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Alternative computation of the Seidel aberration coefficients using the Lie algebraic method

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We give a brief introduction to Hamiltonian optics and Lie algebraic methods. We use these methods to describe the operators governing light propagation, refraction, and reflection in phase space. The method offers a systematic way to find aberration coefficients of any order for arbitrary rotationally symmetric optical systems. The coefficients from the Lie method are linked to the Seidel aberration coefficients. Furthermore, the property of summing individual surface contributions is preserved by the Lie algebraic theory. Two examples are given to validate the proposed methodology with good results. © 2022 Optica Publishing Group

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1. INTRODUCTION

The calculation of Seidel aberrations of rotationally symmetric optical systems is well known in the optical design literature [1–3]. Seidel sums provide a clear insight into the contribution of each optical surface of the analyzed system to the third order transverse ray aberrations at the image plane. Some recently published methods determine aberration coefficients numerically in terms of ray data in pupil coordinates [4,5] or in phase space [6]. Alternatively, differences in optical path lengths can be measured via ray tracing [7] or the use of total aberration formulas [2,8] from which values of Zernike aberrations can be deduced. Most methods derive closed form expressions for aberration coefficients utilizing the expansion of ray-tracing equations [9–11] or of optical path length differences between the principal and a marginal ray [1–3].

In this paper, we aim to derive closed form expressions of the Seidel aberration coefficients using the Lie algebraic method. To this purpose, we present a concise introduction to the Lie algebraic method, pioneered and developed mainly by Dragt and Wolf [12–16], applied to geometrical optics. We also link this formulation to the widely known Seidel coefficients. In [15], a first step towards the classification of optical elements using the Lie method has been made.

We introduce the concept of a fundamental optical map in the framework of the Lie method. The map is composed of propagation from an intermediate object plane, refraction or reflection by a surface, and subsequent propagation to an intermediate image plane. We determine operators that approximate the analytic ray-tracing maps analogously to first order matrix formulation [1,2,17]. Additional operators that also take higher order phenomena into consideration will be calculated. The

Table 1. Correspondence between Matrix Formalism and the Lie Algebraic Method^a

	Matrix (First Order)	Lie (First Order)	Lie (Third Order)
Ray propagation	$\begin{pmatrix} I_{2 \times 2} & \frac{d}{n} I_{2 \times 2} \\ O_{2 \times 2} & I_{2 \times 2} \end{pmatrix}$	$\exp(-d[b_2, \cdot])$ (49)	$\exp(-d[b_4, \cdot])$ (49)
Refraction	$\begin{pmatrix} I_{2 \times 2} & O_{2 \times 2} \\ 2\beta(n - n') I_{2 \times 2} & I_{2 \times 2} \end{pmatrix}$	$\exp([g_2, \cdot])$ (55)	$\exp([g_4, \cdot])$ (57), (60)

^aThe third column contains maps that correspond to third order ray optics.

description of these maps will be discussed in the following sections, but to give the reader an idea, we refer to Table 1 to show the relations between the matrix method and the Lie maps. In Table 1, the matrix in the first column and the Lie map in the second column are equivalent. The map in the third column is an extension to higher order optics.

Additionally, by considering rotationally symmetric optical systems as a concatenation of fundamental optical elements, we will reduce the analysis of the complete system to the determination of the sole fundamental map, thus significantly simplifying the treatment of arbitrary rotationally symmetric systems.

The Lie approach provides a mathematical theory that enables us to systematically compute aberration coefficients of rotationally symmetric systems and link them to the well-known Seidel coefficients. It will be shown how the property of summing up individual surface contributions to the Seidel coefficients, as in traditional optical design theory [1,2], is a direct consequence of the presented mathematical framework.

In Sections 2 and 3, a brief description of geometrical optics and the Lie algebraic approach will be given. In Section 4, the

reader will find the methodology necessary to formulate propagation, refraction, and reflection within the context of the Lie algebraic method. The description of the fundamental element can be found in Section 5. An optical system can then be viewed as the concatenation of multiple optical elements as described in Section 6. The link between the Lie framework and the Seidel coefficients is presented in Section 7. Two examples to validate the presented method will be shown in Section 8 with very satisfactory results. Section 9 offers concluding observations and an outlook to future applications to off-axis systems.

2. CLASSICAL FORMULATION OF GEOMETRICAL OPTICS IN PHASE SPACE

In this section, we will summarize the classical theory of geometrical optics describing light propagation, refraction, and reflection. These results are what we aim to reproduce in Sections 4 and 5 with the use of Lie algebraic tools.

First, we describe free propagation of a light ray. Consider a general ray in three-dimensional space with coordinates (q_1, q_2, z) and let s represent the arc length along said ray. We can then describe the ray path using z as the propagation parameter for $q_1(z)$ and $q_2(z)$. The z axis will also be called the optical axis. Let \mathbf{P}^i and \mathbf{P}^f be the initial and final points, respectively, of a ray path \mathcal{C} ; then its optical path length is defined as

$$\text{OPL} = \int_{\mathcal{C}} n(\mathbf{q}, z) ds = \int_{z^i}^{z^f} n(\mathbf{q}, z) \sqrt{1 + |\dot{\mathbf{q}}|^2} dz, \quad (1)$$

where $\mathbf{q} = (q_1, q_2)$, $\mathbf{P}^i = \mathbf{P}^i(\mathbf{q}(z^i), z^i)$, $\mathbf{P}^f = \mathbf{P}^f(\mathbf{q}(z^f), z^f)$, and $n(\mathbf{q}, z)$ is the refractive index of the medium through which the ray propagates. Fermat's principle tells us that the ray path is a stationary point of Eq. (1) [18]. As such, the ray path satisfies the Euler–Lagrange equations [18]

$$\frac{\partial \mathcal{L}}{\partial \mathbf{q}} - \frac{d}{dz} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} = \mathbf{0}, \quad (2a)$$

with the Lagrangian \mathcal{L} given by

$$\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, z) = n(\mathbf{q}, z) \sqrt{1 + |\dot{\mathbf{q}}|^2}. \quad (2b)$$

The canonical conjugates of $\dot{\mathbf{q}}$, also called momenta, read

$$\mathbf{p} = \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}} = n(\mathbf{q}, z) \frac{\dot{\mathbf{q}}}{\sqrt{1 + |\dot{\mathbf{q}}|^2}}. \quad (3)$$

The conjugates $\mathbf{p} = (p_1, p_2)$ are the projections of the unit direction vector of the ray onto a plane $z = \text{const.}$, e.g., $z = 0$, times the refractive index. The Hamiltonian H is defined in terms of \mathcal{L} by the relation

$$H(\mathbf{q}, \mathbf{p}, z) = \mathbf{p} \cdot \dot{\mathbf{q}} - \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, z), \quad (4)$$

where $\dot{\mathbf{q}}$ is expressed in terms of $\mathbf{q}, \mathbf{p}, z$ through a Legendre transformation [18].

Combining the Lagrangian system Eq. (2) with the definition of \mathbf{p} and H in Eq. (3) and Eq. (4), respectively, we obtain

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}, \quad (5a)$$

where the Hamiltonian H is given by

$$H(\mathbf{q}, \mathbf{p}, z) = -\sqrt{n(\mathbf{q}, z)^2 - |\mathbf{p}|^2}. \quad (5b)$$

A ray is completely defined by its position and direction coordinates along the z axis. Hence, its initial values $(\mathbf{q}^i, \mathbf{p}^i)$ at the plane $z = z^i$ are related to its final coordinates at the plane $z = z^f$ by following the trajectory $(\mathbf{q}(z), \mathbf{p}(z), z)$ governed by the Hamiltonian system Eq. (5). From now on, we will refer to \mathbf{q}, \mathbf{p} as phase space variables. Let p_z be the z component of the unit direction vector along the ray, multiplied by the refractive index n . In an optical medium, it holds true that $n(\mathbf{q}(z), z) = |(\mathbf{p}(z), p_z(z))|$. As such, p_z can be defined as

$$p_z = \sqrt{n(\mathbf{q}, z)^2 - |\mathbf{p}|^2}, \quad (6)$$

and by substitution into Eq. (5b), we get $H = -p_z$. We consider propagation in only the positive z direction, since we assume rays to be traveling only forward. Furthermore, note that if the Hamiltonian is independent of z , then it is constant and thus also p_z is.

Next, we continue this section with the refraction of rays, where we will consider the refractive index to be constant within each respective medium. To this purpose, we introduce two quantities that are conserved at refraction: the position coordinates $\bar{\mathbf{q}}$ of the point of impact of the ray with the refracting surface and the tangential momentum $\bar{\mathbf{p}}$ at this point. We denote with the unprimed values (\mathbf{q}, \mathbf{p}) the phase space coordinates of the incoming ray, with $(\bar{\mathbf{q}}, \bar{\mathbf{p}})$ the conserved ray quantities at the refracting interface and with $(\mathbf{q}', \mathbf{p}')$ the phase space coordinates of the outgoing ray.

When compared to other ray quantities in geometrical optics, we have that the momenta \mathbf{p} and \mathbf{p}' are related to the incoming and outgoing ray angles, respectively. In fact,

$$|\mathbf{p}| = n \sin \theta \quad \text{and} \quad p_z = n \cos \theta, \quad (7)$$

where θ is the angle between the incoming ray and the optical axis. In Eq. (7), we find the relation between phase space coordinates and the more traditionally used ray angles for rotationally symmetric optical systems. Similarly, \mathbf{q} and \mathbf{q}' track the position of the ray along the optical axis, and $\bar{\mathbf{q}}$ is the incidence point of the ray at the optical surface. Information about other optical quantities as, for instance, incidence angles of rays on the surface can be deduced from the phase space coordinates we just introduced.

The position coordinates \mathbf{q} are measured by (back)propagating the ray onto the so-called standard screen defined by $z = 0$ (see Fig. 1). Let $z = \zeta(\mathbf{q})$ be the refracting surface, then the conservation of the point of impact is described through ray propagation:

$$\mathbf{q} + \zeta(\bar{\mathbf{q}}) \frac{\mathbf{p}}{p_z} = \bar{\mathbf{q}} = \mathbf{q}' + \zeta(\bar{\mathbf{q}}) \frac{\mathbf{p}'}{p'_z}. \quad (8)$$

This is the solution to the Hamiltonian system Eq. (5) in a medium of constant refractive index subject to $\mathbf{q}(0) = \mathbf{q}, \mathbf{p}(0) = \mathbf{p}$.

