solve grows with increasing order: while there are only 3 different unknown functions, the first-order problem possesses already 6 unknown first-order derivatives, then there are 9 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

$$\begin{aligned} \mathbf{A}\left(\mathbf{p}(x_{\mathrm{tp}}, y_{\mathrm{tp}})\right)\mathbf{p}^{(1,0)}(x_{\mathrm{tp}}, y_{\mathrm{tp}}) &= \mathbf{b}_x \\ \mathbf{A}\left(\mathbf{p}(x_{\mathrm{tp}}, y_{\mathrm{tp}})\right)\mathbf{p}^{(0,1)}(x_{\mathrm{tp}}, y_{\mathrm{tp}}) &= \mathbf{b}_y \end{aligned} \tag{309}$$

where the different inhomogeneities are given as column vectors

$$\mathbf{b}_x = -\frac{\partial \mathbf{f}}{\partial x_{\mathrm{tp}}} = \begin{pmatrix} -1 & 0 & 0 \end{pmatrix}^T, \quad \mathbf{b}_y = -\frac{\partial \mathbf{f}}{\partial y_{\mathrm{tp}}} = \begin{pmatrix} 0 & -1 & 0 \end{pmatrix}^T. \tag{310}$$

The structure of $\mathbf{b}_x$ and $\mathbf{b}_y$ arises because the original and propagated wavefronts do not have a tilt.

The Jacobian matrix $\mathbf{A}(\mathbf{p}(x_{\mathrm{tp}}, y_{\mathrm{tp}}))$ with elements $A_{ij} := \partial f_i / \partial p_j$ is the same for both equations and analogous to Eq. (274) but now of size 3×3.

$$\mathbf{A}\big(\mathbf{p}(x_{\mathrm{p}},y_{\mathrm{p}})\big)=-\begin{pmatrix} 1+\frac{\tau_{\mathrm{o}}^{(1,0)}}{n}n_{w,x}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,x}^{(0,1)}\tau_{\mathrm{o}}^{(1,1)}+n_{w,x}^{(1,0)}\tau_{\mathrm{o}}^{(2,0)}) & \frac{\tau_{\mathrm{o}}^{(0,1)}}{n}n_{w,x}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,x}^{(0,1)}\tau_{\mathrm{o}}^{(0,2)}+n_{w,x}^{(1,0)}\tau_{\mathrm{o}}^{(1,1)}) & -\frac{n_{w,x}}{n} \\ \frac{\tau_{\mathrm{o}}^{(1,0)}}{n}n_{w,y}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,y}^{(0,1)}\tau_{\mathrm{o}}^{(1,1)}+n_{w,y}^{(1,0)}\tau_{\mathrm{o}}^{(2,0)}) & 1+\frac{\tau_{\mathrm{o}}^{(0,1)}}{n}n_{w,y}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,y}^{(0,1)}\tau_{\mathrm{o}}^{(0,2)}+n_{w,y}^{(1,0)}\tau_{\mathrm{o}}^{(1,1)}) & -\frac{n_{w,y}}{n} \\ \frac{\tau_{\mathrm{o}}^{(1,0)}}{n}n_{w,z}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,z}^{(0,1)}\tau_{\mathrm{o}}^{(1,1)}+n_{w,z}^{(1,0)}\tau_{\mathrm{o}}^{(2,0)}) & \frac{\tau_{\mathrm{o}}^{(0,1)}}{n}n_{w,z}+\frac{\tau+\tau_o-\tau_p}{n}(n_{w,z}^{(0,1)}\tau_{\mathrm{o}}^{(0,2)}+n_{w,z}^{(1,0)}\tau_{\mathrm{o}}^{(1,1)}) & -\frac{n_{w,z}}{n} \end{pmatrix} \tag{311}$$

7.2.4. Solutions for the General Propagation Equations

The direct solutions analogously to Eq. (278) are now given by

$$\begin{aligned}
&\mathbf{p}^{(1,0)}(0,0)=\mathbf{A}^{-1}\mathbf{b}_x\\
&\mathbf{p}^{(0,1)}(0,0)=\mathbf{A}^{-1}\mathbf{b}_y\\
&\mathbf{p}^{(2,0)}(0,0)=\left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_x\\
&\mathbf{p}^{(1,1)}(0,0)=\left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_x=\left(\mathbf{A}^{-1}\right)^{(1,0)}\Big|\mathbf{b}_y\\
&\mathbf{p}^{(0,2)}(0,0)=\left(\mathbf{A}^{-1}\right)^{(0,1)}\mathbf{b}_y\\
&\qquad\qquad\ldots\\
&\mathbf{p}^{(k_x,k_y)}(0,0)=\begin{cases}\left(\mathbf{A}^{-1}\right)^{(k_x-1,0)}\mathbf{b}_x & ,\quad k_x\neq 0,k_y=0\\ \left(\mathbf{A}^{-1}\right)^{(k_x-1,k_y)}\mathbf{b}_x=\left(\mathbf{A}^{-1}\right)^{(k_x,k_y-1)}\mathbf{b}_y & ,\quad k_x\neq 0,k_y\neq 0\\ \left(\mathbf{A}^{-1}\right)^{(0,k_y-1)}\mathbf{b}_y & ,\quad k_x=0,k_y\neq 0\end{cases}
\end{aligned} \tag{312}$$

