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Symmetry in Lie Optics

KURT BERNARDO WOLF*

Departamento de Matemáticas, Universidad Autónoma Metropolitana, Iztapalapa DF, Mexico

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Optical systems produce nonlinear canonical transformations in optical phase space. Free propagation in a homogeneous medium has Euclidean symmetry and dynamical algebras under the Poisson–Lie bracket. Refracting interfaces between homogeneous media exhibit invariants; in particular, a spherical surface possesses an $so(3)$ symmetry algebra which allows the recursive computation of its aberration coefficients to arbitrarily high order. We present explicit results for aberration order nine. © 1986 Academic Press, Inc.

1. INTRODUCTION

The development of Lie methods applied to optics is very recent, and was motivated by problems in accelerator design [1]. Through studying nonlinear transformations of optical phase space which model optical systems, Lie theory can provide insight into the *symmetry* and *dynamics* of such systems as well. These names are taken from the familiar applications of group theory to classical and quantum mechanical systems; their meaning has be rediscovered in optics, though.

The Hamiltonian treatment of optics, surveyed in Section 2, historically preceded its applications in mechanics [2]; so should have the wave treatment of classical systems, yet the quantization of mechanics became a necessity apart from "wavization" of geometrical optics. This section presents the optics of homogeneous media in terms of Euclidean symmetry considerations. It also recalls the factorization theorem of Dragt and Finn [3, 4] which factors the optical transformation into a Gaussian (paraxial, linear) part, and a succession of aberrations of increasing order.

Optical systems, moreover, have elements which do not have a precise counterpart in mechanics: refracting surfaces. These are "instantaneous" finite canonical transformations of phase space. These transformations are nonlinear (and globally non-bijective); under rather broad conditions, however, they are one-to-one in a finite neighborhood of the optical axis of the system. Section 3 introduces the treatment of these surface transformations, their newly discovered factorization [5] and

* Permanent address: Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, Universidad Nacional Autónoma de México, Apdo. Postal 20-726, 01000 México DF, Mexico.

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finds invariants: the Petzval invariant and two so-defined Snell invariants. These close into an $so(3)$ algebra if the surface is spherical. In Section 4 we apply such symmetry considerations to find the well-known aplanatic points of the sphere.

The essential nonlinearity of the general refracting surface transformation satisfies, nevertheless, certain general conditions at the optical axis, and these imply certain "selection rules" for the aberration coefficients which have been noticed before [1, 6–8]. Section 5 uses the Snell invariants for the purpose of calculating the Gaussian parameters and third-order Seidel aberration coefficients of a spherical surface transformation. Section 6 extends this algorithmically to arbitrarily high aberration order, making the "selection rule" explicit.

In Section 7 we present a symplectic classification of aberrations [6], closely related to the Raccah-algebraic treatment of multipole expansions. In this basis we give, in a table, the explicit aberration coefficients of a spherical surface to aberration order nine. (These particularize results obtained by Navarro-Saad [7] for axis-symmetric tenth-degree surfaces; similar results have also been reported by Forest [8] to aberration order seven.) The last section offers some concluding remarks in connection with current developments.

2. Optical Phase Space, Free Propagation, and Lie Series

The Hamiltonian formulation of geometrical optics [1] describes light rays as points $(\mathbf{p}, \mathbf{q})$ in an optical *phase space*, evolving along the *optical axis* z of the system (which takes the role of time in the classical mechanics of point particles). See Fig. 1. At every $z = \text{constant}$ plane, the *configuration* subspace has coordinates $\mathbf{q}$, and is 2-dimensional in actual optical systems. Fermat's principle leads to an optical Lagrangian [1, 2, 9] from which the canonical momentum $\mathbf{p}$ is shown to be a vector *in* the $z = \text{constant}$ plane, along the projection of the ray on the plane, and of magnitude $p = n \sin \theta$, where n is the *refraction index* of the medium at $(\mathbf{q}, z)$, and θ is the angle between the ray and the z axis.

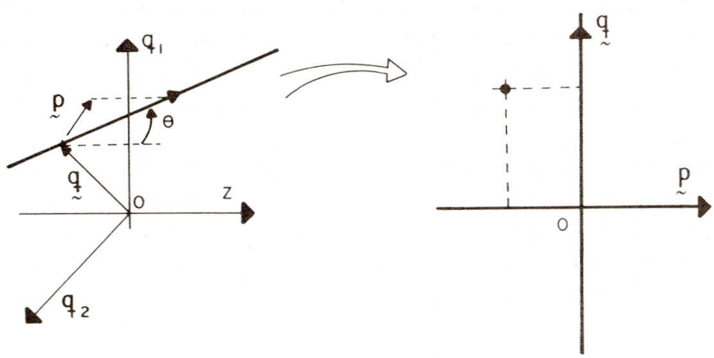

FIG. 1. The Hamiltonian treatment of geometric optics maps light rays (left) onto points in (4-dimensional) phase space (right).

The optical Hamiltonian is shown to be [1]

$$h = -n\cos\theta = -\sqrt{n^2 - p^2}$$
$$\simeq -n + \frac{1}{2n}p^2 + \frac{1}{8n^3}p^4 + \frac{1}{16n^5}p^6 + \cdots. \tag{2.1}$$

The Hamiltonians of classical pointparticle systems contain only one term of order two in $\mathbf{p}$; this is the *Gaussian*, or paraxial, approximation to optics; this allows only *linear* transformations of phase space under free propagation in homogeneous media (n = constant). Terms of order higher than two in the Hamiltonian generate *nonlinear* transformations in optical phase space, which are defined as *aberrations*. Free propagation itself, therefore, aberrates.

Lie optics uses the structure of Hamiltonian optics associating [1, 10, 11] *Lie operators* $\hat{f}$ to every continuously differentiable observable $f(\mathbf{p}, \mathbf{q})$ of phase space, through defining

$$\hat{f} := \sum_{i=1}^{2} \left(\frac{\partial f}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial}{\partial q_i} \right) =: \{f, \cdot\}, \tag{2.2}$$

where $\{\cdot, \cdot\}$ is the Poisson bracket. For the operators $\hat{f}$ we have hence a *Lie structure* of commutators, since [12] $[\hat{f}, \hat{g}] = (\{f, g\})\hat{}$. (Note: The Lie operator associated to f is also denoted by f_{op} by Katz [10], $:f:$ by Dragt [1], $\{f, \cdot\}$ or $[\hat{f}, \cdot]$ by Steinberg [11]. When f is a longish explicit expression, Dragt's notation, $:f:$, is advantageous. In such cases we use $(f)\hat{}$.)

Free propagation through a distance z in a homogeneous medium is thus described with the operator *generated* by h,

$$H_z := \exp(-z\hat{h}), \tag{2.3}$$

whose action is given by the Lie exponential series, or *Lie transformation* [3, 4, 11]:

$$H_z f(\mathbf{p}, \mathbf{q}) = \sum_{n=0}^{\infty} \frac{(-z)^n}{n!} (\hat{h})^n f(\mathbf{p}, \mathbf{q}) = f(H_z\mathbf{p}, H_z\mathbf{q}). \tag{2.4}$$

In particular, on the phase-space coordinates, this series may be summed to

$$H_z\colon \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \mapsto \begin{pmatrix} \mathbf{p}'(\mathbf{p}, \mathbf{q}; z) \\ \mathbf{q}'(\mathbf{p}, \mathbf{q}; z) \end{pmatrix} = \begin{pmatrix} \mathbf{p} \\ \mathbf{q} + z\mathbf{p}/\sqrt{n^2 - p^2} \end{pmatrix}. \tag{2.5}$$

Ray direction obviously does not change in free propagation, and the last summand is simply $z\tan\theta$ along the direction of $\mathbf{p}$, a fact which is clear from simple geometry. For small θ, $\tan\theta \approx \sin\theta$ and H_z is approximated by a lower-triangular block-matrix with $z/n\,\mathbf{1}$ and units on the diagonal; this is the Gaussian approximation to free propagation.