Note that the standard screen can be placed at any distance from the optical surface. However, the assumption that the

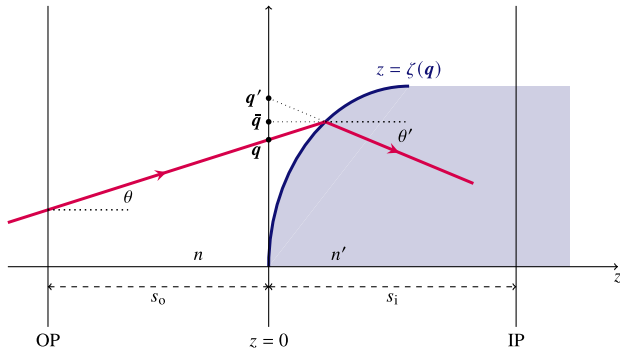


Fig. 1. Refraction at the surface $z = \zeta(\mathbf{q})$, where $n' > n$. Position coordinates are projected along the ray onto the standard screen $z = 0$. Intermediate object and image planes are displayed.

standard screen and the surface both intersect at $\mathbf{q} = \mathbf{0}$ simplifies the expressions in Eq. (8). Equation (8) states that by propagating from the standard screen to the surface in object space, or by propagating from the standard screen to the surface in image space, we reach the same point of impact $(\bar{\mathbf{q}}, \zeta(\bar{\mathbf{q}}))$ at the surface.

Conservation of tangential momentum can be described through the following cross product between the surface normal, to be taken opposite to the incoming rays, and the ray direction coordinates. Let $\nabla\zeta(\bar{\mathbf{q}})$ be the gradient of our refracting surface at the point of impact; then

$$\begin{pmatrix} \nabla\zeta(\bar{\mathbf{q}}) \\ -1 \end{pmatrix} \times \begin{pmatrix} \mathbf{p} \\ p_z \end{pmatrix} = \begin{pmatrix} \nabla\zeta(\bar{\mathbf{q}}) \\ -1 \end{pmatrix} \times \begin{pmatrix} \mathbf{p}' \\ p'_z \end{pmatrix}. \quad (9)$$

Equation (9) is the vectorial form of Snell's Law. The first two components give

$$\mathbf{p} + \nabla\zeta(\bar{\mathbf{q}})p_z = \bar{\mathbf{p}} = \mathbf{p}' + \nabla\zeta(\bar{\mathbf{q}})p'_z. \quad (10)$$

With the results in Eqs. (8) and (10), we can define the root transformation $\mathcal{R}_{n,\zeta}$ that acts upon the incident ray coordinates for a medium with refractive index n and gives us the conserved quantities $(\bar{\mathbf{q}}, \bar{\mathbf{p}})$ at the interface $z = \zeta(\mathbf{q})$ [14,16]:

$$\mathcal{R}_{n,\zeta} \mathbf{q} = \bar{\mathbf{q}} = \mathbf{q} + \zeta(\bar{\mathbf{q}}) \frac{\mathbf{p}}{\sqrt{n^2 - |\mathbf{p}|^2}}, \quad (11a)$$

$$\mathcal{R}_{n,\zeta} \mathbf{p} = \bar{\mathbf{p}} = \mathbf{p} + \nabla\zeta(\bar{\mathbf{q}}) \sqrt{n^2 - |\mathbf{p}|^2}. \quad (11b)$$

Note that these definitions are implicit, because the expression for $\bar{\mathbf{q}}$ is dependent on $\bar{\mathbf{q}}$ itself. Once the position coordinate of the point of impact is known, then the expression for $\bar{\mathbf{p}}$ can be computed explicitly. The root transformation $\mathcal{R}_{n',\zeta}$ is defined analogously to Eq. (11), but has the refracted phase space coordinates $(\mathbf{q}', \mathbf{p}')$ and the refractive index n' as arguments [see Eqs. (8) and (10)]. In this formulation, we can summarize the conservation at the point of impact as

$$\mathcal{R}_{n,\zeta} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \bar{\mathbf{q}} \\ \bar{\mathbf{p}} \end{pmatrix} = \mathcal{R}_{n',\zeta} \begin{pmatrix} \mathbf{q}' \\ \mathbf{p}' \end{pmatrix}. \quad (12)$$

The inverse transformation of $\mathcal{R}_{n',\zeta}$ is derived from Eqs. (8) and (10) by bringing to the other side the necessary terms and reads

$$\mathcal{R}_{n',\zeta}^{-1} \bar{\mathbf{q}} = \mathbf{q}' = \bar{\mathbf{q}} - \zeta(\bar{\mathbf{q}}) \frac{\bar{\mathbf{p}}}{\sqrt{n'^2 - |\bar{\mathbf{p}}|^2}}, \quad (13a)$$

$$\mathcal{R}_{n',\zeta}^{-1} \bar{\mathbf{p}} = \mathbf{p}' = \bar{\mathbf{p}} - \nabla\zeta(\bar{\mathbf{q}}) \sqrt{n'^2 - |\bar{\mathbf{p}}|^2}. \quad (13b)$$

This is again defined implicitly, since the expression for \mathbf{p}' is dependent on \mathbf{p}' itself. We are interested in the refraction mapping $S_{n,n',\zeta}$ between the incoming and outgoing phase space coordinates after refraction by the surface $z = \zeta(\mathbf{q})$ at the standard screen. This is achieved by combining the root transformations in Eq. (11) and their inverses in Eq. (13) into [13,14,19]

$$S_{n,n',\zeta} = \mathcal{R}_{n',\zeta}^{-1} \circ \mathcal{R}_{n,\zeta}. \quad (14)$$

At this point, we assume that the surface intersects the standard screen at the origin, i.e., $\zeta(\mathbf{0}) = 0$, and that the surface is tangential to the standard screen at the origin, i.e., $\nabla\zeta(\mathbf{0}) = \mathbf{0}$. The first assumption is without any loss of generality since the root transformations can be reformulated according to the position of the standard screen, which can therefore be moved freely along the z axis. The second assumption limits the possible surface representations to functions with no first order terms in their Taylor expansion at $\mathbf{q} = \mathbf{0}$. The motivation behind these assumptions will become apparent in the following sections, but the first immediate consequence is that the origin of phase space is mapped onto itself by $S_{n,n',\zeta}$, i.e., if $\mathbf{q} = \mathbf{0} = \mathbf{p}$, then $\mathbf{q}' = \mathbf{0} = \mathbf{p}'$.

The implicit form of the root transformations makes it necessary to compute them recursively up to the desired order of accuracy. We start with a fixed point iteration using $\bar{\mathbf{q}} = \mathbf{q}$ as our first guess. Solving Eq. (11a) iteratively allows us to find an expansion for $\bar{\mathbf{q}}$ up to the desired order. Substituting this result into Eq. (11b) gives us an expansion for $\bar{\mathbf{p}}$. We then proceed similarly to derive expansions of \mathbf{q}' , \mathbf{p}' in terms of $\bar{\mathbf{q}}$, $\bar{\mathbf{p}}$ using Eq. (13). Combining these results yields an expansion of the outgoing ray coordinates in terms of the incoming ones up to the desired order of accuracy. A rotationally symmetric refracting surface can be described by

$$z = \zeta(\mathbf{q}) = \beta|\mathbf{q}|^2 + \delta(|\mathbf{q}|^2)^2 + \dots \quad (15)$$

Here, β is half the curvature. If we consider the surface description in Eq. (15), then the third order expansion of $S_{n,n',\zeta}$ in Eq. (14) applied to the phase space variables of an incoming ray reads

$$\mathbf{q}' = \mathbf{q} + \beta \left(\frac{1}{n} - \frac{1}{n'} \right) |\mathbf{q}|^2 \mathbf{p} + 2\beta^2 \left(1 - \frac{n}{n'} \right) |\mathbf{q}|^2 \mathbf{q}, \quad (16a)$$

$$\begin{aligned} \mathbf{p}' = & \mathbf{p} + 2\beta(n - n')\mathbf{q} - \beta \left(\frac{1}{n} - \frac{1}{n'} \right) |\mathbf{p}|^2 \mathbf{q} \\ & + 2\beta^2 \left(1 - \frac{n'}{n} \right) |\mathbf{q}|^2 \mathbf{p} - 4\beta^2 \left(1 - \frac{n}{n'} \right) (\mathbf{p} \cdot \mathbf{q}) \mathbf{q} \\ & + 4(n - n') \left(\delta + \beta^3 \frac{n - n'}{n'} \right) |\mathbf{q}|^2 \mathbf{q}, \end{aligned} \quad (16b)$$

and is in agreement with [13,16]. The linear part of Eq. (16) describes refraction within the limits of Gaussian optics [17]. We will refer to the linear components of propagation and refraction as the Gaussian part of said mappings.

To illustrate the procedure, we will show the first steps necessary to derive the expressions in Eq. (16). We start by solving Eq. (11) up to third order using the surface expansion in Eq. (15). As previously noted, Eq. (11a) is implicit. The first order guess of the iterative process reads $\bar{\mathbf{q}} = \mathbf{q} + \mathcal{O}(2)$, where $\mathcal{O}(2)$ stands for terms of order two or higher in \mathbf{q}, \mathbf{p} . The second step therefore is to use the intermediate result $\bar{\mathbf{q}} = \mathbf{q} + \mathcal{O}(2)$ in Eq. (11a) and to expand the square root:

$$\begin{aligned}\bar{\mathbf{q}} &= \mathbf{q} + \zeta(\mathbf{q} + \mathcal{O}(2)) \frac{\mathbf{p}}{\sqrt{n^2 - |\mathbf{p}|^2}} \\ &= \mathbf{q} + (\beta|\mathbf{q} + \mathcal{O}(2)|^2 + \mathcal{O}(4)) \left(\frac{\mathbf{p}}{n} + \frac{|\mathbf{p}|^2}{2n^3} \mathbf{p} + \mathcal{O}(5) \right) \\ &= \mathbf{q} + \frac{\beta}{n} |\mathbf{q}|^2 \mathbf{p} + \mathcal{O}(4).\end{aligned}\quad (17)$$

Substituting Eq. (17) into Eq. (11b) gives, up to third order,

$$\bar{\mathbf{p}} = \mathbf{p} + 2\beta n \mathbf{q} + 2\beta^2 |\mathbf{q}|^2 \mathbf{p} - \frac{\beta}{n} |\mathbf{p}|^2 \mathbf{q} + 4n\delta |\mathbf{q}|^2 \mathbf{q} + \mathcal{O}(5).\quad (18)$$

Performing similar computations for Eq. (13) and combining them with the results in Eqs. (17) and (18) will result, up to third order, in the expressions given in Eq. (16).