where $\mathbf{A}^{-1}=\mathbf{A}(\mathbf{p}(0,0))^{-1}=\mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1,0)}=\frac{d}{dx_{\mathrm{tp}}}\mathbf{A}\big(\mathbf{p}(x_{\mathrm{tp}},y_{\mathrm{tp}})\big)^{-1}\Big|_{x_{\mathrm{tp}}=0,y_{\mathrm{tp}}=0}$,

$\left(\mathbf{A}^{-1}\right)^{(k_x,k_y)}=\frac{d^{k_x+k_y}}{dx_{\mathrm{tp}}^{k_x}dy_{\mathrm{tp}}^{k_y}}\mathbf{A}\big(\mathbf{p}(x_{\mathrm{tp}},y_{\mathrm{tp}})\big)^{-1}\Big|_{x_{\mathrm{tp}}=0,y_{\mathrm{tp}}=0}$, etc. The fact that there are two starting equations (309) 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. (308), for each $\mathbf{p}^{(k_x,k_y)}$ both 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. (281),(282) for the 2D case, we provide here the explicit results

$$\mathbf{A}(\mathbf{0})=\begin{pmatrix} -1+\frac{\tau\tau_{\text{o}}^{(2,0)}}{n^2} & \frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} & 0 \\ \frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} & -1+\frac{\tau\tau_{\text{o}}^{(0,2)}}{n^2} & 0 \\ 0 & 0 & \frac{1}{n} \end{pmatrix} \quad \mathbf{A}(\mathbf{0})^{-1}=\begin{pmatrix} \gamma\begin{pmatrix} -1+\frac{\tau\tau_{\text{o}}^{(0,2)}}{n^2} & -\frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} \\ -\frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} & -1+\frac{\tau\tau_{\text{o}}^{(2,0)}}{n^2} \end{pmatrix} & \begin{matrix} 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 & \quad 0 \end{matrix} & n \end{pmatrix} \tag{313}$$

with $\gamma=\frac{1/n}{\det(\mathbf{A}(\mathbf{0}))}=\frac{1}{1-(\frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2})^2-\frac{\tau\tau_{\text{o}}^{(2,0)}}{n^2}-\frac{\tau\tau_{\text{o}}^{(0,2)}}{n^2}+\frac{\tau^2\tau_{\text{o}}^{(2,0)}\tau_{\text{o}}^{(0,2)}}{n^4}}$

and after application of Eqs. (310),(312) the solutions

$$\mathbf{p}^{(1,0)}(0,0)=\gamma\begin{pmatrix} 1-\frac{\tau\tau_{\text{o}}^{(0,2)}}{n^2} \\ \frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} \\ 0 \end{pmatrix}, \qquad \mathbf{p}^{(0,1)}(0,0)=\gamma\begin{pmatrix} \frac{\tau\tau_{\text{o}}^{(1,1)}}{n^2} \\ 1-\frac{\tau\tau_{\text{o}}^{(2,0)}}{n^2} \\ 0 \end{pmatrix} \tag{314}$$

For the orders $k\geq 2$ we apply Eqs. (312). The derivatives $\mathbf{A}^{(1,0)}=\frac{d}{dx_{\text{tp}}}\mathbf{A}(\mathbf{p}(x_{tp},y_{\text{tp}}))\Big|_{x_{\text{tp}}=0,y_{\text{tp}}=0}$ etc. are directly obtained by total derivative of Eq. (311) with respect to x_{tp} and y_{tp}, evaluated for $x_{\text{tp}}=0$ and $y_{\text{tp}}=0$. For the orders $k\geq 2$ especially the results $\tau_{\text{p}}^{(k_x,k_y)}(0,0)$ for the propagated wavefront are interesting, therefore we directly provide those result. The resulting second-order law is (omitting the argument '(0)')