When the medium is homogeneous, $\hat{h}$ evidently commutes with the generators of translations in the plane, $\hat{p}_1$ and $\hat{p}_2$. It is also commutes with the generator of *rotations around the optical axis*

$$\hat{m}_3 := (\mathbf{q}\times\mathbf{p})\hat{\ } = (q_1 p_2 - q_2 p_1)\hat{\ } \\ = p_2 \partial p_1 - p_1 \partial p_2 + q_2 \partial q_1 - q_1 \partial q_2. \tag{2.6}$$

Correspondingly, the classical observable

$$m_3(\mathbf{p}, \mathbf{q}) = \mathbf{q}\times\mathbf{p} = \mathbf{q}'\times\mathbf{p}' = m_3(\mathbf{p}', \mathbf{q}'), \tag{2.7}$$

is conserved under z-evolution generated by $\hat{h}$. It is called [9] the *skewness*, or *Petzval*, invariant.

Conversely, $[\hat{m}_3, \hat{h}] = 0$ implies that the Hamiltonian $h(\mathbf{p}, \mathbf{q})$ may only depend on quantities invariant under joint rotations of the $\mathbf{p}$ and $\mathbf{q}$ planes, namely p^2, $\mathbf{p}\cdot\mathbf{q}$, q^2, and $\mathbf{q}\times\mathbf{p}$. Then $[\hat{p}_i, \hat{h}] = 0$ reduces h to depend on p^2 only.

In a homogeneous, isotropic medium, the choice of the z axis is clearly arbitrary. For simplicity, we may draw the situation in one dimension, as depicted in Fig. 2: the *same* ray has coordinates (θ, q) with respect to the q axis, and (θ^R, q^R) with respect to the q^R axis, rotated by α. For the angles, $\theta^R = \theta + \alpha$, while from the law of sines, $q/\cos\theta^R = q^R/\cos\theta$. As a result, the transformation of optical phase space due to a rotation by α is, in one dimension,

$$p \mapsto p^R = p\cos\alpha + \sqrt{n^2 - p^2}\sin\alpha \tag{2.8a}$$

$$q \mapsto q^R = (\cos\alpha - \sin\alpha\, p/\sqrt{n^2 - p^2})^{-1} q. \tag{2.8b}$$

The full transformation in two dimensions requires dot and cross products between vectors $\mathbf{p}$, $\mathbf{q}$, $\boldsymbol{\alpha}$, but the *generator* of (2.8) is easily brought to 2-vector form as

$$\mathbf{m} := \mathbf{q}\sqrt{n^2 - p^2}. \tag{2.9}$$

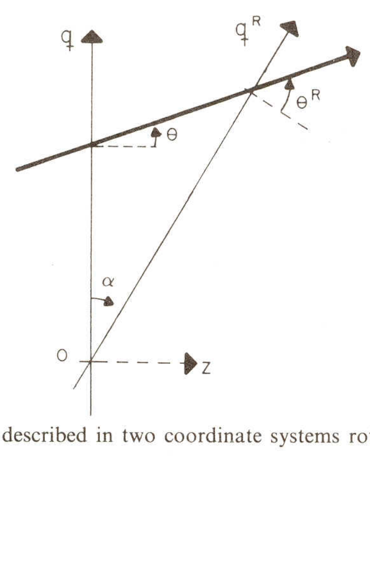

FIG. 2. A fixed light ray as described in two coordinate systems rotated with respect to each other around O.

One may verify that the two operator generators in (2.9) and the Petzval invariant (2.6) satisfy the commutation relations of the rotation algebra [13] $so(3)$:

$$[\hat{m}_1, \hat{m}_2] = \hat{m}_3, \qquad [\hat{m}_2, \hat{m}_3] = \hat{m}_1, \qquad [\hat{m}_3, \hat{m}_1] = \hat{m}_2. \tag{2.10}$$

Under these, the following commuting operators transform as a 3-vector:

$$\hat{p}_1, \hat{p}_2, \hat{p}_3 = (\sqrt{n^2 - p^2})\hat{} = -\hat{h}. \tag{2.11}$$

The Hamiltonian, thus, is identified with the generator of translations in the z direction, and its form is therefore fixed. The $so(3)$ invariant magnitude of the translation 3-vector is n.

The *symmetry* algebra of optical free propagation is therefore the 2-dimensional Euclidean algebra $iso(2)$, generated by $\{\hat{p}_1, \hat{p}_2; \hat{m}_3\}$. The *dynamical* algebra, of which $\hat{h} = -\hat{p}_3$ is an element, is the 3-dimensional Euclidean algebra $iso(3)$ generated by $\{\hat{p}_1, \hat{p}_2, \hat{p}_3 = -\hat{h}; \hat{m}_1, \hat{m}_2, \hat{m}_3\}$.

As we exemplified above for the free propagation operator $H_z = \exp(-z\hat{h})$, any continuously differentiable $f(\mathbf{p}, \mathbf{q})$ may be used to construct a *Lie transformation* $F_t = \exp(t\hat{f})$. These operators are [11] linear: $F_t(c_1 g_1 + c_2 g_2) = c_1 F_t g_1 + c_2 F_t g_2$, they preserve function products and Poisson brackets: $F_t(g_1 g_2) = (F_t g_1)(F_t g_2)$, $F_t\{g_1, g_2\} = \{F_t g_1, F_t g_2\}$, and act on function arguments as $(F_t g)(x) = g(F_t x)$. If we describe two optical elements or systems, A and B, by Lie series operators S_A and S_B whose action on $x = (\mathbf{p}, \mathbf{q})$ is $S_A x = x_A(x)$ and $S_B x = x_B(x)$, with known functions x_A and x_B of x, then their composition, i.e., the compound system AB obtained by acting first with A and second with B, is

$$\begin{aligned} S_{AB} x &:= S_A S_B x = S_A x_B(x) \\ &= x_B(S_A x) = x_B(x_A(x)) =: x_{AB}(x). \end{aligned} \tag{2.12}$$

The action of Lie series operators S on Poisson brackets insures that $Sx = x'(x)$ is a symplectic map [2], or canonical transformation [3], i.e., $\{q'_i, q'_j\} = 0$, $\{p'_i, p'_j\} = 0$, $\{q'_i, p'_j\} = \delta_{ij}$. A converse result has been given as a *factorization theorem* by Dragt and Finn [3, Theorem 2]. This may be parapharased in the following form. Let $x'(x) = Sx$ be a symplectic map having a power series expansion about the origin. Then there exist unique homogeneous polynomials s_n of degrees $n = 1, 2, \ldots$ such that $x'(x) = (\cdots S_4 S_3 S_2 S_1)x$, where $S_n = \exp \hat{s}_n$. When S sends the origin into itself, i.e., when there are no constant terms in the power series expansion, then $s_1 = 0$.

We should note that $S_2 x$ is linear in the components of x (the Gaussian, or linear, approximation), while $S_n x$ is x plus terms of order $n-1, 2n-1, \ldots$ in the components of x. The symplectic map $S^a := \cdots S_5 S_4 S_3$ may be called the *aberration* part of $S = S^a S_2$. (The original presentation of this result [3] was in the form $S = S_2 S^{a'}$, $S^{a'} = S'_3 S'_4 \cdots$. The advantage here of acting *first* with the aberration part on the "object" phase space, and *second* with the Gaussian part S_2, is that the coefficients in $S_3, S_4, \ldots$, will give the magnitude and sign of the aberration of the object, *before* it undergoes its major size transformation under the main, Gaussian part of the system.)