In the case of a reflecting surface, similar calculations can be performed. The corresponding reflection relations read [14]

$$\begin{aligned}\mathbf{q} + \zeta(\bar{\mathbf{q}}) \frac{\mathbf{p}}{\sqrt{n^2 - |\mathbf{p}|^2}} &= \bar{\mathbf{q}} = \mathbf{q}' - \zeta(\bar{\mathbf{q}}) \frac{\mathbf{p}'}{\sqrt{n^2 - |\mathbf{p}'|^2}}, \\ \mathbf{p} + \nabla\zeta(\bar{\mathbf{q}}) \sqrt{n^2 - |\mathbf{p}|^2} &= \bar{\mathbf{p}} = \mathbf{p}' - \nabla\zeta(\bar{\mathbf{q}}) \sqrt{n^2 - |\mathbf{p}'|^2}.\end{aligned}\quad (19)$$

We notice that Eq. (19) considers a backpropagation of the reflected ray compared to Eq. (11). Following the steps presented in the case of refraction, expressions similar to Eq. (16) can be calculated. A way to promptly derive the reflection expansion from Eq. (16) is to substitute $n' = -n$ in Eq. (16) [19], but we encourage the reader to perform the calculations themselves to get better acquainted with the procedure. We will focus on the treatment of refractive optics, but each step made using Eq. (11) can be applied analogously to Eq. (19).

3. LIE ALGEBRAIC TOOLS

This section serves as a brief introduction to the theory of Lie algebraic tools needed to describe light propagation and refraction introduced in Section 2. We first define the Poisson bracket and the Lie algebra structure it generates for functions in phase space. Next, the concepts of Lie operators and Lie transformations are explained. Important results connecting Lie transformations and symplectic mappings are presented

together with some essential tools for the treatment of Lie transformation products. From this section onward, all functions in phase space are assumed to be sufficiently smooth for any differentiation they might be subjected to.

The Poisson bracket is an operator $[\cdot, \cdot]$ that maps any pair of functions f, g in (\mathbf{q}, \mathbf{p}) to a single function of (\mathbf{q}, \mathbf{p}) , denoted by $[f, g]$:

$$[f, g] := \sum_{i=1}^2 \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) = \frac{\partial f}{\partial \mathbf{q}} \cdot \frac{\partial g}{\partial \mathbf{p}} - \frac{\partial f}{\partial \mathbf{p}} \cdot \frac{\partial g}{\partial \mathbf{q}}.\quad (20)$$

The above definition of the Poisson bracket implies that $[q_i, p_j] = \delta_{ij}$. The Poisson bracket has the following properties:

$$[\alpha f + \beta g, h] = \alpha [f, h] + \beta [g, h] \quad (\text{linear in first component}),\quad (21a)$$

$$[f, \alpha g + \beta h] = \alpha [f, g] + \beta [f, h] \quad (\text{linear in second component}),\quad (21b)$$

$$[f, f] = 0 \quad (\text{alternating}),\quad (21c)$$

$$[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = 0 \quad (\text{Jacobi identity}).\quad (21d)$$

As a consequence of Eq. (21c), the Poisson bracket is also anti-symmetric, i.e., $[f, g] = -[g, f]$. Thus, the Poisson bracket turns the space of functions defined in phase space into Lie algebra [20].

Propagation and refraction as described in Section 2 are transformations of phase space variables. Let us therefore establish some mathematical concepts about these transformations. The transformation to new phase space variables $(\mathbf{q}, \mathbf{p}) \mapsto (\mathbf{Q}(\mathbf{q}, \mathbf{p}), \mathbf{P}(\mathbf{q}, \mathbf{p}))$ is said to be a canonical transformation, if it satisfies [12,14]

$$\begin{aligned}[Q_i, Q_j] &= [q_i, q_j] = 0 \\ [P_i, P_j] &= [p_i, p_j] = 0 \\ [Q_i, P_j] &= [q_i, p_j] = \delta_{ij}.\end{aligned}\quad (22)$$

Consequently, the value of Poisson brackets is preserved under canonical transformations [21]. We now collect the two sets of variables q_i, p_i and Q_i, P_i into a single set of four variables w_1, \dots, w_4 and W_1, \dots, W_4 , respectively, where

$$\mathbf{w} = (q_1, q_2, p_1, p_2)^T, \quad \mathbf{W} = (Q_1, Q_2, P_1, P_2)^T.\quad (23)$$

Using the notation of Eq. (23), the rules in Eq. (22) can be summarized by

$$[w_i, w_j] = J_{ij}, \quad \text{where } J = \begin{pmatrix} O_{2 \times 2} & I_{2 \times 2} \\ -I_{2 \times 2} & O_{2 \times 2} \end{pmatrix}.\quad (24)$$

The Poisson bracket operation Eq. (20) in terms of \mathbf{w} can be represented as

$$[f, g] = \sum_{k,l=1}^4 \frac{\partial f}{\partial w_k} J_{kl} \frac{\partial g}{\partial w_l} = \left(\frac{\partial f}{\partial \mathbf{w}} \right)^T J \frac{\partial g}{\partial \mathbf{w}}.\quad (25)$$

Let us consider a canonical transformation $\mathbf{w} \mapsto \mathbf{W}(\mathbf{w})$, which therefore satisfies Eq. (22). Combining the relations in Eq. (24) with the just introduced representation of the Poisson bracket in Eq. (25) yields

$$J_{ij} = [W_i, W_j] = \sum_{k,l=1}^4 \frac{\partial W_i}{\partial w_k} J_{kl} \frac{\partial W_j}{\partial w_l}. \quad (26)$$

Let M be the Jacobian matrix of the transformation from \mathbf{w} to \mathbf{W} , i.e.,

$$M_{ik}(\mathbf{w}) = \frac{\partial W_i}{\partial w_k}, \quad (27)$$

then according to Eq. (26), the following must hold:

$$MJM^T = J. \quad (28)$$

The relation in Eq. (28) means that the matrix M belongs to the symplectic group in four dimensions [12], which implies that the phase space transformation is volume preserving. Accordingly, the necessary and sufficient condition for a transformation to be canonical is for its Jacobian matrix to be symplectic, and a canonical transformation is therefore often called a symplectic map.

Let f and g be two functions in phase space. We define the linear Lie operator $[f, \cdot]$ associated with f acting on g as follows:

$$[f, \cdot]g = [f, g].$$

For instance, we have that $[q_1, \cdot] = \partial/\partial p_1$. If the argument of $[f, \cdot]$ is a vector-valued function \mathbf{g} , then it acts component-wise on \mathbf{g} . We now introduce the main Lie algebraic tool used in this work: the Lie transformation. The Lie transformation $\exp([f, \cdot])$ associated with f and generated by $[f, \cdot]$ is defined as

$$\exp([f, \cdot]) = \sum_{k=0}^{\infty} \frac{[f, \cdot]^k}{k!}. \quad (29)$$

The powers in Eq. (29) follow the recursive definition

$$[f, \cdot]^0 = I, \quad [f, \cdot]^k = [f, [f, \cdot]^{k-1}], \quad k = 1, 2, \dots$$

It can be proven that the Lie transformation associated with a function $f(\mathbf{q}, \mathbf{p})$ in phase space has the following properties for any differentiable functions g, h in phase space [14]:

$$\begin{aligned} \exp([f, \cdot])[g, h] &= [\exp([f, \cdot])g, \exp([f, \cdot])h], \\ &\text{(Conservation of Poisson bracket),} \end{aligned} \quad (30a)$$

$$\begin{aligned} \exp([f, \cdot])g(\mathbf{q}, \mathbf{p}) &= g(\exp([f, \cdot])\mathbf{q}, \exp([f, \cdot])\mathbf{p}). \\ &\text{(Action on function arguments).} \end{aligned} \quad (30b)$$

The motivation for introducing Lie transformations becomes clear with the following two theorems by Dragt and Finn [12], which are pivotal for the discussion to follow. They will allow us to establish a direct link between symplectic maps and their representation as Lie transformations. The first theorem ([12], Theorem 1) gives us a result regarding maps derived from Lie transformations for a given f of the form

$$W_i = \exp([f, \cdot])w_i. \quad (31)$$

Provided the series in Eq. (31) converges, the resulting map is symplectic [12]. In fact, using property Eq. (30a) of Lie transformations and their definition in Eq. (29), we have

$$\begin{aligned} [W_i, W_j] &= [\exp([f, \cdot])w_i, \exp([f, \cdot])w_j] \\ &= \exp([f, \cdot])[w_i, w_j] \\ &= \exp([f, \cdot])J_{ij} \\ &= J_{ij}, \end{aligned} \quad (32)$$

since $[f, \cdot]^k J_{ij} = 0$ for any $k \neq 0$. The result in Eq. (32) states that maps of the form Eq. (31) are symplectic. Conversely, the second theorem ([12], Theorem 2) gives us a sufficient condition for representing symplectic maps in terms of Lie transformations. Suppose that each component of a symplectic map $\mathbf{w} \mapsto \mathbf{W}(\mathbf{w})$ allows for a representation as

$$W_i = \sum_{|\sigma|>0} a_i(\sigma)w^\sigma, \quad (33)$$

where σ denotes a 4-tuple of exponents in \mathbb{N} , and

$$|\sigma| = \sum_{k=1}^4 \sigma_k, \quad w^\sigma = w_1^{\sigma_1} w_2^{\sigma_2} w_3^{\sigma_3} w_4^{\sigma_4}. \quad (34)$$

Then, W_i can be represented as an infinite product of Lie transformations:

$$W_i = (\exp([g_2, \cdot]) \exp([g_3, \cdot]) \cdots) w_i, \quad (35)$$

where the generators g_2, g_3 , etc., are homogeneous polynomials in the variables w_i of degree 2,3, etc. Here, we omit the concatenation symbol \circ , as it is clear from the context that we are concatenating operators. Recall that a homogeneous polynomial $p_m(\mathbf{w})$ of degree m satisfies the following condition:

$$p_m(\lambda \mathbf{w}) = \lambda^m p_m(\mathbf{w}) \quad (36)$$

for every $\lambda \in \mathbb{R}$. Note that the symplectic map described in Eq. (33) maps the origin of phase space onto itself, i.e., $\mathbf{W}(\mathbf{0}) = \mathbf{0}$. The core information to be taken from these two theorems is that any analytic symplectic map of the form Eq. (33) can be represented as an infinite product of Lie transformations with homogeneous polynomials as generators and that the truncated product is still a symplectic map, since it is a product of symplectic maps [12].