$$\begin{aligned} \tau_{\text{p}}^{(2,0)} &= \gamma\left(\tau\left(\frac{\tau_{\text{o}}^{(1,1)}}{n}\right)^2+\left(1-\tau\frac{\tau_{\text{o}}^{(0,2)}}{n^2}\right)\tau_{\text{o}}^{(2,0)}\right) \\ \tau_{\text{p}}^{(1,1)} &= \gamma\,\tau_{\text{o}}^{(1,1)} \\ \tau_{\text{p}}^{(0,2)} &= \gamma\left(\tau\left(\frac{\tau_{\text{o}}^{(1,1)}}{n}\right)^2+\left(1-\tau\frac{\tau_{\text{o}}^{(2,0)}}{n^2}\right)\tau_{\text{o}}^{(0,2)}\right) \end{aligned} \tag{315}$$

which are identical with the results of Eqs. (159) using Eqs. (324) to transform OPD aberrations to wavefront (saggita) aberrations.

If the coordinate axis coincides with the directions of principal curvature of the wavefront, which means that $\tau_{\text{o}}^{(1,1)}=0$, Eq. (315) can be simplified to

$$\begin{aligned}
\tau_{\mathrm{p}}^{(2,0)} &= \frac{1}{1-\dfrac{\tau\tau_{\mathrm{o}}^{(2,0)}}{n^2}}\tau_{\mathrm{o}}^{(2,0)} \\
\tau_{\mathrm{p}}^{(1,1)} &= 0 \\
\tau_{\mathrm{p}}^{(0,2)} &= \frac{1}{1-\dfrac{\tau\tau_{\mathrm{o}}^{(0,2)}}{n^2}}\tau_{\mathrm{o}}^{(0,2)}
\end{aligned} \tag{316}$$

The resulting higher-order laws can be written in a similar fashion. Now for the special case that the coordinate axis coincide with the directions of principal curvature of the wavefront the third-order law is

$$\begin{aligned}
\tau_{\mathrm{p}}^{(3,0)} &= \frac{1}{\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(2,0)}}{n^2}\right)^3}\tau_{\mathrm{o}}^{(3,0)} \\
\tau_{\mathrm{p}}^{(2,1)} &= \frac{1}{\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(2,0)}}{n^2}\right)^2\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(0,2)}}{n^2}\right)}\tau_{\mathrm{o}}^{(2,1)} \\
\tau_{\mathrm{p}}^{(1,2)} &= \frac{1}{\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(2,0)}}{n^2}\right)\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(0,2)}}{n^2}\right)^2}\tau_{\mathrm{o}}^{(1,2)} \\
\tau_{\mathrm{p}}^{(0,3)} &= \frac{1}{\left(1-\dfrac{\tau\tau_{\mathrm{o}}^{(0,2)}}{n^2}\right)^3}\tau_{\mathrm{o}}^{(0,3)}
\end{aligned} \quad . \tag{317}$$

8. Summary

In the present thesis we have developed a general method for generating refraction, propagation and reflection equations for local wavefront aberrations of any order under arbitrarily oblique incidence conditions, which are published in [25,26,27]. **The main advantage of the approach presented in this thesis is that it is based exclusively on <u>analytical</u> formulas which are novel.** This saves much computation time compared to numerical iteration routines which would otherwise be necessary for determining the higher order aberrations. These results include as a special case the well-known scalar Vergence equation as well as the Coddington equation and the classical Transfer equation (order $k=2$), **but <u>extend</u> these equations to aberrations of any arbitrary higher order $k>2$.**

For convenience, we have distinguished between the two-dimensional and the three-dimensional problem in deriving the refraction, propagation and reflection equations. we have provided the general formulism and for the orders $k \le 6$, we have provided explicit formulas for the resulting terms in the two-dimensional case.

In chapter 3 we have demonstrated <u>for the first time</u> the derivation of analytical refraction equations for Higher Order Aberrations and in chapter 6 the derivation of analytical reflection equations for Higher Order Aberrations. The refraction and reflection equations are relations between an incoming wavefront, a refractive or reflective surface and an outgoing or reflected 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, respectively. The general refraction equations are established as a sequence of analytical relations between these series coefficients. **We have been able to show that for each given order $k \ge 2$ 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 only aberrations of one single order k are present, then the generalization of the Coddington equation will be exact for that order k, which reads for the two-dimensional problem $E'_k \cos^k \varepsilon' = E_k \cos^k \varepsilon + \nu \cdot \overline{E}_k$ in case of refraction and in case of reflection $\overline{E}_k = \cos^{k-1} \varepsilon \left(E'_k{}' - E_k \right)$, and in the three-dimensional case the vector-valued version of which reads $\mathbf{C}'_k\, \mathbf{e}'_k = \mathbf{C}_k \mathbf{e}_k + \nu\, \overline{\mathbf{e}}_k$ for refraction and $\overline{\mathbf{e}}_k = \widetilde{\mathbf{C}}_k (\mathbf{e}'_k - \mathbf{e}_k)$ for reflection. These results include as a special case the well-known scalar Vergence equation as well as the Coddington equation (order $k=2$), but **<u>extend</u> these refraction equations to aberrations of any arbitrary higher order $k>2$ which is done for the first time and published in [25,27].**