The factorization theorem of Dragt and Finn also allows us to *approximate* a system S by considering *up-to-Nth order aberrations*. We replace S^a by $S^a_N := S_{N+1} S_N \cdots S_4 S_3$, and thus S by $\bar{S}_N := S^a_N S_2$. The transformation $x \mapsto \bar{S}_N x =: x'_N(x)$ is still a symplectic map. Conversely, if we know the Taylor series of the map $x'(x)$ up to Nth order terms, $\bar{x}'_N(x)$, we may in principle reconstitute the symplectic map S up to Nth aberration order $\bar{S}_N$. Of course, $x \mapsto \bar{x}'_N(x)$ is *not*, by itself (for $N > 1$), a symplectic map. Poisson brackets between the $\bar{\mathbf{p}}'_N$ and $\bar{\mathbf{q}}'_N$ components of $\bar{x}'_N(x)$ will in general yield Poisson brackets with 0 or 1, plus terms of order $N+1$ and higher. They may be called *canonical to order N*.

3. Refracting Surfaces

A *refracting surface* is here a continuously differentiable interface $z = \zeta(\mathbf{q})$ between two homogeneous media of refraction indices n and n'. The geometric process of light refraction is described, as is well known, by Snell's law

$$n \sin \phi = n' \sin \phi' \tag{3.1}$$

where ϕ and ϕ' are the angles between the incident and refracted rays, and the surface normal at the point of incidence. The three directions lie in a plane.

The description of refraction at a sharp interface ζ might seem to be troublesome in Lie optics, since the process involves a discontinuity in the Hamiltonian. Indeed, even the symplecticity of the phase-space transformation does not seem to have been proven directly until recently. We may denote this transformation by $S(n, n'; \zeta)$. It appears, moveover, that in neighborhoods excluding caustics, the refracting-surface map has a convergent power series expansion; this will allow us to apply the Dragt–Finn factorization theorem.

In what follows, we shall exploit the following theorem due to Navarro-Saad and Wolf [5], which is based on the rather simple geometric construction of Fig. 3, and which we shall partially sketch below. It states that the refracting surface transformation S may be *factorized* as

$$S(n, n; \zeta) = R(n; \zeta)\, R(n'; \zeta)^{-1}, \tag{3.2}$$

where the "root" transformation $R(n, \zeta)$ acts as

$$\bar{\mathbf{p}}(\mathbf{p}, \mathbf{q}) := R(n, \zeta)\mathbf{p} = \mathbf{p} + \sqrt{n^2 - p^2}(\nabla\zeta)(\bar{\mathbf{q}}), \tag{3.3a}$$

$$\bar{\mathbf{q}}(\mathbf{p}, \mathbf{q}) := R(n; \zeta)\mathbf{q} = \mathbf{q} + \zeta(\bar{\mathbf{q}})\, \mathbf{p}/\sqrt{n^2 - p^2}, \tag{3.3b}$$

and is locally *canonical* at all its points of continuity. Note that the root transformation is defined *implicitly* by (3.3), since $\bar{\mathbf{q}}$ appears on both sides of (3.3b).

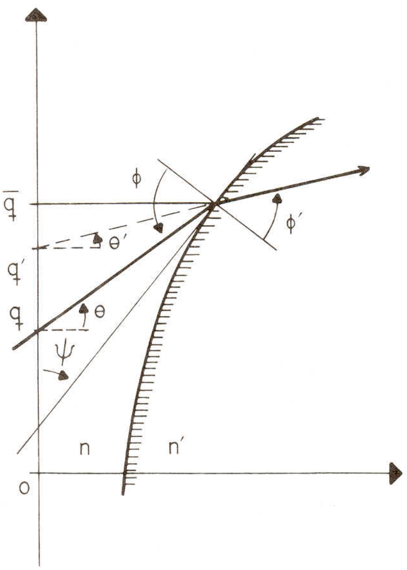

FIG. 3. Geometric meaning of the factorization for refracting surfaces. The action of the surface on the refracted ray is described as a finite transformation at the reference plane. The refracted ray is continued back to this plane; the point of intersection, $\bar{q}$, is shown.

The meaning of the surface factorization (3.2) is rather intuitive: there is a reference surface $z=0$, through which the ray $(\mathbf{p}, \mathbf{q})$ propagates to ζ; as it refracts, its regression *back* to the reference surface $z=0$ is the ray $(\mathbf{p}', \mathbf{q}')$. The effect of ζ is thus described by $(\mathbf{p}, \mathbf{q}) \mapsto (\mathbf{p}', \mathbf{q}')$ at $z=0$, quite independently of whether the actual refracting surface $z=\zeta(\mathbf{q})$ is "near" to $z=0$ or not. Its effect is that of a sudden transformation at the chosen reference point along the optical axis.

Regarding the composition through (2.12), if $R(n; \zeta)x = \bar{x}_{(n)}(x)$ and its inverse is denoted by $R(n; \zeta)^{-1}x = \tilde{x}_{(n)}(x)$ (so $R(s, n)^{-1}\, \bar{x}_{(n)}(x) = x$), then $S(n, n'; \zeta)x = R(n; \zeta)\, R(n'; \zeta)^{-1}x = R(n; \zeta)\, \tilde{x}_{(n')}(x) = \tilde{x}_{(n')}(R(n; \zeta)x) = \tilde{x}_{(n')}(\bar{x}_{(n)}(x)) = x'(x; n, n')$.

This factorization theorem is also valid when the two media are *not* homogeneous, but $n = n(\mathbf{q}, z)$, $n' = n'(\mathbf{q}, z)$. In that case, however, the root transformation takes a form which replaces (3.3) by the appropriate propagation in the inhomogeneous media [15].

This construction provides us with a very obvious way of building optical invariants: $\bar{\mathbf{q}}$ *itself* is a conserved (vector) quantity for the surface transformation S in the sense that, due to the factorization (3.2),

$$\bar{\mathbf{q}}(\mathbf{p}, \mathbf{q}; n) = \bar{\mathbf{q}}(\mathbf{p}', \mathbf{q}'; n') = S\bar{\mathbf{q}}(\mathbf{p}, \mathbf{q}; n'). \tag{3.4}$$

Next, the incidence angle in Snell's law (3.1) is $\phi = \theta + \psi$ and the refracted angle is $\phi' = \theta' + \psi$ with $\tan \psi = (\nabla\zeta)(\bar{q})$. In one dimension, we thus define

$$k := n \sin(\theta + \psi) = [p + \sqrt{n^2 - p^2}(\nabla\zeta)(\bar{q})] \cos \psi =: \bar{p} \cos \psi. \tag{3.5}$$

This leads to (3.3a), and establishes also $\bar{\mathbf{p}}$ (in two dimensions) as a conserved (vector) quantity

$$\bar{\mathbf{p}}(\mathbf{p}, \mathbf{q}; n) = \bar{\mathbf{p}}(\mathbf{p}', \mathbf{q}'; n') = S\bar{\mathbf{p}}(\mathbf{p}, \mathbf{q}; n'). \tag{3.6}$$

Indeed, *any* function $\mathbf{f}$ of $\bar{\mathbf{p}}$ and $\bar{\mathbf{q}}$ only, will be conserved in the sense that, when (3.4) and (3.6) are replaced,

$$\mathbf{g}(\mathbf{p}, \mathbf{q}; n) := \mathbf{f}(\bar{\mathbf{p}}, \bar{\mathbf{q}}) = \mathbf{g}(\mathbf{p}', \mathbf{q}'; n') = S\mathbf{g}(\mathbf{p}, \mathbf{q}; n'). \tag{3.7}$$

This general statement may be operationally vacuous unless we be able to write concrete functions $\mathbf{g}$ which are *explicit* in the arguments, and not merely defined implicitly. This will be done for the spherical surface in the next section. Here we want to exploit the general construction in implicit form using the second result of the above theorem: the canonicity of (3.3).