We conclude this section with some results that are necessary for the derivations in the sections to follow. The first is the Baker–Campbell–Hausdorff (BCH) formula [12]. Given two functions g and f , the function k satisfying

$$\exp([k, \cdot]) = \exp([g, \cdot]) \exp([f, \cdot]) \quad (37a)$$

is given by

$$k = g + f + [g, f]/2 + ([g, [g, f]] + [f, [f, g]])/12 + \dots \quad (37b)$$

If f and g commute, i.e., $[f, g] = 0$, then we have that

$$\exp([g, \cdot]) \exp([f, \cdot]) = \exp([g + f, \cdot]). \quad (38)$$

Note that the Lie transformation associated with a constant generates only the identity operator. Thus, the inverse of a Lie transformation follows from Eq. (38):

$$\exp(-[f, \cdot]) \exp([f, \cdot]) = \exp([f, \cdot]) \exp(-[f, \cdot]) = I. \quad (39)$$

From Eq. (39), we deduce that

$$\exp([f, \cdot])^{-1} = \exp(-[f, \cdot]). \quad (40)$$

The second Lie algebraic tool of relevance is the following result, which will facilitate considerably the treatment of products of Lie transformations. Theorem 3 of Dragt and Finn [12] states that for any two Lie operators $[f, \cdot]$ and $[g, \cdot]$, we have that

$$\begin{aligned} \exp([f, \cdot]) \exp([g, \cdot]) \exp(-[f, \cdot]) &= \exp([k, \cdot]), \\ k &= \exp([f, \cdot])g. \end{aligned} \quad (41)$$

This implies that whenever we have three Lie transformations as on the left-hand side of Eq. (41), it is then possible to exactly compute their concatenation without the need of the BCH formula.

Lastly, we make a remark about the order of approximation that we will consider in this work. All the expansions of phase space variables will be performed up to third order terms, i.e., $|\sigma| \leq 3$ in Eq. (34). This decision imposes some restrictions on the degree of the generators g_2, g_3, \dots of the Lie transformations in Eq. (44). All stems from the observation that if we consider the space \mathcal{P}_m spanned by monomials of degree $m \geq 1$, then for $f \in \mathcal{P}_m$ and $g \in \mathcal{P}_n$, we have that

$$[f, g] \in \mathcal{P}_{m+n-2}. \quad (42)$$

As such, if we decide to consider polynomial expansions in phase space only up to third order, then we can restrict the degree of homogeneous polynomials in Eq. (35) to four. Any Lie transformation whose associated polynomial is of a degree higher than four will generate terms of orders higher than three and can therefore be neglected. As another consequence of property Eq. (42), Lie transformations associated with homogeneous polynomials of second degree do not change the degree of their arguments. In fact, $f \in \mathcal{P}_2$ means that $m = 2$, and therefore, for any $g \in \mathcal{P}_n$, we have $[f, g] \in \mathcal{P}_n$. Thus, Lie transformations with second degree generators can be represented by linear transformations when applied to phase space variables, i.e., $n = 1$. We will refer to these Lie transformations as the Gaussian part of the mapping.

4. LIE ALGEBRAIC FORMULATION OF GEOMETRICAL OPTICS IN PHASE SPACE

Using the results in Section 3, we will describe how to formulate the propagation and refraction shown in Section 2 in terms of Lie transformations. All the results that follow are calculated up to third order terms in the phase space variable expansions for rotationally symmetric optical systems.

We start by proving that the Hamiltonian defined in Eq. (5b) is the generator of the solution of free propagation in a medium of constant refractive index. First, note that the Hamiltonian system Eq. (5a) can be represented in terms of Poisson brackets:

$$\dot{\mathbf{q}} = -[H, \mathbf{q}], \quad \dot{\mathbf{p}} = -[H, \mathbf{p}]. \quad (43)$$

Using the notation of Eq. (23), we can use the even more compact representation

$$\dot{\mathbf{w}} = -[H, \mathbf{w}]. \quad (44)$$

Consider the Taylor expansion of \mathbf{w} at the final image screen $z = z^f$:

$$\mathbf{w}(z^f) = \mathbf{w}(z^i) + \sum_{m=1}^{\infty} \frac{1}{m!} (z^f - z^i)^m \left. \frac{d^m \mathbf{w}}{dz^m} \right|_{z=z^i}. \quad (45)$$

We know from Eq. (44) that

$$\begin{aligned} \frac{d\mathbf{w}}{dz} &= -[H, \cdot]\mathbf{w}, \\ \frac{d^2\mathbf{w}}{dz^2} &= -[H, \cdot] \frac{d\mathbf{w}}{dz} = (-[H, \cdot])^2 \mathbf{w}, \\ &\dots, \\ \frac{d^m \mathbf{w}}{dz^m} &= (-[H, \cdot])^m \mathbf{w}. \end{aligned} \quad (46)$$

Upon substitution of Eq. (46) into the Taylor expansion Eq. (45), we get the series representation of a Lie transformation as in Eq. (29) with the Hamiltonian H as the generator. This means that the mapping \mathcal{M} , such that $\mathbf{w}(z^f) = \mathcal{M}(\mathbf{w}(z^i))$ and which is a solution to Eq. (44), is defined as

$$\mathcal{M} = \exp(-(z^f - z^i)[H, \cdot]). \quad (47)$$

Given the result of Eq. (47), we have that free propagation from a standard screen at $z = z^i$ to a standard screen at $z = z^f$ is described by

$$\exp(-(z^f - z^i)[H, \cdot])\mathbf{q} = \mathbf{q} + (z^f - z^i) \frac{\mathbf{p}}{\sqrt{n^2 - |\mathbf{p}|^2}}, \quad (48a)$$

$$\exp(-(z^f - z^i)[H, \cdot])\mathbf{p} = \mathbf{p}. \quad (48b)$$

The solution in Eq. (48) is in agreement with Eq. (8). Note that the Hamiltonian can be expanded as follows:

$$\begin{aligned} -H &= \sqrt{n^2 - |\mathbf{p}|^2} = n - \frac{|\mathbf{p}|^2}{2n} - \frac{(|\mathbf{p}|^2)^2}{8n^3} - \dots \\ &= -b_0 - b_2(\mathbf{p}) - b_4(\mathbf{p}) - \dots \end{aligned} \quad (49)$$

Thus, the transit through a slab of thickness d made of a homogeneous medium with refractive index n can alternatively be written as an infinite product of Lie transformations:

$$\begin{aligned} \mathcal{M} &= \exp\left(d \left[\sqrt{n^2 - |\mathbf{p}|^2}, \cdot \right]\right) \\ &= \exp(-d/(2n)[|\mathbf{p}|^2, \cdot]) \exp(-d/(8n^3)[(|\mathbf{p}|^2)^2, \cdot]) \dots \\ &= \exp(-d[b_2, \cdot]) \exp(-d[b_4, \cdot]) \dots \end{aligned} \quad (50)$$

The identity in Eq. (50) holds because the generators in the sole variable $|\mathbf{p}|^2$, present in the expansion Eq. (49), commute by the

property Eq. (21c), and therefore the BCH formula Eq. (37) is significantly simplified [see Eq. (38)]. The term h_0 clearly does not generate any Lie transformation other than identity.

Lastly, recall that by the argument following from Eq. (42), the linear part of the mapping \mathcal{M} is entirely generated by h_2 . The linear, or Gaussian, part of the mapping therefore reads

$$\mathcal{M}_G = \exp(-d[h_2, \cdot]). \tag{51}$$

Evaluating the map in Eq. (51) gives

$$\exp(-d[h_2, \cdot])\mathbf{w} = \begin{pmatrix} I_{2 \times 2} & \frac{d}{n} I_{2 \times 2} \\ O_{2 \times 2} & I_{2 \times 2} \end{pmatrix} \mathbf{w}, \tag{52}$$

which is equal to the propagation matrix in the conventional matrix formulation of Gaussian optics [17]. In fact, the traditional matrix formulation uses position coordinates and ray angles times the refractive index to trace the rays. Since the momenta \mathbf{p} are the sines of the ray angles times the refractive index, momenta and the angles themselves times refractive index are equal in the setting of Gaussian optics, i.e., first order expansions where $\sin \theta \approx \theta$.

We now turn our attention to the refraction mapping described in Eq. (16). The optical surface is given by Eq. (15), where terms of order higher than four will not influence the third order aberrations. Thus we consider only

$$z = \zeta(\mathbf{q}) = \beta|\mathbf{q}|^2 + \delta(|\mathbf{q}|^2)^2. \tag{53}$$

$$\begin{aligned} \begin{pmatrix} \mathbf{q}_{g_4}(\mathbf{q}, \mathbf{p}) \\ \mathbf{p}_{g_4}(\mathbf{q}, \mathbf{p}) \end{pmatrix} &= \exp([g_4, \cdot]) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} + \begin{pmatrix} [g_4, \mathbf{q}] \\ [g_4, \mathbf{p}] \end{pmatrix} + \mathcal{O}(w^5) \\ &= \begin{pmatrix} \mathbf{q} - 4A|\mathbf{p}|^2\mathbf{p} - B(2(\mathbf{p} \cdot \mathbf{q})\mathbf{p} + |\mathbf{p}|^2\mathbf{q}) - 2C(\mathbf{p} \cdot \mathbf{q})\mathbf{q} - 2D|\mathbf{q}|^2\mathbf{p} - E|\mathbf{q}|^2\mathbf{q} \\ \mathbf{p} + B|\mathbf{p}|^2\mathbf{p} + 2C(\mathbf{p} \cdot \mathbf{q})\mathbf{p} + 2D|\mathbf{p}|^2\mathbf{q} + E(2(\mathbf{p} \cdot \mathbf{q})\mathbf{q} + |\mathbf{q}|^2\mathbf{p}) + 4F|\mathbf{q}|^2\mathbf{q} \end{pmatrix} + \mathcal{O}(w^5), \end{aligned} \tag{58}$$