It is important to note that the formalism presented in this work in general allows to determine each of the three surfaces (incoming wavefronts, refractive or reflective surface, outgoing or reflected wavefront) 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 or reflective surface are given and that the outgoing or reflected wavefront is to be determined, as we have illustrated by examples. However, the reverse problem can likewise be treated. As we have shown explicitly in examples, if the incoming and the outgoing or reflected wavefront are both given without deviation from an ideal sphere up to the order $k = 6$, our equations directly allow to determine the refractive or reflective surface necessary for this imagery.

In chapter 3 we have demonstrated <u>for the first time</u> the derivation of analytical propagation equations for Higher Order Aberrations. For propagation only analytical equations exist which are still restricted by some approximations. As is written by Dai et al [44], further study is necessary to obtain a unified formulation for wavefronts containing both low-order and high-order aberrations. **<u>In the present work we have succeeded to develop such a unified and novel analytical propagation method.</u>** These results include as a special case the classical scalar vertex correction formula as well as the well-known Transfer Matrix equation (order $k = 2$), but <u>extend</u> these propagation equations to aberrations of higher order $k > 2$ which is done for the first time and published in [26].

The propagation equations are relations between the original wavefront and the propagated wavefront. In detail, we have defined local aberrations of those two wavefronts in terms of local power series coefficients, which describe the wavefronts in a general coordinate systems aligned with the chief rays normal. The general propagation equations are established as a sequence of analytical relations between these series coefficients. **We have been able to show that for each given order $k \geq 2$ it is possible to assign one equation taken from that sequence whose leading-order terms represent a straightforward generalization of the Transfer 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 only aberrations of one single order k $(k > 2)$ are present, then the aberrations are not changed by propagation, which reads $E_{p,k} = E_{o,k}$ for the two-dimensional problem, and the vector-valued version of which reads $\mathbf{e}_{p,k} = \mathbf{e}_{o,k}$ in the three-dimensional case.

In chapter 4 we have demonstrated how to calculate the aberration coefficients in a rotated coordinate system directly from the original aberration coefficients. Also in this chapter we have derived the relation between the coefficients of Zernike series polynomials and the coefficients of power series polynomials. In Appendix A: Relation between sagitta derivatives and OPD derivatives" are equations provided for transforming wavefront (sagitta) aberrations to OPD aberrations. **The method, used in this thesis, has also the capability to derive directly the equations for Higher Order OPD aberrations. This is done exemplarily in the case of propagation in chapter 7 which is done for the first time.**

With the method developed in this work, it is now possible to calculate in an analytical way the local Higher Order Aberrations of the outgoing or reflected wavefront directly from the aberrations of the incoming wavefront and the refractive or reflective surface and the aberrations of the propagated wavefront from the aberrations of the original wavefront. Although our method is based on local techniques, it yields results which are by no means restricted to small apertures, as shown theoretically as well as in two examples.

9. Appendix

Appendix A: Relation between sagitta derivatives and OPD derivatives

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 Figure 16 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 $w_{\mathrm{In}}(y_{\mathrm{In}})$, the coordinate in the tangential plane is $\bar{y}_{\mathrm{t}}$ instead of $\bar{y}_{\mathrm{S}}$, and the wavefront's OPD is $\tau_w(\bar{y}_{\mathrm{t}})$ instead of $\tau(\bar{y}_{\mathrm{S}})$ (see Figure 37).

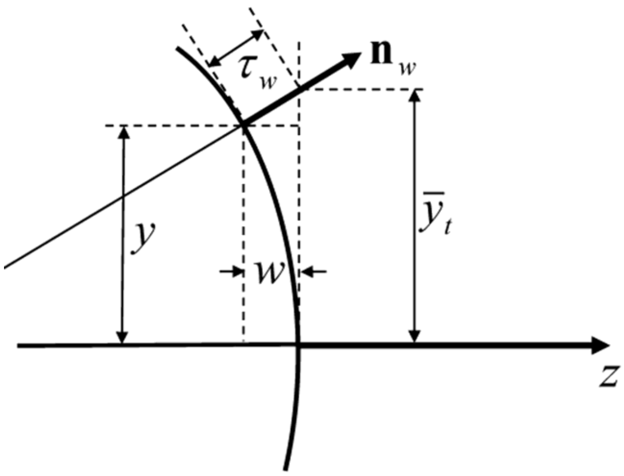

Figure 37: Relationship between the sagitta $w(y)$ of a wavefront and its OPD given by the function $\tau_w(\bar{y})$. There exists a unique relation between the aberration coefficients in terms of the wavefront (by the definition the sagitta derivatives) and the aberration coefficients in terms of the aberration function (to be defined as the OPD derivatives).