The two sides of Snell's equation (3.1) are the statement of invariance of (3.5), namely (in two dimensions) of

$$\mathbf{k} := \bar{\mathbf{p}}/\sqrt{1+\zeta'^2}, \qquad \zeta'^2 := [(\nabla\zeta)(\bar{\mathbf{q}})]^2, \tag{3.8}$$

which we call *Snell's invariant*, since it has the property (3.7). We now calculate the Poisson bracket between the two components of $\mathbf{k}$, k_1, and k_2, with respect to the canonically conjugate variables $(\bar{\mathbf{p}}, \bar{\mathbf{q}})$. This is

$$\{k_1, k_2\} = \tfrac{1}{2}(1+\zeta'^2)^{-2}(\bar{\mathbf{p}} \times \bar{\nabla})\zeta'^2 \tag{3.9}$$

(where $\bar{\nabla}$ indicates that derivatives are taken with respect to $\bar{q}$).

If the surface ζ is axially symmetric, so that $\zeta(\bar{\mathbf{q}})$ is a function of $\bar{q} := |\bar{\mathbf{q}}|$ only, then $(\bar{\nabla}\zeta)(\bar{\mathbf{q}}) = \bar{\mathbf{q}}\zeta'/\bar{q}$ and $\bar{\nabla}\zeta'^2 = 2(\bar{\mathbf{q}}/\bar{q})\,\zeta'\zeta''$, with $\zeta'(\bar{\mathbf{q}}) = d\zeta(\bar{q})/d\bar{q}$. Then we may write (3.9) as

$$\{k_1, k_2\} = \left[\frac{d}{d(\bar{q}^2)}\left(\frac{-1}{1+\zeta'^2}\right)\right]\bar{\mathbf{q}} \times \bar{\mathbf{p}}. \tag{3.10}$$

For axially symmetric surfaces too, from (3.3), the ray *skewness*

$$m_3 = \mathbf{q} \times \mathbf{p} = \bar{\mathbf{q}} \times \bar{\mathbf{p}} = \mathbf{q}' \times \mathbf{p}' = Sm_3 \tag{3.11}$$

is an invariant under the surface transformation which, in contradistinction to the general invariant (3.7), does not depend on the two refraction indices n, n'. The Petzval invariant (3.11) intertwines the two Snell invariants, since

$$\{m_3, k_1\} = k_2, \qquad \{m_3, k_2\} = -k_1, \tag{3.12}$$

but does not in general close into a finite-dimensional algebra with them, unless the bracketed expression in (3.10) be a constant.

4. Spherical Surfaces

Consider the surface of a sphere of radius r centered at $z=c$,

$$z=\zeta(q)=c-\sqrt{r^2-q^2}, \tag{4.1}$$

defined for $q^2 \leqslant r^2$. In that case, in (3.9), $\nabla\zeta(\bar{q})=\bar{q}/\sqrt{r^2-\bar{q}^2}$ and $\zeta'^2=\bar{q}^2/(r^2-\bar{q}^2)$; the quantity in brackets in (3.10) is $1/r^2$, and so the three quantities $\{rk_1, rk_2, m_3\}$ of last section close into an $so(3)$ algebra under the Poisson bracket. So do the associated Lie operators under commutation.

In this case, the Snell invariants (3.8) become $\bar{\mathbf{p}}\sqrt{r^2-\bar{q}^2}/r$ and may thus be written *explicitly* in terms of the unbarred ray coordinates, using (3.3a) for (4.1), as

$$r\mathbf{k}=\mathbf{p}c+\mathbf{q}\sqrt{n^2-p^2}=\mathbf{p}'c+\mathbf{q}'\sqrt{n'^2-p'^2}. \tag{4.2}$$

The Lie operators associated to (4.2) are the generators of rotations around the center of the sphere at $z=c$, as may be seen comparing with (2.9),

$$\exp(-c\hat{h})\,\hat{\mathbf{m}}\exp(c\hat{h})=r\hat{\mathbf{k}}, \tag{4.3}$$

i.e., $r\hat{\mathbf{k}}$ is obtained moving the center of rotation to the position $z=c$. The equality in (4.2) means, quite obviously, that the incident and refracted rays move in unison as they are rotated around the center of the refracting sphere. The $so(3)$ Casimir operator is

$$\mathbf{m}^2+m_3^2=(\mathbf{p}c+\mathbf{q}\sqrt{n^2-p^2})^2+(\mathbf{q}\times\mathbf{p})^2=n^2(c^2+q^2)-(\mathbf{q}\cdot\mathbf{p}-c\sqrt{n^2-p^2})^2 \tag{4.4}$$

Now, a pencil of *meridional* rays (i.e., rays which lie in a plane with the optical axis, so $\mathbf{p}/\!/\mathbf{q}$ and $m_3=0$) converging towards an intersection point at z_i, have their position and direction bound by the relation $q=-z_i\tan\theta$ or, vectorially, $\mathbf{q}\sqrt{n^2-p^2}=-z_i\mathbf{p}$. Their Snell invariant is thus

$$r\mathbf{k}=(c-z_i)\mathbf{p}. \tag{4.5}$$

Those rays which converge towards the center $z_i=c$ of the refracting spherical surface ζ have zero Snell invariants: $\mathbf{k}=\mathbf{0}$, before and after refraction.

This property of all the rays in a pencil through a point, to have their Snell invariant proportional to their momentum times the distance to the reference plane, Eq. (4.5), may be used to furnish a simple derivation of the location of the *aplanatic points* of a refracting sphere. Pairs of aplanatic points [16], —see Fig. 4—are such that rays converging to one of them will, upon refraction, converge to the other. A refracting sphere has one such pair. (This property is used to build the objective lens of oil-immersion microscopes.) Placing the reference plane $z=0$ at the center of the sphere, the two pencils must satisfy $r\mathbf{k}=-z_i\mathbf{p}=-z_i'\mathbf{p}'$ or $z_i n\sin\theta=z_i'n'\sin\theta'$. If $n<n'$ as in the figure, the maximum of $r\mathbf{k}$ is achieved at $\theta_m'=\pi/2$, corresponding to tangency at T, so $z_i n\sin\theta_m=z_i'n'$; but $\sin\theta_m=r/z_i$, and so it follows that

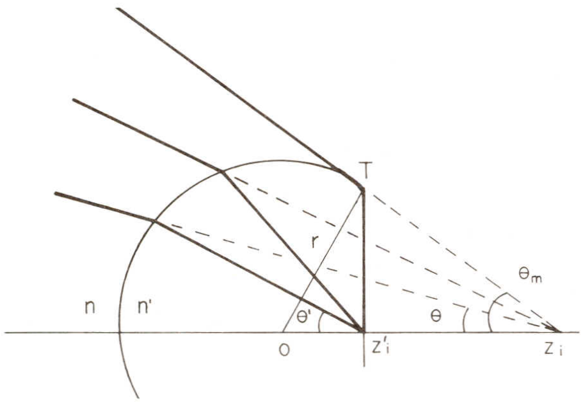

FIG. 4. The geometry of the aplanatic points of a sphere. A pencil of rays aimed to intersect at z_i, refracts and intersects at z_i'.

$z_i' = rn/n'$. Since θ_m is also the angle to the normal of refracted tangent rays, $\sin\theta_m = n/n'$ and it also follows that $z_i = rn'/n$. Replacement into $z_i \mathbf{p} = z_i' \mathbf{p}'$ verifies the Abbe sine condition [17] $\sin\theta/\sin\theta' = n/n'$ for perfect imaging.