The root transformations $\mathcal{R}_{n;\zeta}$, $\mathcal{R}_{n';\zeta}$ are canonical as long as the considered ray lies in the Descartes sphere $|\mathbf{p}|^2 < n^2$ and intersects the surface [13,14,16]. Consequently, their inverses are canonical too. Thus, the refraction mapping $\mathcal{S}_{n,n';\zeta}$ is canonical since it is a composition of canonical operators [13,14]. Furthermore, under the appropriate conditions on the surface, i.e., $\zeta(\mathbf{0}) = 0$, $\nabla\zeta(\mathbf{0}) = \mathbf{0}$, the phase space origin is mapped onto itself. As such, the results of Eq. (35) can be applied [15]. It is now a matter of finding the appropriate homogeneous polynomials that generate the mapping. We can already make a few statements. Since in this paper we will restrict ourselves to the treatment of third order aberrations by considering only third order expansion terms, any Lie transformations generated by homogeneous polynomials of degree five or higher can be neglected. Additionally, we will consider rotationally symmetric systems. This implies that the polynomials themselves can depend only on the variables $|\mathbf{p}|^2$, $|\mathbf{q}|^2$, $\mathbf{p} \cdot \mathbf{q}$, and $\mathbf{p} \times \mathbf{q}$ [14,15,22]. Since $\mathbf{p} \times \mathbf{q}$ is a preserved quantity in rotationally symmetric systems, we will omit it. As such, refraction can be associated only with polynomials of even degree, and we will now search for the two polynomials g_2, g_4 such that the product of the associated Lie transformations applied to our initial phase space variables reproduces the results in Eq. (16) up to third order, i.e.,

$$\mathbf{w}' = \exp([g_2, \cdot]) \exp([g_4, \cdot])\mathbf{w} + \mathcal{O}(w^5), \tag{54}$$

where w^5 is defined according to Eq. (34), and the \mathcal{O} terms are to be considered in each component of the vector \mathbf{w}' . It can be verified [13,15,16] that Gaussian refraction is associated with

$$g_2(\mathbf{q}, \mathbf{p}) = \beta(n - n')|\mathbf{q}|^2, \tag{55}$$

where 2β is the curvature of the surface at the origin [see Eq. (53)]. The corresponding linear transformation modifies the initial variables according to

$$\begin{aligned} \exp([g_2, \cdot]) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} &= \begin{pmatrix} I_{2 \times 2} & O_{2 \times 2} \\ 2\beta(n - n')I_{2 \times 2} & I_{2 \times 2} \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{q} \\ \mathbf{p} + 2\beta(n - n')\mathbf{q} \end{pmatrix}, \end{aligned} \tag{56}$$

which corresponds to the Gaussian part in Eq. (16) and also to the conventional matrix formulation of refraction in Gaussian optics [17].

Next, let us consider the third order transverse ray aberrations as being associated with a fourth degree polynomial $g_4(\mathbf{q}, \mathbf{p})$ of the general form

$$\begin{aligned} g_4(\mathbf{q}, \mathbf{p}) &= A(|\mathbf{p}|^2)^2 + B(\mathbf{p} \cdot \mathbf{q})|\mathbf{p}|^2 + C(\mathbf{p} \cdot \mathbf{q})^2 \\ &\quad + D|\mathbf{p}|^2|\mathbf{q}|^2 + E(\mathbf{p} \cdot \mathbf{q})|\mathbf{q}|^2 + F(|\mathbf{q}|^2)^2. \end{aligned} \tag{57}$$

The generated transformation up to third order reads

where we need only the first two terms of the exponential series of g_4 and use that $[g_4, \mathbf{q}] = -\partial g_4/\partial \mathbf{p}$, $[g_4, \mathbf{p}] = \partial g_4/\partial \mathbf{q}$. In fact, any subsequent term is of order greater than three and can be omitted. We now concatenate the two transformations in Eq. (54) to find

$$\begin{aligned} &\exp([g_2, \cdot]) \exp([g_4, \cdot]) \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \\ &= \exp([g_2, \cdot]) \begin{pmatrix} \mathbf{q}_{g_4}(\mathbf{q}, \mathbf{p}) \\ \mathbf{p}_{g_4}(\mathbf{q}, \mathbf{p}) \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{q}_{g_4}(\exp([g_2, \cdot])\mathbf{q}, \exp([g_2, \cdot])\mathbf{p}) \\ \mathbf{p}_{g_4}(\exp([g_2, \cdot])\mathbf{q}, \exp([g_2, \cdot])\mathbf{p}) \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{q}' \\ \mathbf{p}' \end{pmatrix}. \end{aligned} \tag{59}$$

Here we used the property of “jumping into arguments” of Lie transformations described in Eq. (30b). Thus, the operations in Eq. (59) tell us to substitute $\mathbf{q} \rightarrow \exp([g_2, \cdot])\mathbf{q} = \mathbf{q}$ and $\mathbf{p} \rightarrow \exp([g_2, \cdot])\mathbf{p} = \mathbf{p} + 2\beta(n - n')\mathbf{q}$ into Eq. (58). Comparing the resulting polynomials with the expressions in Eq. (16), we get the following results for coefficients A, \dots, F in Eq. (57), which are consistent with [13,16]:

$$\begin{aligned}
A &= 0, \quad B = 0, \quad C = 0, \\
D &= \frac{\beta}{2} \left(\frac{1}{n'} - \frac{1}{n} \right), \quad E = 2\beta^2 \left(1 - \frac{n'}{n} \right), \\
F &= \delta(n - n') - 2\beta^3 \frac{(n - n')^2}{n}.
\end{aligned} \tag{60}$$

We have now fully determined the generators of free propagation in a homogeneous medium [see Eqs. (49) and (50)] and refraction by a rotationally symmetric surface [see Eqs. (54), (55), (57), and (60)]. The coefficients of the generating polynomials are completely defined by the geometric parameters of the underlying system. Before concluding this section, note that in Eq. (58), the coefficient F of g_4 is the only one that does not influence the final position coordinates, and A does not influence the final direction coordinates.

5. FUNDAMENTAL REFRACTOR ELEMENT

With the description of free propagation and refraction up to third order, we now aim to describe what may be the most fundamental refractive optical element: a single refractive surface. The resulting map \mathcal{M} will be split into a Gaussian and a higher order part. Once we have developed the treatment for one surface, the extension to rotationally symmetric refractive optical systems will be straightforward.

We split refraction through an optical interface into three steps: propagation from the object to the interface, refraction at the interface, and propagation of the refracted ray to the image plane (see Fig. 1). The object and image distances will be denoted by s_o and s_i , respectively, and they satisfy the Gaussian imaging condition [17]

$$\frac{n}{s_o} + \frac{n'}{s_i} = \frac{n' - n}{R}, \tag{61}$$

where $R = (2\beta)^{-1}$ is the radius of curvature of the interface. By combining the results in Eqs. (49), (50), (55), and (60), the symplectic mapping \mathcal{M} with generators up to fourth degree for a single refracting optical element reads

$$\begin{aligned}
\mathcal{M} &= \underbrace{\exp\left(-\frac{s_o}{2n} [|\mathbf{p}|^2, \cdot]\right) \exp\left(-\frac{s_o}{8n^3} [(|\mathbf{p}|^2)^2, \cdot]\right)}_{\text{propagation from object plane}} \\
&\quad \times \underbrace{\exp(\beta(n - n') [|\mathbf{q}|^2, \cdot]) \exp([g_4, \cdot])}_{\text{refraction}} \\
&\quad \times \underbrace{\exp\left(-\frac{s_i}{2n'} [|\mathbf{p}|^2, \cdot]\right) \exp\left(-\frac{s_i}{8n'^3} [(|\mathbf{p}|^2)^2, \cdot]\right)}_{\text{propagation to image plane}},
\end{aligned} \tag{62}$$

where g_4 is completely defined by the coefficients in Eq. (60). Using Lie algebra techniques described in Section 3, it is possible to express Eq. (62) in the product form

$$\mathcal{M} \approx \mathcal{M}_G \exp([t_4, \cdot]), \tag{63}$$

where \mathcal{M}_G contains all information regarding the Gaussian approximation, and t_4 contains all the higher order aberration information of the complete fundamental element (up to third order transverse ray aberrations). Generators of degree five or higher are omitted, since their action on the arguments generates terms of order four or higher.

By considering only the contributions of the Gaussian part \mathcal{M}_G in Eq. (63), we recover the traditional matrix formulation for refraction of rays at an interface [17], where

$$\begin{aligned}
\mathcal{M}_G &= \exp\left(-\frac{s_o}{2n} [|\mathbf{p}|^2, \cdot]\right) \exp(\beta(n - n') [|\mathbf{q}|^2, \cdot]) \\
&\quad \times \exp\left(-\frac{s_i}{2n'} [|\mathbf{p}|^2, \cdot]\right).
\end{aligned} \tag{64}$$

Since matrices do not commute and do not “jump into arguments” like Lie transformations, their order needs to be inverted compared to the associated Lie transformations’ product. Using the matrix representations given in Eqs. (52) and (56), we rewrite the operator in Eq. (64) as

$$\begin{aligned}
\mathcal{M}_G &= \begin{pmatrix} I_{2 \times 2} & \frac{s_o}{n'} I_{2 \times 2} \\ O_{2 \times 2} & I_{2 \times 2} \end{pmatrix} \begin{pmatrix} I_{2 \times 2} & O_{2 \times 2} \\ 2\beta(n - n') I_{2 \times 2} & I_{2 \times 2} \end{pmatrix} \\
&\quad \times \begin{pmatrix} I_{2 \times 2} & \frac{s_i}{n} I_{2 \times 2} \\ O_{2 \times 2} & I_{2 \times 2} \end{pmatrix}.
\end{aligned} \tag{65}$$

Let us introduce the dioptric power of a surface $\mathcal{D} = (n' - n)/R$ and magnification $m = -ns_i/(n's_o)$, and recall that $2\beta = 1/R$, where R is the radius of curvature of the surface [17]. Then the Gaussian imaging condition Eq. (61) turns Eq. (65) into

$$\mathcal{M}_G = \begin{pmatrix} -\frac{ns_i}{n's_o} I_{2 \times 2} & O_{2 \times 2} \\ -\mathcal{D} I_{2 \times 2} & -\frac{n's_o}{ns_i} I_{2 \times 2} \end{pmatrix} = \begin{pmatrix} m I_{2 \times 2} & O_{2 \times 2} \\ -\mathcal{D} I_{2 \times 2} & \frac{1}{m} I_{2 \times 2} \end{pmatrix}. \tag{66}$$

The matrix in Eq. (66) represents the traditional matrix formulation of Gaussian optics [17].