The first one of Eqs. (39) then takes the form

$$\begin{pmatrix} y \\ w(y) \end{pmatrix} - \frac{\tau_w}{n}\mathbf{n}_w = \begin{pmatrix} \bar{y}_{\mathrm{t}} \\ 0 \end{pmatrix}. \tag{318}$$

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. (318). Inserting $\mathbf{n}_w(y) = (-w^{(1)}(y),1)^T / \sqrt{1+w^{(1)}(y)^2}$ (see Eq. (36)), the second row of Eq. (318) can be solved for $\tau_w(\bar{y}_{\mathrm{t}}(y))$, yielding

$$\tau_w(\bar{y}_t(y)) = n\,w(y)\sqrt{1+w^{(1)}(y)^2}\;. \tag{319}$$

Inserting then Eq. (319) into the first row of Eq. (318) leads to

$$\bar{y}_t(y) = y + w(y)w^{(1)}(y)\;. \tag{320}$$

For obtaining a relationship between the derivatives $\tau_w^{(k)}(\bar{y}_t) \equiv \partial^k \tau_w / \partial \bar{y}_t^k$ and the derivatives $w^{(k)}(y)$, we insert Eq. (320) into the argument of τ_w in Eq. (319), yielding

$$\tau_w\left(y + w(y)w^{(1)}(y)\right) = n\,w(y)\sqrt{1+w^{(1)}(y)^2}\;. \tag{321}$$

As is generally the key ingredient in this thesis, we take now the subsequent derivatives of Eq. (321) and evaluate at the position $y = 0$. Making use of $w(0) = 0, w^{(1)}(0) = 0$, this leads to

$$\begin{aligned}
\tau_w(0) &= 0 \\
\tau_w^{(1)}(0) &= 0 \\
\tau_w^{(2)}(0) &= n\,w^{(2)}(0) \\
3w^{(2)}(0)^2\,\tau_w^{(1)}(0) + \tau_w^{(3)}(0) &= n\,w^{(3)}(0) \\
10w^{(2)}(0)w^{(3)}(0)\tau_w^{(1)}(0) + 12w^{(2)}(0)^2\,\tau_w^{(2)}(0) + \tau_w^{(4)}(0) &= n\left(6w^{(2)}(0)^3 + w^{(4)}(0)\right) \\
&\ldots,
\end{aligned} \tag{322}$$

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 $\tau_w^{(1)}(0)$ in the successive equations in Eq. (322), then the one for $\tau_w^{(2)}(0)$, and so on, yields the result (omitting the argument '(0)')

$$\begin{aligned}
\tau_w &= 0 \\
\tau_w^{(1)} &= 0 \\
\tau_w^{(2)} &= n\,w^{(2)} \\
\tau_w^{(3)} &= n\,w^{(3)} \\
\tau_w^{(4)} &= n\left(w^{(4)} - 6{w^{(2)}}^3\right) \\
\tau_w^{(5)} &= n\left(w^{(5)} - 40{w^{(2)}}^2 w^{(3)}\right) \\
&\ldots
\end{aligned} \tag{323}$$

Eq. (323) 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 $k \geq 4$, there occur more and more transformation terms. In the 3D case the procedure is analogous, and the result reads