5. The Spherical Surface, Its Gaussian Part, and Third-Order Aberrations

The factorization theorem of [5] for refracting surface transformations was instrumental in setting up the characterization of invariance in the form (3.7). Through the introduction of the "root" transformation phase-space variables $(\bar{\mathbf{p}}, \bar{\mathbf{q}})$, applied to the Snell invariant (3.8) in a spherical refracting surface, we obtain Eq. (4.2). We restate this as

$$pc + q\sqrt{n^2 - p^2} = S(pc + q\sqrt{n'^2 - p^2}). \tag{5.1}$$

We should remark that whereas the numerical value of $\mathbf{k}$ is conserved in (4.2) its functional form is changed by S, from that in a medium n to that in a medium n'. Phase space is by no means invariant under S, but only the refracting surface $\zeta(\bar{q})$.

We now use the factorization theorem of Dragt and Finn for symplectic maps [3] to inquire into the coefficients of the homogeneous polynomials $S_2, S_3, S_4, \ldots$ present in

$$S = \cdots \exp \hat{S}_5 \exp \hat{S}_4 \exp \hat{S}_3 \exp \hat{S}_2, \tag{5.2}$$

i.e., the *aberration coefficients*. The theorem's requirement that the origin of phase space map onto itself means that a ray along the optical axis must remain there. The center of the sphere, as above, must be on it too.

The spherical surface transformation S for a fixed value of the radius r is one particular element (or a line—*not* a subgroup—of elements parametrized by the radius r) of the infinite-parameter group of general (nonlinear, classic) canonical transformations, $\mathscr{C}$, of optical phase space. Now, S lies in the *commutant* of m_3 in $\mathscr{C}$, the Petzval invariant, generator of axis rotations, due to (3.11). The Snell vector conservation, we saw, is a statement of *co*-variance of the function space, so that the function $\mathbf{g}(\mathbf{p}, \mathbf{q}; n)$ is mapped by $S(n, n'; \zeta)$ to the function $\mathbf{g}(\mathbf{p}, \mathbf{q}; n')$. This is the case of Eq. (4.2), in particular, with the only peculiarity that the functions can be written explicitly and developed thus in Taylor series. It will be seen below that S is determined by this requirement, and computable by explicit use of this $so(3)$ covariance statement.

The decomposition of S into $S^a S_2$ is a subgroup decomposition into nonlinear and linear transformations, respectively, and so is the aberration subgroup nesting $\tilde{S}_N := \cdots S_{N+2} S_{N+1} \subset \tilde{S}_{N-1} \subset \tilde{S}_{N-2} \subset \cdots \subset S^a$, since $\{s_m, s_n\} = s_{m+n-2}$ and $m+n-2 > m, n$ for $m, n > 2$. As we argued intuitively at the end of Section 2, the *group* of up-to-Nth order aberrations is now defined as the *factor* group $\tilde{S}_N \backslash \mathscr{C} =: \bar{S}_N$. Due to the nesting, each S_N must be generated by algebra elements $\hat{s}_N$ in the commutant of $\hat{m}_3$. Now, $s_n(\mathbf{p}, \mathbf{q})$ is of polynomial form and order n in the components of $\mathbf{p}$ and $\mathbf{q}$, and must satisfy $\hat{m}_3 s_n = 0$, but $\hat{m}_3 \mathbf{p} \neq \mathbf{p}$ and $\hat{m}_3 \mathbf{q} \neq \mathbf{q}$, however, $\hat{m}_3 f(p^2, \mathbf{p}\cdot\mathbf{q}, q^2) = 0$. This means that all odd-n $s_n(\mathbf{p}, \mathbf{q})$ must have vanishing coefficients (since every combination of monomials $p_1^{k_1} p_2^{k_2} q_1^{l_1} q_2^{l_2}$, $k_1 + k_2 + l_1 + l_2 = n$, must have "unbalanced" vector indices). In the even-n $s_n(\mathbf{p}, \mathbf{q})$, only and all monomials $(p^2)^{n_+}(\mathbf{p}\cdot\mathbf{q})^{n_0}(q^2)^{n_-}$, $2(n_+ + n_0 + n_-) = n$, may be present. The axis-symmetric subgroup of $\mathscr{C}$ is thus defined and has the decomposition $\cdots S_6 S_4 S_2$, with $S_n = \exp s_n(p^2, \mathbf{p}\cdot\mathbf{q}, q^2)$, n even. We now narrow the requirements for S by imposing (3.7) to a corresponding requirement on each of the S_n's, which will be algorithmic and will fully determine them sequentially.

First note that, for any fixed order n of s_n,

$$\begin{aligned} \exp \hat{s}_n f(\mathbf{p}, \mathbf{q}) &= \sum_{m=0}^{\infty} \frac{1}{m!} \{s_n, \{s_n, \cdots \{s_n, f\} \cdots \}\}(\mathbf{p}, \mathbf{q}) \\ &= f\left(\sum_{m=0}^{\infty} \mathbf{p}'_{m(n-2)+1}(\mathbf{p}, \mathbf{q}), \sum_{m=0}^{\infty} \mathbf{q}'_{m(n-2)+1}(\mathbf{p}, \mathbf{q}) \right) \\ &= f(\mathbf{p}', \mathbf{q}'), \end{aligned} \tag{5.3}$$

where $x'_l(x)$ ($x'_l = \mathbf{p}'_l$ and $\mathbf{q}'_l$) is a polynomial vector function which is a homogeneous polynomial of order $l = m(n-2)+1$ in the components of x ($x = \mathbf{p}$ and $\mathbf{q}$). For order $n = 2$ above, we are applying the *Gaussian* part S_2 of the surface transformation S, and there one obtains a series of linear polynomials, $m(n-2)+1 = 1$ for all m; this series can be summed [6] to

$$\begin{pmatrix} \mathbf{p}'_2 \\ \mathbf{q}'_2 \end{pmatrix} = S_2 \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \exp[v_{+1} p^2 + v_0 p \cdot q + v_{-1} q^2]^{\wedge} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}. \tag{5.4a}$$

$$= \begin{pmatrix} \alpha^1 & \beta^1 \\ \gamma^1 & \delta^1 \end{pmatrix} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}, \quad \begin{pmatrix} \alpha^1 & \beta^1 \\ \gamma^1 & \delta^1 \end{pmatrix} = \begin{pmatrix} \cosh v + v_0 \operatorname{sinch} v & 2v_{-1} \operatorname{sinch} v \\ -2v_{+1} \operatorname{sinch} v & \cosh v - v_0 \operatorname{sinch} v \end{pmatrix} \tag{5.4b}$$

$$v = \sqrt{v_0^2 - 4v_{+1}v_{-1}}, \qquad \operatorname{sinch} v = v^{-1} \sinh v. \tag{5.4c}$$

when keeping up to third-order terms in (5.11). We now use these to replace into the key equation (5.8), the expressions for $\mathbf{p}^a = \mathbf{p} + \mathbf{p}_3 + \mathcal{O}(x^5)$ and $\mathbf{q}^a = \mathbf{q} + \mathbf{q}_3 + \mathcal{O}(x^5)$ obtaining

$$\mathbf{p}r + \mathbf{q}\left(n - \frac{1}{2n}p^2\right) = \left(\mathbf{p} + \mathbf{p}_3 + \frac{n-n'}{r}[\mathbf{q} + \mathbf{q}_3]\right) r + (\mathbf{q} + \mathbf{q}_3)\left(n' - \frac{1}{2n'}[\mathbf{p} + \frac{n-n'}{r}\mathbf{q}]^2\right) + \mathcal{O}(x^5). \quad (5.13a)$$