To group the Gaussian parts together, we have to apply some manipulations to the original mapping \mathcal{M} . We use the result of Eq. (40) to insert identity operators. Thus, we “create” triplets that enable the use of Eq. (41). We simplify the notation by substituting the generators of propagation to the object plane $-s_o[b_2, \cdot]$, $-s_o[b_4, \cdot]$, the generators of refraction $[g_2, \cdot]$, $[g_4, \cdot]$, and the generators of propagation to the image plane $-s_i[b'_2, \cdot]$, $-s_i[b'_4, \cdot]$. Here, the subscript represents the degree of the respective homogeneous polynomial, and the b' polynomials take into consideration the image space refractive index n' [cf. Eq. (49)]. We rewrite Eq. (62) as

$$\begin{aligned}
 \mathcal{M} &= \exp(-s_o[b_2, \cdot]) \exp(-s_o[b_4, \cdot]) \exp([g_2, \cdot]) \exp([g_4, \cdot]) \\
 &\quad \times \exp(-s_i[b'_2, \cdot]) \exp(-s_i[b'_4, \cdot]) \\
 &= \exp(-s_o[b_2, \cdot]) \exp([g_2, \cdot]) \exp(-s_i[b'_2, \cdot]) \\
 &\quad \times \exp(s_i[b'_2, \cdot]) \exp(-[g_2, \cdot]) \exp(-s_o[b_4, \cdot]) \\
 &\quad \times \exp([g_2, \cdot]) \exp([g_4, \cdot]) \exp(-s_i[b'_2, \cdot]) \exp(-s_i[b'_4, \cdot]) \\
 &= \mathcal{M}_G \\
 &\quad \times \exp(s_i[b'_2, \cdot]) \exp(-[g_2, \cdot]) \exp(-s_o[b_4, \cdot]) \\
 &\quad \times \exp([g_2, \cdot]) \exp([g_4, \cdot]) \\
 &\quad \times \exp(-s_i[b'_2, \cdot]) \exp(-s_i[b'_4, \cdot]).
 \end{aligned} \tag{67}$$

We rewrite the mapping in Eq. (67) and insert one more time an identity operator of the form $I = \exp(-s_i[b'_2, \cdot]) \exp(s_i[b'_2, \cdot])$:

$$\begin{aligned}
 \mathcal{M} &= \mathcal{M}_G \\
 &\quad \times \exp(s_i[b'_2, \cdot]) \exp(-[g_2, \cdot]) \exp(-s_o[b_4, \cdot]) \\
 &\quad \times \exp([g_2, \cdot]) \exp(-s_i[b'_2, \cdot]) \\
 &\quad \times \exp(s_i[b'_2, \cdot]) \exp([g_4, \cdot]) \exp(-s_i[b'_2, \cdot]) \\
 &\quad \times \exp(-s_i[b'_4, \cdot]).
 \end{aligned} \tag{68}$$

In Eq. (68), there are multiple instances in which we can apply the result given in Eq. (41): twice in the second and third line and once in the fourth one. This leads to

$$\mathcal{M} = \mathcal{M}_G \exp(-s_o[\tilde{h}_4, \cdot]) \exp([\tilde{g}_4, \cdot]) \exp(-s_i[b'_4, \cdot]), \tag{69}$$

where \tilde{h}_4 and \tilde{g}_4 are given by

$$\begin{aligned}
 \tilde{h}_4 &= -s_o \exp(s_i[b'_2, \cdot]) \exp(-[g_2, \cdot]) b_4, \\
 \tilde{g}_4 &= \exp(s_i[b'_2, \cdot]) g_4.
 \end{aligned} \tag{70}$$

Recall that Lie transformations associated with homogeneous polynomials of second degree do not change the degree of their arguments, and hence, \tilde{h}_4, \tilde{g}_4 are of degree four. The last necessary step to derive the desired expression Eq. (63) is to apply the BCH formula Eq. (37) to combine the three fourth degree Lie transformations into one. This step is straightforward, since Poisson brackets between fourth degree generators are generating homogeneous polynomials of degree six or higher and can therefore be neglected; see the discussion at the end of Section 3. It follows from Eq. (69), that we can write t_4 in Eq. (63) as

$$t_4 = -s_o \tilde{h}_4 + \tilde{g}_4 - s_i b'_4. \tag{71}$$

After explicitly performing the computations given in Eqs. (70) and (71), we denote with A^*, \dots, F^* the coefficients of t_4 , analogous to the representation of g_4 in Eq. (57), and find

$$\begin{cases}
 A^* = -\frac{s_o}{8n^3} m^4 + \frac{s_i^2}{n^2} D - \frac{s_i^3}{n^2} E + \frac{s_i^4}{n^4} F - \frac{s_i}{8n^3}, \\
 B^* = -\frac{s_o D}{2n^3} m^3 - 2\frac{s_i}{n} D + 3\frac{s_i^2}{n^2} E - 4\frac{s_i^3}{n^3} F, \\
 C^* = -\frac{s_o D^2}{2n^3} m^2 - 2\frac{s_i}{n} E + 4\frac{s_i^2}{n^2} F, \\
 D^* = -\frac{s_o D^2}{4n^3} m^2 + D - \frac{s_i}{n} E + 2\frac{s_i^2}{n^2} F, \\
 E^* = -\frac{s_o D^3}{2n^3} m + E - 4\frac{s_i}{n} F, \\
 F^* = -\frac{s_o D^4}{8n^3} + F,
 \end{cases} \tag{72}$$

where D, E, F are defined in Eq. (60). It is now possible to represent our fundamental element in the form Eq. (63) with the Gaussian part described by Eq. (64), or equivalently Eq. (66), and the fourth degree polynomial defined by its coefficients in Eq. (72).

We conclude this section with a brief comment about higher order aberrations. The methods described in Sections 4 and 5 allow for further investigation of the aberrations of optical interfaces. The derivation of generating polynomials of order six and higher, which correspond to transverse ray aberrations of order five and higher, follows the same steps as described so far. It needs to be noted that the composition of operators via the BCH formula becomes increasingly more complicated as lower order aberrations compose into higher order contributions in addition to the intrinsic aberrations of the surface. For instance, composing the generators of third order aberrations will lead to additional contributions to the generators of fifth order aberrations. The necessary machinery needed for these computations is, however, already contained in the mathematical framework of the Lie algebraic method.

6. OPTICAL SYSTEMS

With the results of Section 5, it is possible to concatenate multiple fundamental elements into a complete optical system. The necessary tools have already been presented and used in the previous sections.

A rotationally symmetric refractive optical system is simply a composition of fundamental elements as described in Section 5. We therefore consider an optical system with k interfaces. Each interface can be described in up to fourth order terms by its coefficients $\beta_j, \delta_j, j = 1, \dots, k$ according to

$$z = \zeta_j(\mathbf{q}) = \beta_j |\mathbf{q}|^2 + \delta_j (|\mathbf{q}|^2)^2, \quad j = 1, \dots, k. \tag{73}$$

With the surface Eq. (73) at the vertex of each surface, we can determine the paraxial quantities. At each interface j , the Gaussian imaging conditions are satisfied:

$$\frac{n_j}{s_{o,j}} + \frac{n_{j+1}}{s_{i,j}} = \frac{n_{j+1} - n_j}{R_j}. \tag{74}$$

In Eq. (74), it holds that $2\beta_j = R_j^{-1}$. The additional quantities necessary for the calculations are

$$m_j = -\frac{n_j s_{i,j}}{n_{j+1} s_{o,j}}, \quad s_{o,j+1} = d_j - s_{i,j}, \quad D_j = \frac{n_{j+1} - n_j}{R_j}, \tag{75}$$

where m_j is the magnification of the optical surface j , D_j its dioptric power, $c_j = 1/R_j$ its curvature, and d_j the distance between interface j and interface $j + 1$ along the optical axis.

As previously shown, we can derive a symplectic mapping that describes ray propagation up to operators generated by fourth degree polynomials. We divide the contribution of each interface j into a second degree, \mathcal{M}_{G_j} , and fourth degree, $\exp([\sigma_j, \cdot])$, contribution. Here, σ_j is a fourth degree polynomial whose coefficients are completely defined by the geometry of the interface j and the system according to Eq. (72). Let us denote with \mathcal{M} the symplectic map describing ray propagation through our optical system up to fourth order; then we have

$$\begin{aligned} \mathcal{M} = & \mathcal{M}_{G_1} \exp([\sigma_1, \cdot]) \mathcal{M}_{G_2} \exp([\sigma_2, \cdot]) \cdots \mathcal{M}_{G_{k-1}} \\ & \times \exp([\sigma_{k-1}, \cdot]) \mathcal{M}_{G_k} \exp([\sigma_k, \cdot]). \end{aligned} \quad (76)$$

Similar to previous discussions, we want all second degree components, which describe the paraxial regime, to be grouped together. We introduce the notation

$$\mathcal{M}_{G_{1 \rightarrow j}} = \mathcal{M}_{G_1} \cdots \mathcal{M}_{G_j}, \quad j = 2, \dots, k. \quad (77)$$

The operator describing the Gaussian propagation of the complete system will be denoted by $\mathcal{M}_{G_{1 \rightarrow k}}$. Using the notation introduced in Eq. (77), the following holds true:

$$\begin{aligned} \mathcal{M} = & \mathcal{M}_{G_{1 \rightarrow k}} (\mathcal{M}_{G_{2 \rightarrow k}})^{-1} \exp([\sigma_1, \cdot]) \mathcal{M}_{G_{2 \rightarrow k}} (\mathcal{M}_{G_{3 \rightarrow k}})^{-1} \\ & \times \exp([\sigma_2, \cdot]) \mathcal{M}_{G_{3 \rightarrow k}} (\mathcal{M}_{G_{4 \rightarrow k}})^{-1} \\ & \times \exp([\sigma_3, \cdot]) \cdots \mathcal{M}_{G_k} \exp([\sigma_k, \cdot]). \end{aligned} \quad (78)$$

The mappings in Eqs. (76) and (78) are equivalent, but in Eq. (78), it is possible to apply multiple times the identity given in Eq. (41). We define σ_j^* such that

$$\begin{aligned} \exp([\sigma_j^*, \cdot]) = & (\mathcal{M}_{G_{j+1 \rightarrow k}})^{-1} \\ & \times \exp([\sigma_j, \cdot]) \mathcal{M}_{G_{j+1 \rightarrow k}} \quad j = 1, \dots, k-1. \end{aligned} \quad (79)$$