$$
\begin{aligned}
&\tau_w = 0 \\
&\begin{pmatrix} \tau_w^{(1,0)} \\ \tau_w^{(0,2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\
&\begin{pmatrix} \tau_w^{(2,0)} \\ \tau_w^{(1,1)} \\ \tau_w^{(0,2)} \end{pmatrix} = n \begin{pmatrix} w^{(2,0)} \\ w^{(1,1)} \\ w^{(0,2)} \end{pmatrix} \\
&\begin{pmatrix} \tau_w^{(3,0)} \\ \tau_w^{(2,1)} \\ \tau_w^{(1,2)} \\ \tau_w^{(0,3)} \end{pmatrix} = n \begin{pmatrix} w^{(3,0)} \\ w^{(2,1)} \\ w^{(1,2)} \\ w^{(0,3)} \end{pmatrix} \\
&\begin{pmatrix} \tau_w^{(4,0)} \\ \tau_w^{(3,1)} \\ \tau_w^{(2,2)} \\ \tau_w^{(1,3)} \\ \tau_w^{(0,4)} \end{pmatrix} = n \left(\begin{pmatrix} w^{(4,0)} \\ w^{(3,1)} \\ w^{(2,2)} \\ w^{(1,3)} \\ w^{(0,4)} \end{pmatrix} - \begin{pmatrix} 6w^{(2,0)}\left(w^{(1,1)^2} + w^{(2,0)^2}\right) \\ 3w^{(1,1)}\left(w^{(1,1)^2} + w^{(2,0)}\left(w^{(0,2)} + 2w^{(2,0)}\right)\right) \\ \left(w^{(0,2)} + w^{(2,0)}\right)\left(5w^{(1,1)^2} + w^{(0,2)}w^{(2,0)}\right) \\ 3w^{(1,1)}\left(w^{(1,1)^2} + w^{(0,2)}\left(2w^{(0,2)} + w^{(2,0)}\right)\right) \\ 6w^{(0,2)}\left(w^{(1,1)^2} + w^{(0,2)^2}\right) \end{pmatrix} \right) \\
&\quad \ldots
\end{aligned}
\tag{324}
$$

For calculation of the relations between the OPD and saggita aberrations of the wavefront in the 2D case, the results of Eq. (323), describing the relations between sagitta derivatives and the OPD derivatives, can be transformed to relations between the wavefront and OPD aberrations, shown in Table 10.

Relation between OPD aberrations and Wavefront aberrations	
OPD aberration	Wavefront aberration
S^{OPD}	S
E_3^{OPD}	E_3
E_4^{OPD}	$E_4 - 6\frac{S^3}{n^2}$
E_5^{OPD}	$E_5 - 40\frac{S^2 E_3}{n^2}$

Table 10: Relation between OPD aberrations and wavefront aberrations up to order 5 in the 2D case. the results of Eq. (323), describing the relations between sagitta derivatives and the OPD derivatives, can be transformed to relations between the wavefront and OPD aberrations

Appendix B

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

$$\mathbf{r}_3 = \begin{pmatrix} 0 \\ -\dfrac{\sin\varepsilon\left(n\cos\varepsilon\, S'_{xx}\,(n^2 S'_{xx} - n'^2\, S) + n'\cos\varepsilon'(n' S^2 - n^2 (S'^2_{xx} + S\, S'_{yy} - S'_{xx}\, S'_{yy}))\right)}{nn'^2\,(n'\cos\varepsilon' - n\cos\varepsilon)} \\ 0 \\ -\dfrac{3\cos\varepsilon\cos\varepsilon'\sin\varepsilon\,(n'\cos\varepsilon\, S - n\cos\varepsilon'\, S'_{yy})(n'^2\, S - n^2 S'_{yy})}{nn'^2\,(n'\cos\varepsilon' - n\cos\varepsilon)} \end{pmatrix}. \qquad (325)$$

Appendix C

$$\mathbf{p}^{(1)}(y_\mathrm{p}) = \mathbf{A}(\mathbf{p}(y_\mathrm{p}))^{-1}\mathbf{b}\,. \tag{326}$$

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b} \\
\mathbf{p}^{(2)}(0) &= \left(\mathbf{A}^{-1}\right)^{(1)}\mathbf{b} \\
&\ldots \\
\mathbf{p}^{(k)}(0) &= \left(\mathbf{A}^{-1}\right)^{(k-1)}\mathbf{b},
\end{aligned} \tag{327}$$

where $\mathbf{A}^{-1} = \mathbf{A}(\mathbf{p}(0))^{-1} = \mathbf{A}(\mathbf{0})^{-1}$, and $\left(\mathbf{A}^{-1}\right)^{(1)} = \frac{d}{dy_\mathrm{p}}\mathbf{A}\left(\mathbf{p}(y_\mathrm{p})\right)^{-1}\Big|_{y_\mathrm{p}=0}$, …,

$$\left(\mathbf{A}^{-1}\right)^{(k-1)} = \frac{d^{k-1}}{dy_\mathrm{p}^{k-1}}\mathbf{A}\left(\mathbf{p}(\bar{y}_\mathrm{S})\right)^{-1}\Big|_{y_\mathrm{p}=0}$$