The Gaussian terms cancel as they should, and certain other terms simplify to

$$-\frac{1}{2n}p^2\mathbf{q} = \mathbf{p}_3 r + \mathbf{q}_3 n - \frac{1}{2n'}\left(\mathbf{p} + \frac{n-n'}{r}\mathbf{q}\right)^2 \mathbf{q} + \mathcal{O}(x^5). \quad (5.13b)$$

Here we replace $\mathbf{p}_3$ and $\mathbf{q}_3$ from (5.12), equating the coefficients of the four independent monomials $p^2\mathbf{q}$, $q^2\mathbf{p}$, $\mathbf{p}\cdot\mathbf{q}\mathbf{q}$, and $q^2\mathbf{q}$ (the other two, $p^2\mathbf{p}$ and $\mathbf{p}\cdot\mathbf{q}\mathbf{p}$ are absent since $A = B = C = 0$). We obtain, from the first, third, and fourth,

$$D = \frac{1}{4r}\left(\frac{1}{n'} - \frac{1}{n}\right), \quad (5.14a)$$

$$E = \frac{1}{2r^2}\frac{n-n'}{n'}, \quad (5.14b)$$

$$F = \frac{1}{8r^3}\left[(n-n') + 2\frac{(n-n')^2}{n'}\right], \quad (5.14c)$$

in complete accordance with [6]. (Note that the coefficients A, B,..., F used in [9] and re-obtained in [5] refer to the decomposition $S = S_2 S^{a'}$, rather than $S^a S_2$ as used here.)

Each of the above coefficients corresponds to one of the third-order Seidel aberrations [9]. They have been examined individually in some detail in [6]. Thus, A is the spherical aberration coefficient, B is the coma coefficient, C astigmatism, D curvature of field, and E distortion; F does not seem to have been given a Seidel name, since it keeps $\mathbf{q}$ fixed and has no effect on a focused image. In [6] we used the name "pocus," as it refers to unfocusing in $\mathbf{p}$, diminishing the depth of field at the edges of the screen. It is the Fourier conjugate to spherical aberration. Note that the vanishing of A, B, and C was a consequence only of the placement of the optical center of the surface at $z = 0$ (free propagation thereafter will produce them, however). The vanishing of the first three coefficients is valid for any axis-symmetric surface. What was specific of the sphere is the use of Snell's conservation statement in explicit form, namely the key equation (5.8), reduced to (5.13). We note that of the four independent equations derived from the latter, one of them—the coefficient of $q^2\mathbf{p}$—is identically satisfied when the other three are.

The algorithm presented here shortens that which was used previously [5, 6, 7] when the surface is not spherical: (i) finding of $\bar{x}(x)$ through self-replacement in (3.3) to some agreed order, (ii) finding the inverse $x'(\bar{x})$ through an analogous procedure, (iii) concatenation, and (iv) comparison with the coefficients of $x_3(x)$ in (5.11). Here, (i)–(iii) is replaced by expanding the root and powers in the key equation (5.8) in Taylor series. As we sketch the case for Nth order aberrations, this leads to increasing economy in the symbolic computation [18, 19].

6. Nth-Order Aberrations

Third-order (Seidel) aberration terms are the most important corrections to Gaussian optics. Yet it is of interest to proceed systematically further. The task is to use the key equation (5.8) for aberration orders larger than three. We wrote $S^a = \cdots S_{10} S_8 S_6 S_4$; if we want to go to ninth aberration order, the ellipses $(\cdots)$ must be disregarded or, equivalently, the classical Poisson-bracket algebra must be factored modulo polynomials in x of order $n \geqslant 11$. Then, the series $\exp \hat{s}_4$ must be taken up to $(\hat{s}_4)^4$ in x, the series $\exp \hat{s}_6$ up to $(\hat{s}_6)^2$, and $\exp \hat{s}_8$ and $\exp \hat{s}_{10}$ up to the linear term. Properly concatenated, this generalizes the third-order expression (5.9):

$$x^a(x) = [1 + \hat{s}_{10}][1 + \hat{s}_8]\left[1 + \hat{s}_6 + \frac{1}{2!}(\hat{s}_6)^2\right]$$

$$\times\left[1 + \hat{s}_4 + \frac{1}{2!}(\hat{s}_4)^2 + \frac{1}{3!}(\hat{s}_4)^3 + \frac{1}{4!}(\hat{s}_4)^4\right] x + \mathcal{O}(x^{11})$$

$$= x + x_3(x) + x_5(x) + x_7(x) + x_9(x) + \mathcal{O}(x^{11}); \tag{6.1a}$$

$$x_3(x) = \hat{s}_4 x, \tag{6.1b}$$

$$x_5(x) = \hat{s}_6 x + \frac{1}{2!}\hat{s}_4^2 x, \tag{6.1c}$$

$$x_7(x) = \hat{s}_8 x + \hat{s}_6 \hat{s}_4 x + \frac{1}{3!}\hat{s}_4^3 x, \tag{6.1d}$$

$$x_9(x) = \hat{s}_{10} x + \hat{s}_8 \hat{s}_4 x + \frac{1}{2!}\hat{s}_6^2 x + \frac{1}{2!}\hat{s}_6 \hat{s}_4^2 x + \frac{1}{4!}\hat{s}_4^4 x, \tag{6.1e}$$

where $x_N(x)$ contains only terms of order x^N. Generalizing (5.10), we may write the general $(2N)$th order polynomial function of p^2, $\mathbf{p}$, $\mathbf{q}$, and q^2, as

$$s_{2N}(\mathbf{p}, \mathbf{q}) = \sum_{n_+ + n_0 + n_- = N} c^N_{n_+ n_0 n_-} M_{n_+ n_0 n_-}(\mathbf{p}, \mathbf{q}), \tag{6.2a}$$

$$M_{n_+ n_0 n_-}(\mathbf{p}, \mathbf{q}) := (p^2)^{n_+} (\mathbf{p} \cdot \mathbf{q})^{n_0} (q^2)^{n_-}. \tag{6.2b}$$

First we shall see which restrictions correspond to the selection rule $A = B = C = 0$ of last section, setting "essential zeros" among the coefficients; these are to be valid for any aberration order and for surfaces which are only axis-symmetric. We start with s_4, as we did in the last section, and impose on $x_3(x)$ in (6.1b) the optical center conditions (5.6). Then, if Eqs. (5.6) are made to hold for $x_3 = \hat{s}_4 x$, they also hold replacing x by $\hat{s}_4 x$ or $(\hat{s}_4)^n x$, since the latter is composed of factors of the former. This eliminates the summand with $\hat{s}_4$ in the expression (6.1c) and below. When the optical center condition is applied to x_5 in (6.1d), it will yield restrictions on the coefficients in $\hat{s}_6$ which, when satisfied, elliminate all further summands in $\hat{s}_6$ down the ladder in (6.1). Thus the conditions (5.6) hold indeed, for every aberration order. It is then sufficient to consider one monomial at a time in (6.2). From

$$\mathbf{p}' := \{M_{n_+ n_0 n_-}, \mathbf{p}\} = n_0 M_{n_+, n_0 - 1, n_-} \mathbf{p} + 2n_- M_{n_+, n_0, n_- - 1} \mathbf{q}, \tag{6.3a}$$

$$\mathbf{q}' := \{M_{n_+ n_0 n_-}, \mathbf{q}\} = -2n_+ M_{n_+ - 1, n_0, n_-} \mathbf{p} - n_0 M_{n_+, n_0 - 1, n_-} \mathbf{q}, \tag{6.3b}$$

we obtain

$$\left.\frac{\partial q_i'}{\partial p_j}\right|_{q=0} = 2n_+ (p^2)^{n_+ - 2} [p^2 \delta_{ij} - 2(n_+ - 1)\, p_i p_j]\, \delta_{n_0,0}\, \delta_{n_-,0}, \tag{6.4a}$$

$$\left.\frac{\partial x_i'}{\partial x_j}\right|_{q=0} = \delta_{ij} - n_0 (p^2)^{n_+ - 1} [p^2 \delta_{ij} \mp 2n_+\, p_i p_j]\, \delta_{n_0,1}\, \delta_{n_-,0}, \tag{6.4b}$$

$$\left.\frac{\partial p_i'}{\partial q_j}\right|_{q=0} = 2(p^2)^{n_+}\, p_i p_j\, \delta_{n_0,2}\, \delta_{n_-,0} + 2(p^2)^{n_+}\, \delta_{ij}\, \delta_{n_0,0}\, \delta_{n_-,1}, \tag{6.4c}$$

$$\left.\frac{\partial^k p_i'}{\partial q_{j_1} \cdots \partial q_{j_k}}\right|_{q=0} = n_0(n_0 - 1) \cdots (n_0 - k)(p^2)^{n_+}\, p_i p_{j_1} \cdots p_{j_k}\, \delta_{n_0,k+1}\, \delta_{n_-,0} + \cdots \tag{6.4d}$$