The mapping \mathcal{M} can therefore be rewritten as

$$\begin{aligned} \mathcal{M} = & \mathcal{M}_{G_{1 \rightarrow k}} \exp([\sigma_1^*, \cdot]) \exp([\sigma_2^*, \cdot]) \cdots \exp([\sigma_{k-1}^*, \cdot]) \\ & \times \exp([\sigma_k, \cdot]). \end{aligned} \quad (80)$$

A computationally convenient procedure to compute σ_j^* is to consider that $\mathcal{M}_{G_{j+1 \rightarrow k}}$ can be treated as both a Lie transformation and a matrix—beware of the inversion of concatenation order when composing the matrices instead of the Lie transformations. Applying the result in Eq. (41) to the definition in Eq. (79) gives

$$\sigma_j^* = (\mathcal{M}_{G_{j+1 \rightarrow k}})^{-1} \sigma_j. \quad (81)$$

The function σ_j is a fourth degree homogeneous polynomial in \mathbf{q} and \mathbf{p} , i.e., $\sigma_j(\mathbf{q}, \mathbf{p})$. Using the property of “jumping into arguments” in Eq. (30b), we rewrite Eq. (81) as

$$\sigma_j^*(\mathbf{q}, \mathbf{p}) = \sigma_j((\mathcal{M}_{G_{j+1 \rightarrow k}})^{-1} \mathbf{q}, (\mathcal{M}_{G_{j+1 \rightarrow k}})^{-1} \mathbf{p}). \quad (82)$$

The action of $(\mathcal{M}_{G_{j+1 \rightarrow k}})^{-1}$ on the phase space variables in Eq. (82) can be described via the associated matrix, and finding

the coefficients of $\sigma_j^*(\mathbf{q}, \mathbf{p})$ reduces to expanding and grouping terms on the right-hand side of Eq. (82). All the σ_j^* and σ_k are homogeneous polynomials of fourth degree since the Gaussian parts of the mapping do not change the degree of their arguments. We claim that these fourth degree polynomials contain the necessary information regarding the Seidel sums, as will be proven in the coming section, and therefore, the expressions in Eqs. (79) and (80) tell us that the aberrations of each fundamental element are propagated through the system via the Gaussian mappings of the subsequent elements.

We conclude this section by stating that the symplectic map \mathcal{M} given in Eq. (80) can be approximated up to fourth degree generators by

$$\mathcal{M} \approx \mathcal{M}_{G_{1 \rightarrow k}} \exp([\tau, \cdot]). \quad (83)$$

With the BCH formula Eq. (37) and the fact that higher degree polynomials can be neglected, we get

$$\tau = \sum_{j=1}^{k-1} \sigma_j^* + \sigma_k. \quad (84)$$

A physical interpretation as to why the form in Eq. (83) might be desirable is that the Gaussian part $\mathcal{M}_{G_{1 \rightarrow k}}$ acts first on both the phase space coordinates and subsequently also on the Lie transformations by the “jumping into arguments” property. At this point, we are left with a mapping defined on the Gaussian image space variables, which applies aberrations to these coordinates. To summarize, we first propagate through the complete system to the Gaussian image space via $\mathcal{M}_{G_{1 \rightarrow k}}$ and then aberrate. Since aberrations are traditionally given with respect to Gaussian coordinates [1,2], the ordering in Eq. (83) comes naturally.

7. LIE TRANSFORMATIONS AND SEIDEL SUMS

The performance of an optical system is often investigated by computing its Seidel coefficients [1,2]. These coefficients completely describe the third order transverse ray aberrations of monochromatic light through a rotationally symmetric refractive system [1,2]. In this section, we will show the relation between the coefficients of the fourth degree polynomial τ derived in Eq. (84) and the Seidel aberration coefficients. Furthermore, it will be shown how the property of summing Seidel contributions over all interfaces is a direct consequence of the described mathematical framework.

We start by recalling, that the wavefront aberration expansion is traditionally given in exit pupil and Gaussian image position coordinates [1,2]. Transverse ray aberration in the Lie approach is instead given in terms of the Gaussian phase space coordinates. We therefore need to be able to express the Gaussian momentum coordinates in terms of the exit pupil coordinates \mathbf{q}' and the Gaussian image position coordinates \mathbf{q}_G . Up to first order, we can express the Gaussian momentum coordinate \mathbf{p}_G as follows:

$$\mathbf{p}_G = \frac{n}{R_S} (\mathbf{q}_G - \mathbf{q}'). \quad (85)$$

Here, n and R_S refer to the refractive index and exit pupil distance with respect to the last image plane, respectively. This

means that $n = n_{k+1}$. Similar to [23], we consider aberrations to be departures from the ideal Gaussian image point. As such, third order aberrations are the difference at the ideal image plane between the third order position coordinates $\mathbf{q}^{(3)} = \mathcal{M}_{G_1 \rightarrow k} \exp([\tau, \cdot])\mathbf{q}$ and the Gaussian position coordinates $\mathbf{q}_G = \mathcal{M}_{G_1 \rightarrow k} \mathbf{q}$. The full third order aberration expansion reads

$$\begin{aligned} \Delta \mathbf{q}^{(3)} &= \exp([\tau(\mathbf{q}_G, \mathbf{p}_G), \cdot])\mathbf{q}_G - \mathbf{q}_G + \mathcal{O}(w^5) \\ &= [\tau, \mathbf{q}_G] + \mathcal{O}(w^5) \\ &= -4A_\tau |\mathbf{p}_G|^2 \mathbf{p}_G - B_\tau (2(\mathbf{p}_G \cdot \mathbf{q}_G) \mathbf{p}_G + |\mathbf{p}_G|^2 \mathbf{q}_G) \\ &\quad - 2C_\tau (\mathbf{p}_G \cdot \mathbf{q}_G) \mathbf{q}_G - 2D_\tau |\mathbf{q}_G|^2 \mathbf{p}_G - E_\tau |\mathbf{q}_G|^2 \mathbf{q}_G + \mathcal{O}(w^5), \end{aligned} \tag{86}$$

where A_τ, \dots, E_τ are the coefficients of τ as defined in Eq. (84). As in Eq. (58), we notice that F_τ does not influence the position coordinates. Substituting the identity Eq. (85) into Eq. (86) will yield an expression dependent on exit pupil and Gaussian image coordinates that is derived from the Lie approach:

$$\begin{aligned} \Delta \mathbf{q}^{(3)} &= \left(4 \frac{n^3}{R_S^3} A_\tau\right) |\mathbf{q}'|^2 \mathbf{q}' + \left(-8 \frac{n^3}{R_S^3} A_\tau - 2 \frac{n^2}{R_S^2} B_\tau\right) (\mathbf{q}' \cdot \mathbf{q}_G) \mathbf{q}' \\ &\quad + \left(4 \frac{n^3}{R_S^3} A_\tau + 2 \frac{n^2}{R_S^2} B_\tau + 2 \frac{n}{R_S} D_\tau\right) |\mathbf{q}_G|^2 \mathbf{q}' \\ &\quad + \left(-4 \frac{n^3}{R_S^3} A_\tau - \frac{n^2}{R_S^2} B_\tau\right) |\mathbf{q}'|^2 \mathbf{q}_G \\ &\quad + \left(8 \frac{n^3}{R_S^3} A_\tau + 4 \frac{n^2}{R_S^2} B_\tau + 2 \frac{n}{R_S} C_\tau\right) (\mathbf{q}' \cdot \mathbf{q}_G) \mathbf{q}_G \\ &\quad + \left(-4 \frac{n^3}{R_S^3} A_\tau - 3 \frac{n^2}{R_S^2} B_\tau - 2 \frac{n}{R_S} C_\tau - 2 \frac{n}{R_S} D_\tau - E_\tau\right) \\ &\quad \times |\mathbf{q}_G|^2 \mathbf{q}_G. \end{aligned} \tag{87}$$

To connect the Lie algebraic approach with the theory of Seidel sums, we express third order aberrations in terms of the Seidel aberration coefficients. Following [1,2], we write the fourth order expansion of the wavefront in terms of Seidel sums S_I, \dots, S_V as

$$\begin{aligned} W(\hat{\rho}, \varphi; \hat{\eta}) &= \frac{1}{8} S_I \hat{\rho}^4 + \frac{1}{2} S_{II} \hat{\eta} \hat{\rho}^3 \cos \varphi + \frac{1}{2} S_{III} \hat{\eta}^2 \hat{\rho}^2 \cos^2 \varphi \\ &\quad + \frac{1}{4} (S_{III} + S_{IV}) \hat{\eta}^2 \hat{\rho}^2 + \frac{1}{2} S_V \hat{\eta}^3 \hat{\rho} \cos \varphi, \end{aligned} \tag{88}$$

where $\hat{\rho} = (x^2 + y^2)/\rho_{\max}$ are the normalized pupil coordinates, $\hat{\eta} = \eta/\eta_{\max}$ is the normalized image height, and $\hat{\rho} \cos \varphi = y/\rho_{\max}$. Here, η is the image height, and η_{\max} is the maximum image height. Last, ρ_{\max} is the exit pupil radius. It is possible to relate wavefront aberrations to transverse ray aberrations [1,2] through

$$\Delta \mathbf{q} = -\frac{R_S}{n} \nabla_{(x,y)} W, \tag{89}$$

where $\nabla_{(x,y)}$ represents the gradient in the (x, y) coordinates, and R_S is the radius of the reference sphere, or equivalently, the

exit pupil distance with respect to the last image plane. If we substitute Eq. (88) into Eq. (89), we have up to third order

$$\begin{aligned} \Delta \mathbf{q}^{(3)} &= -\frac{R_S}{n} \left[\frac{1}{2} \frac{S_I}{\rho_{\max}^4} (x^2 + y^2) \begin{pmatrix} x \\ y \end{pmatrix} \right. \\ &\quad + \frac{1}{2} \frac{S_{II}}{\rho_{\max}^3 \eta_{\max}} \left((x^2 + y^2) \begin{pmatrix} 0 \\ \eta \end{pmatrix} + 2y\eta \begin{pmatrix} x \\ y \end{pmatrix} \right) \\ &\quad + \frac{S_{III}}{\rho_{\max}^2 \eta_{\max}^2} y\eta \begin{pmatrix} 0 \\ \eta \end{pmatrix} + \frac{1}{2} \frac{S_{III} + S_{IV}}{\rho_{\max}^2 \eta_{\max}^2} \eta^2 \begin{pmatrix} x \\ y \end{pmatrix} \\ &\quad \left. + \frac{1}{2} \frac{S_V}{\rho_{\max} \eta_{\max}^3} \eta^2 \begin{pmatrix} 0 \\ \eta \end{pmatrix} \right]. \end{aligned} \tag{90}$$