$$\begin{aligned}
\mathbf{A}\mathbf{p}^{(1)}(0) &= \mathbf{b} && \text{(a)} \\
\mathbf{A}^{(1)}\mathbf{p}^{(1)}(0) + \mathbf{A}\mathbf{p}^{(2)}(0) &= \mathbf{0} && \text{(b)} \\
\mathbf{A}^{(2)}\mathbf{p}^{(1)}(0) + 2\mathbf{A}^{(1)}\mathbf{p}^{(2)}(0) + \mathbf{A}\mathbf{p}^{(3)}(0) &= \mathbf{0} && \text{(c)} \\
&\ldots \\
\sum_{j=1}^{k}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0) &= \mathbf{0}, \quad k \ge 2 && \text{(d)}
\end{aligned} \tag{328}$$

$$\begin{aligned}
\mathbf{p}^{(1)}(0) &= \mathbf{A}^{-1}\mathbf{b}, && k = 1 \\
\mathbf{p}^{(k)}(0) &= -\mathbf{A}^{-1}\sum_{j=1}^{k-1}\binom{k-1}{j-1}\mathbf{A}^{(k-j)}\mathbf{p}^{(j)}(0), && k \ge 2.
\end{aligned} \tag{329}$$

Local Aberrations (our method)					
		Example A1		Example A2	
Radial order	Symbol	Original wavefront	Propagated wavefront	Original wavefront	Propagated wavefront
k		$value*m^{k-1}$	$value*m^{k-1}$	$value*m^{k-1}$	$value*m^{k-1}$
0	E	0	0	0	0
1	E_x	0	0	0	0
	E_y	0	0	0	0
2	E_{xx}	0	0	0	0
	E_{xy}	0	0	0	0
	E_{yy}	0	0	0	0
3	E_{xxx}	0	0	0	0
	E_{xxy}	0	0	-99.919	99.9191
	E_{xyy}	0	0	0	0
	E_{yyy}	0	0	-311.92	311.924
4	E_{xxxx}	-1.3049×10^{6}	-1.3049×10^{6}	50653	51253
	E_{xxxy}	0	0	0	0
	E_{xxyy}	-4.3498×10^{5}	-4.3498×10^{5}	19729	20752
	E_{xyyy}	0	0	0	0
	E_{yyyy}	-1.3049×10^{6}	-1.3049×10^{6}	68329	74167
5	E_{xxxxx}	0	0	0	0
	E_{xxxxy}	0	0	-1.9975×10^{6}	-2.6475×10^{6}
	E_{xxxyy}	0	0	0	0
	E_{xxyyy}	0	0	-2.1749×10^{6}	-2.9387×10^{6}
	E_{xyyyy}	0	0	0	0
	E_{yyyyy}	0	0	-1.1823×10^{7}	-1.6268×10^{7}
6	E_{xxxxxx}	1.0761×10^{10}	3.5133×10^{11}	1.6856×10^{9}	2.2744×10^{9}
	E_{xxxxxy}	0	0	0	0
	E_{xxxxyy}	2.1522×10^{9}	7.0266×10^{10}	4.6196×10^{8}	6.7583×10^{8}
	E_{xxxyyy}	0	0	0	0
	E_{xxyyyy}	2.1522×10^{9}	7.0266×10^{10}	6.0316×10^{8}	9.3213×10^{8}
	E_{xyyyyy}	0	0	0	0
	E_{yyyyyy}	1.0761×10^{10}	3.5133×10^{11}	3.8114×10^{9}	6.1388×10^{9}

Table 11: Values of the local aberrations based on our method before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) in examples A1 and A2.

Local Aberrations (our method)					
		Example B1		Example B2	
Radial order	Symbol	Original wavefront	Propagated wavefront	Original wavefront	Propagated wavefront
k		$value*m^{k-1}$	$value*m^{k-1}$	$value*m^{k-1}$	$value*m^{k-1}$
0	E	0	0	0	0
1	E_x	0	0	0	0
	E_y	0	0	0	0
2	E_{xx}	-21.669	-15.117	-41.247	-22.602
	E_{xy}	0	0	0	0
	E_{yy}	-21.669	-15.117	-50.877	-25.2174
3	E_{xxx}	0	0	0	0
	E_{xxy}	0	0	-749.20	-111.50
	E_{xyy}	0	0	0	0
	E_{yyy}	0	0	-3420.7	-416.53
4	E_{xxxx}	-1.2881×10^{6}	-3.0828×10^{5}	-8.1744×10^{5}	-87851
	E_{xxxy}	0	0	0	0
	E_{xxyy}	-4.2937×10^{5}	-1.0276×10^{5}	-4.5578×10^{5}	-37337
	E_{xyyy}	0	0	0	0
	E_{yyyy}	-1.2881×10^{6}	-3.0828×10^{5}	-2.3047×10^{6}	-1.4236×10^{5}
5	E_{xxxxx}	0	0	0	0
	E_{xxxxy}	0	0	-7.6008×10^{7}	-1.8204×10^{6}
	E_{xxxyy}	0	0	0	0
	E_{xxyyy}	0	0	-1.2692×10^{8}	-2.2713×10^{6}
	E_{xyyyy}	0	0	0	0
	E_{yyyyy}	0	0	-1.0583×10^{9}	-1.4054×10^{7}
6	E_{xxxxxx}	-5.0085×10^{10}	1.9658×10^{10}	-1.1937×10^{11}	-2.1245×10^{9}
	E_{xxxxxy}	0	0	0	0
	E_{xxxxyy}	-1.0017×10^{10}	3.9317×10^{9}	-4.9496×10^{10}	-5.7487×10^{8}
	E_{xxxyyy}	0	0	0	0
	E_{xxyyyy}	-1.0017×10^{10}	3.9317×10^{9}	-9.9092×10^{10}	-7.6601×10^{8}
	E_{xyyyyy}	0	0	0	0
	E_{yyyyyy}	-5.0085×10^{10}	1.9658×10^{10}	-9.6626×10^{11}	-5.0286×10^{9}