In (3.7b) x' and x are either $\mathbf{q}'$ and $\mathbf{q}$, or $\mathbf{p}'$ and $\mathbf{p}$. Now compare with (5.6). It follows that

$$c^N_{m,N-m,0} = 0, \qquad m = 0, 1, ..., N. \tag{6.5}$$

Hence, s_{2N} contains no terms $(p^2)^N$, $(p^2)^{N-1}\mathbf{p}\cdot\mathbf{q}$,..., $(p^2)^{N-k}(\mathbf{p}\cdot\mathbf{q})^k$,..., $(\mathbf{p}\cdot\mathbf{q})^N$. This eliminates $N+1$ aberration coefficients of order $2N-1$. The "hidden symmetry" selection rule (6.5) has been noted by Forest [8] and Navarro-Saad [7] for aberration orders seven and nine.

Further, the coefficients $c^N_{N-1,0,1}$ for the spherical surface may be calculated noting that (6.4c) must equal the term of order $2N-2$ in the series of the right-hand side of (5.6). Using the series expansion

$$\sqrt{n^2 - p^2} = n - \frac{1}{2}\frac{p^2}{n} - \frac{1 \cdot 1}{2 \cdot 4}\frac{p^4}{n^3} - \cdots - \frac{(2N-5)!!}{(2N-2)!!}\frac{p^{2N-2}}{n^{2N-3}} - \cdots \tag{6.6}$$

we obtain the coefficient of $(p^2)^{N-1}q^2$,

$$c^N_{N-1,0,1} = \frac{(2N-5)!!}{2r(2N-2)!!}\left(\frac{1}{n'^{2N-3}} - \frac{1}{n^{2N-3}}\right). \tag{6.7}$$

Actually, this coefficient holds for general axis-symmetric surfaces as well if we replace the factor $1/2r$ by the coefficient of the quadratic term in the Taylor series expansion of the surface ζ. This term corresponds to the highest power of p^2 in the aberration polynomial, so it is the most important aberration of order $2N-1$ for rays at large angles. It contributes to $\mathbf{p}'$ with a term $2c(p^2)^{N-1}\mathbf{q}$ and to $\mathbf{q}'$ with a term $-2(N-1)\,c(p^2)^{N-2}q^2\mathbf{p}$, where c is given by (6.7), above.

The $N+2$ coefficients we have found above for any aberration order are only the consequence of placing the optical center at the origin, and are valid for any surface $\zeta(q) = \alpha q^2 + \beta q^4 + \gamma q^6 + \cdots$, as stated before. Let us now proceed with the spherical surface. For Gaussian and third-order terms, the procedure was detailed in the previous section and the results are explict. For general aberration order $2N-1$, we assume we know $s_4(x), s_6(x),\ldots$ and $s_{2N-2}(x)$. Following (6.1) we now replace $x^a = x + x_3 + \cdots + x_{2N-3} + x_{2N-1}$ with $x_3,\ldots, x_{2N-3}$ assumed known and

$$x_{2N-1}(x) = \hat{s}_{2N}x + \hat{s}_{2N-2}\hat{s}_4 x + \cdots + \frac{1}{(N-1)!}(\hat{s}_4)^{N-1}x \tag{6.8}$$

into the key equation (5.8) and read off only the terms of order x^{2N-1}, the aberration order. The series (6.6) expands $\sqrt{n^2-p^2}$ in the left-hand side and $\sqrt{n'^2-p'^2}$ in the right-hand side, and power of $p'^2 = (\mathbf{p}^a + (n-n')/r\mathbf{q}^a)^2$ will yield contributions of order x^{2N-1} from the first term up to the Nth (this is the generalization of Eq. (5.13b)). Thus we have an equation homogeneous of degree $2N-1$ involving $\mathbf{p}$, $\mathbf{q}$, in powers and $\hat{s}_{2N}\mathbf{p}$, $\hat{s}_{2N}\mathbf{q}$, linearly. We replace now the general form of $\hat{s}_{2N}$ from (6.2) aided by (6.3), leaving all coefficients $c^N_{n_+n_0n_-}$ to be determined by equating monomials $M_{n_+n_0n_-}(\mathbf{p}, \mathbf{q})$. We are thus to find the $\frac{1}{2}(N+1)(N+2)$ coefficients $c^N_{n_+n_0n_-}$ from $N(N+1)$ possible monomial equations. Of the former, $N+1$ are zero and one more is determined in (6.7). The number of $(2N+1)$th order monomials in which $\mathbf{p}'$ and $\mathbf{q}'$ actually expand is $N(N-1)$ and $N(N-2)$, respectively. There are more equations than coefficients, but each coefficient appears in at most four monomial equations due to (6.3), and the system solves providing a check on the computation.

7. The Symplectic Classification of Aberrations

In this section we propose a classification of higher order aberrations with a Lie-theoretic significance which may lead to a deeper insight into the question of non-linear transformations of phase space. In (5.10) and (6.2) we expanded the polynomial s_{2N} generating aberrations of order $2N-1$ in monomials which are like Cartesian tensors. This is the basis used by Dragt and coworkers [8, 20] which particularizes their work with non-axis-symmetric elements in accelerators and electron microscopes, and serves well to express the zeros of some coefficients [cf. (6.5)].

Ultimately, we want to know the aberration coefficients tabulated in this section for a spherical surface in order to be able to concatenate them with free-flight transformations and with other lens surfaces which constitute the optical system; and to do so efficiently. The *main* part of the system is Gaussian, however, and in attention to the corresponding group we shall classify the aberrations.