Our variables in the Lie approach are $\mathbf{q}' = (x, y)^T$ and $\mathbf{q}_G = (0, \eta)^T$. We therefore rewrite Eq. (90) as

$$\begin{aligned} \Delta \mathbf{q}^{(3)} &= -\frac{R_S}{n} \left[\frac{1}{2} \frac{S_I}{\rho_{\max}^4} |\mathbf{q}'|^2 \mathbf{q}' + \frac{1}{2} \frac{S_{II}}{\rho_{\max}^3 \eta_{\max}} \right. \\ &\quad \times \left(|\mathbf{q}'|^2 \mathbf{q}_G + 2(\mathbf{q}' \cdot \mathbf{q}_G) \mathbf{q}' \right) + \frac{S_{III}}{\rho_{\max}^2 \eta_{\max}^2} (\mathbf{q}' \cdot \mathbf{q}_G) \mathbf{q}_G \\ &\quad \left. + \frac{1}{2} \frac{S_{III} + S_{IV}}{\rho_{\max}^2 \eta_{\max}^2} |\mathbf{q}_G|^2 \mathbf{q}' + \frac{1}{2} \frac{S_V}{\rho_{\max} \eta_{\max}^3} |\mathbf{q}_G|^2 \mathbf{q}_G \right]. \end{aligned} \tag{91}$$

Comparing each term in Eqs. (87) and (91) yields

$$\begin{cases} -\frac{R_S}{n} \frac{1}{2} \frac{S_I}{\rho_{\max}^4} = 4 \frac{n^3}{R_S^3} A_\tau, \\ -\frac{R_S}{n} \frac{S_{II}}{\rho_{\max}^3 \eta_{\max}} = -8 \frac{n^3}{R_S^3} A_\tau - 2 \frac{n^2}{R_S^2} B_\tau, \\ -\frac{R_S}{n} \frac{S_{III}}{\rho_{\max}^2 \eta_{\max}^2} = 8 \frac{n^3}{R_S^3} A_\tau + 4 \frac{n^2}{R_S^2} B_\tau + 2 \frac{n}{R_S} C_\tau, \\ -\frac{R_S}{n} \frac{1}{2} \frac{S_{III} + S_{IV}}{\rho_{\max}^2 \eta_{\max}^2} = 4 \frac{n^3}{R_S^3} A_\tau + 2 \frac{n^2}{R_S^2} B_\tau + 2 \frac{n}{R_S} D_\tau, \\ -\frac{R_S}{n} \frac{1}{2} \frac{S_V}{\rho_{\max} \eta_{\max}^3} = -4 \frac{n^3}{R_S^3} A_\tau - 3 \frac{n^2}{R_S^2} B_\tau - 2 \frac{n}{R_S} C_\tau - 2 \frac{n}{R_S} D_\tau - E_\tau. \end{cases} \tag{92}$$

The system Eq. (92) gives the Seidel sums in terms of the coefficients of the generator τ in the Lie algebraic description.

An advantageous property of Seidel coefficients is that they can be represented as sums of interface contributions [1,2]. It is therefore possible to distinguish the effect of each surface on the Seidel coefficient of the complete system and determine which interfaces need to be modified to reduce the aberrations of the complete system. Modifying one surface will then leave the contribution of the others unchanged. By definition of τ in Eq. (84), we can write

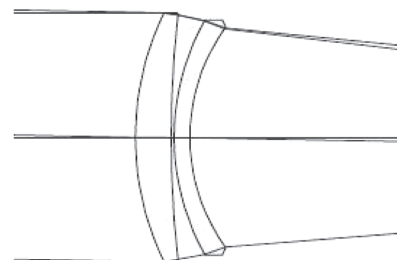


Fig. 2. Gaussian doublet (Fig. 8.11, [24]).

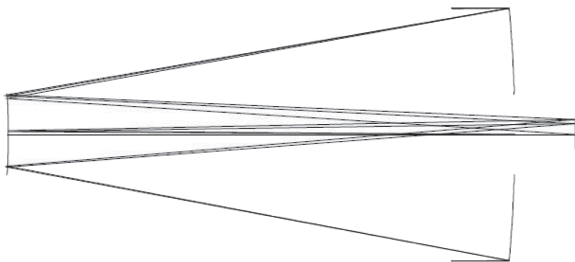
Table 2. Comparison between Kidger ([24], p. 180) and the Lie Method for the Gaussian Doublet

		S_I	S_{II}	S_{III}	S_{IV}	S_V
Surface 1	Kidger [24]	0.191312	0.007686	0.000309	0.000491	0.000032
	Lie	0.191312	0.007687	0.000309	0.000491	0.000032
Surface 2	Kidger [24]	0.005631	−0.001252	0.000278	−0.000130	−0.000033
	Lie	0.005631	−0.001252	0.000278	−0.000130	−0.000033
Surface 3	Kidger [24]	−0.009703	−0.000634	−0.000041	0.000701	0.000043
	Lie	−0.009703	−0.000634	−0.000041	0.000701	0.000043
Surface 4	Kidger [24]	−0.183099	−0.007941	−0.000344	−0.000902	−0.000054
	Lie	−0.183100	−0.007942	−0.000344	−0.000902	−0.000054
Total	Kidger [24]	0.004140	−0.002141	0.000201	0.000160	−0.000012
	Lie	0.004140	−0.002141	0.000201	0.000160	−0.000012

$$A_\tau = \sum_{j=1}^{k-1} A_{\sigma_j^*} + A_{\sigma_k}, \quad (93)$$

and analogously to Eq. (93), we compute the other coefficients B_τ, \dots, F_τ of the polynomial τ . The identities in Eq. (92) give linear relations between the Seidel sums of the system and the coefficients of the polynomial τ . This implies that if we use the identities in Eq. (92) with the coefficients of σ_j^* or σ_k , then we are actually computing the contributions of the individual surfaces to the respective Seidel sum. The property of adding interface contributions is therefore preserved by the Lie approach purely by mathematical argumentation—mainly the BCH formula applied in Eq. (84)—and without the need of physical or geometric justifications (see [1,2]).

To summarize, to derive the Seidel sums and the surface contributions of a rotationally symmetric optical system, it is necessary to first determine all Gaussian quantities in Eq. (75) of the system with the help of the Gaussian imaging conditions in Eq. (74). It is then possible to compute the coefficients of the fourth order generators for each interface using Eq. (72). Once the system is described by its corresponding map as in Eq. (76), we can proceed modifying it into Eq. (80). In this form, it is

**Fig. 3.** Ritchey–Chrétien telescope (Fig. 13.9, [24]).

possible to extract the third order aberration information of each interface and of the complete system according to Eq. (92).

8. EXAMPLES

In this section, we compute the Seidel sums for two examples, where we applied the results given in previous sections. The geometric data of the optical systems and the respective Seidel sums have been taken from [24].

As a first example of a fully refractive system, we take a Gaussian doublet (see Fig. 2). The necessary information is taken from [24], p. 180. To have all parameters for the expressions in Eq. (92), we need to track the exit pupil quantities using the Gaussian part of our mapping. The corresponding Seidel sums given in [24] and the ones derived from the Lie algebraic method are listed in Table 2.

The next example is a fully reflective system in the form of a Ritchey–Chrétien telescope (see Fig. 3). The necessary geometric information is taken from [24], p. 263. The procedure to derive the necessary polynomial coefficients is the same as described in Sections 4 and 5. The only change is that the root transformations considered are those for reflection given in Eq. (19). The corresponding Seidel sums given in [24] are compared with the ones derived from the Lie algebraic method in Table 3.

We have thus shown how we are able to replicate traditional results often recovering all significant digits.

9. CONCLUSION

In the presented work, a new way of computing the Seidel coefficients using the Lie algebraic theory has been presented. We briefly introduced the topics of geometrical optics and the Lie algebraic method. After showing how to reformulate the

Table 3. Comparison between Kidger ([24], p. 263) and the Lie Method for the Ritchey–Chrétien Telescope

		S_I	S_{II}	S_{III}	S_{IV}	S_V
Surface 1	Kidger [24]	−0.258533	−0.220745	0.017983	−0.017983	0.000000
	Lie	−0.258534	−0.220610	0.017961	−0.017961	0.000000
Surface 2	Kidger [24]	0.258574	0.220580	0.001553	0.041525	−0.002062
	Lie	0.258574	0.220446	0.001552	0.041475	−0.002058
Total	Kidger [24]	0.000040	−0.000164	0.019537	0.023542	−0.002062
	Lie	0.000040	−0.000164	0.019513	0.023513	−0.002058

geometrical optics results using Lie algebraic tools, we illustrated how to combine the reformulation of propagation and refraction into arbitrary refractive optical systems with rotational symmetry. The extension to reflective systems can be derived by following the same steps as for refractive systems. The link between the presented Lie framework and the Seidel coefficients has been shown, and the property of adding surface contributions is preserved by the Lie algebraic method. The examples given validate our results for refractive and reflective optical systems with rotational symmetry showing good agreement between our and existing results.

The Lie algebraic method offers a mathematical theory and a systematic procedure to link the aberrations of an optical system directly with the geometric parameters of the system itself. All the necessary ray information, i.e., ray heights at interfaces or image height, can be calculated using the Gaussian part of the mapping. The resulting expressions are given explicitly and can be extended to virtually any order of aberrations. The development of a fundamental element makes it straightforward to treat optical systems. In fact, most of the expensive algebraic computations are needed to determine the polynomials associated with the operators. Once these polynomials have been found for the fundamental element, describing an optical system is reduced to concatenating and reordering operators. It is therefore possible to gain additional insight into the interaction of geometries and aberrations of arbitrary order in a closed form, without resorting to ray tracing after each geometric variable change.

The presented methodology also allows to extend these results to off-axis optical systems. The authors intend to apply the Lie algebraic method to reflective systems with only one plane-symmetry, thus allowing for the optical axis to bend. The aim is to derive closed form aberration coefficients for off-axis optical systems.

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