Table 12: Values of the local aberrations based on our method before propagation (Taylor wavefront sagitta representation of the original wavefront) and after propagation (Taylor wavefront sagitta representation of the propagated wavefront) in examples B1 and B2.

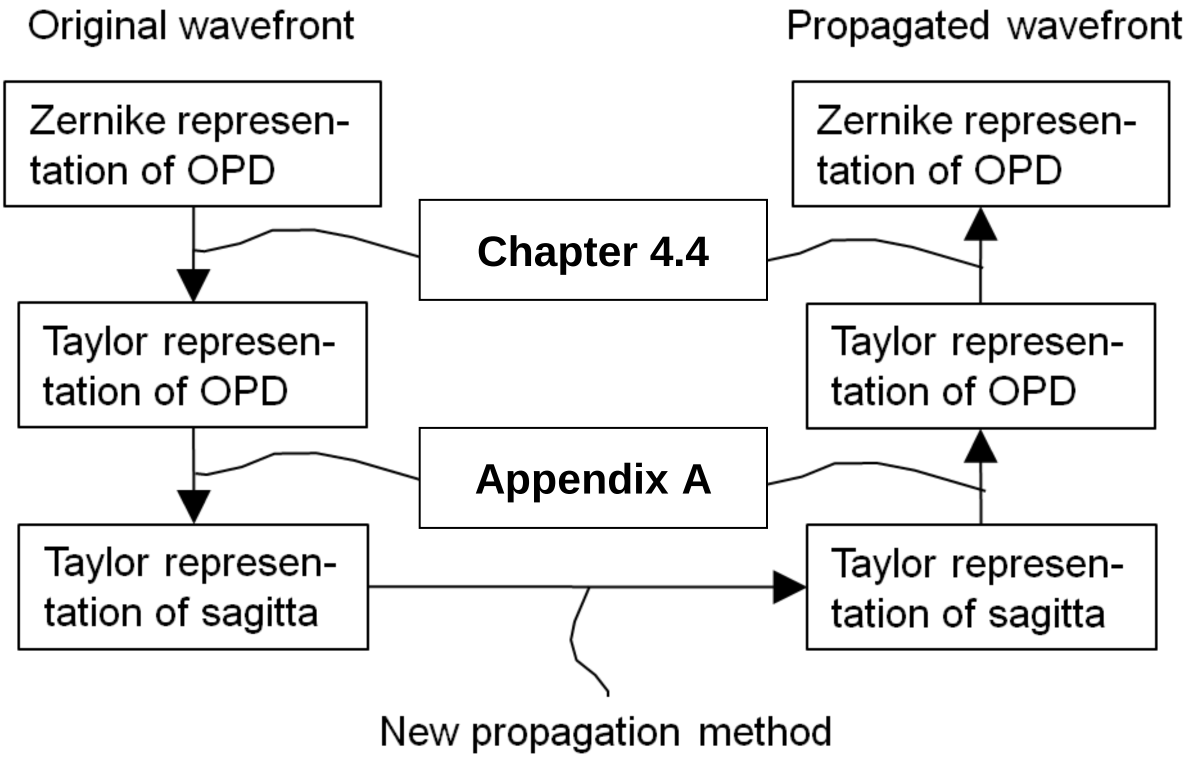

Figure 38: Logical flow of the computation of the Zernike coefficients of a propagated wavefront for given Zernike coefficients of the original wavefront by the derived analytical method.

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