We note that the generators of Gaussian transformations,

$$\hat{K}_+ = \tfrac{1}{2}(p^2)\hat{}, \qquad \hat{K}_0 = \tfrac{1}{2}(\mathbf{p}\cdot\mathbf{q})\hat{}, \qquad \hat{K}_- = \tfrac{1}{2}(q^2)\hat{}, \tag{7.1a}$$

close into an $sp(2, R)$ (2-dimensional real symplectic) algebra under commutation:

$$[\hat{K}_0, \hat{K}_\pm] = \pm\hat{K}_\pm, \qquad [\hat{K}_+, K_-] = -2\hat{K}_0. \tag{7.1b}$$

The last minus sign above distinguishes this algebra from the $so(3)$ symmetry algebra of the spherical surface seen in (2.10) in he Cartesian basis. These operators act on the following 3-dimensional space

$$\xi_+ := -\frac{1}{\sqrt{2}}(\xi_1 + i\xi_2) := \frac{1}{\sqrt{2}}p^2, \tag{7.2a}$$

$$\xi_0 := \xi_3 := \mathbf{p}\cdot\mathbf{q}, \tag{7.2b}$$

$$\xi- := \frac{1}{\sqrt{2}}(\xi_1 - i\xi_2) := \frac{1}{\sqrt{2}}q^2, \tag{7.2c}$$

and leave invariant

$$\begin{aligned}\xi_1^2+\xi_2^2+\xi_3^2 = \xi_0^2 - 2\xi_+\xi_- &= -[p^2q^2 - (\mathbf{p}\cdot\mathbf{q})^2] \\ &= -(\mathbf{p}\times\mathbf{q})^2 = 4(K_0^2 - K_+K_-) =: -2\Xi.\end{aligned} \tag{7.3}$$

This is a sphere of imaginary radius given by the value of the Petzval skewness invariant. The action of the K_σ on the coordinates ξ_τ allow us to realize the former as

$$\hat{K}_+ = -\sqrt{2}\left(\xi_+\frac{\partial}{\partial\xi_0} + \xi_0\frac{\partial}{\partial\xi_-}\right), \tag{7.4a}$$

$$\hat{K}_0 = \xi_+\frac{\partial}{\partial\xi_+} - \xi_-\frac{\partial}{\partial\xi_-}, \tag{7.4b}$$

$$\hat{K}_- = \sqrt{2}\left(\xi_0\frac{\partial}{\partial\xi_+} + \xi_-\frac{\partial}{\partial\xi_0}\right). \tag{7.4c}$$

We now define the *symplectic-basis* nth aberration order polynomial generators ${}^{2N}\chi^j_m$ as polynomials in the ξ_τ of *order* $2N = n + 1$ in the components of $\mathbf{p}$ and $\mathbf{q}$, of *spin* j, and $\hat{K}_0$-eigenvalue m $(m = j, j-1, ..., -j)$ as follows:

$$ {}^{2N}\chi^j_m = \Xi^v \, {}^{2j}\chi^j_m, \qquad 2j + 4v = 2N, \tag{7.5a} $$

$$ {}^{2j}\chi^j_m = \frac{\sqrt{4\pi(2j+1)(j+m)!\,(j-m)!}}{(2j+1)!!}\, \mathcal{Y}^j_m(\xi) $$

$$ = \frac{(j+m)!\,(j-m)!}{(2j-1)!!} \sum_k \frac{1}{2^{2k+m}} \frac{(p^2)^{k+m}(\mathbf{p}\cdot\mathbf{q})^{j-2k-m}(q^2)^k}{(k+m)!\,(j-2k-m)!\,k!}, \tag{7.5b} $$

where all indices are nonnegative integers. Here,

$$ \Xi = \tfrac{1}{2}\,[p^2q^2 - (\mathbf{p}\cdot\mathbf{q})^2] \tag{7.5c} $$

is the symplectic invariant (7.3) of order four in $(\mathbf{p}, \mathbf{q})$, and $\mathcal{Y}^j_m(\xi)$ is the solid spherical harmonic of integer spin j, projection m and of order $2j$ in $(\mathbf{p}, \mathbf{q})$. The normalization has been chosen [6] for the computational convenience of dealing with coefficients as simple as possible, starting with

$$ {}^{2j}\chi^j_j = (p^2)^j, \tag{7.6a} $$

and then lowering or raising in m through

$$ \hat{K}_\mp \, {}^{2N}\chi^j_m = (m \pm j)\, {}^{2N}\chi^j_{m\mp 1}. \tag{7.6b} $$

We note—useful as a numerical check—that the sum of the absolute values of the monomial coefficients is unity. This rule served to build ${}^{2N}\chi^N_m$, and the ${}^{2N}\chi^j_m$ with the lower values of j are obtained through multiplication by this "normalized" skewness invariant Ξ. We note also that for *meridional* ray optics, only these "*stretched*" ${}^{2j}\chi^j_m$ (with $j = N$) are nonzero, since $\Xi = 0$ when $\mathbf{p}/\!/\mathbf{q}$. One-dimensional (or cylindrical-lens) optics [21] require only the latter, therefore.

The symplectic aberration polynomials ${}^{2N}\chi^j_m(\mathbf{p}, \mathbf{q})$ transform under the $sp(2, R)$ algebra (7.1) as $so(2)$-classified bases for (finite-dimensional, nonunitary) irreducible representations of spin j (or $so(2, 1)$ Bargmann [22] label $k = -j$). The $2j + 1$ members of each *aberration multiplet* (of fixed (N, j)), transform among themselves under Gaussian optics with the corresponding finite-dimensional D-matrices (see [6, Eq. (4.7)]), and *do not mix* amongst multiplets. This leads to a block-diagonalization in the composition of the aberration group parameters, which may be computationally significant.

The generator polynomials $S_{2N}(\mathbf{p}, \mathbf{q})$ if $(2N-1)$th order aberrations given in (6.2) is thus written as

$$ S_{2N}(\mathbf{p}, \mathbf{q}) = \sum_{j=N(-2)}^{1 \text{ or } 0} \sum_{m=-j}^{j} V^{2N-1}_{jm} \, {}^{2N}\chi^j_m, \tag{7.7} $$

where for aberration order $2N - 1 = 3, 7, 11, ...,$ the spin j ranges over the values

$j=N, N-2,\ldots, 0$, and for aberration order $2N-1=5, 9, 13,\ldots$, over $j=N$, $N-2,\ldots, 1$. There are $\frac{1}{2}(N+1)(N+2)$ aberrations of order $2N-1$. Their values for the refracting spherical surface are given in the table.

For the important case of third-order aberrations ($N=2$) given as monomials in (5.10), the six aberrations break up into a quintuplet ${}^4\chi^2_m$ and a singlet ${}^4\chi^0_0=\Xi$. Concretely, we have

$$\begin{aligned} &{}^4\chi^2_2=(p^2)^2, \qquad {}^4\chi^2_1=p^2\mathbf{p}\cdot\mathbf{q}, \qquad {}^4\chi^2_0=\tfrac{1}{3}\,[p^2q^2+2(\mathbf{p}\cdot\mathbf{q})^2] \\ &{}^4\chi^2_{-1}=\mathbf{p}\cdot\mathbf{q}q^2, \qquad {}^4\chi^2_{-2}=(q^2)^2; \end{aligned} \tag{7.8a}$$

$${}^4\chi^0_0=\tfrac{1}{2}[p^2q^2-(\mathbf{p}\cdot\mathbf{q})^2]. \tag{7.8b}$$

The $m=0$ quintuplet aberration has been called *curvatism*, the singlet *astigmature*, while the Fourier conjugate of spherical aberration, ${}^4\chi^2_{-2}$ is pocus. The degenerate pair mixes astigmatism and curvature of field through

$$C(\mathbf{p}\cdot\mathbf{q})^2+Dp^2q^2=V^3_{20}\,{}^4\chi^2_0+V^3_{00}\,{}^4\chi^0_0 \tag{7.8c}$$

$$\begin{pmatrix} c^2_{101} \\ c^2_{020} \end{pmatrix}=\begin{pmatrix} 1/3 & 1/2 \\ 2/3 & -1/2 \end{pmatrix}\begin{pmatrix} v^3_{20} \\ v^3_{00} \end{pmatrix}, \qquad \begin{pmatrix} v^3_{20} \\ v^3_{00} \end{pmatrix}=\begin{pmatrix} 1 & 1 \\ 4/3 & -2/3 \end{pmatrix}\begin{pmatrix} c^2_{101} \\ c^2_{020} \end{pmatrix} \tag{7.8d}$$

The selection rule (6.5) and (6.7) bind the quintuplet and singlet contribution as $v^3_{20}=\frac{3}{4}\,v^3_{00}=c^2_{101}$ for any surface transformation.

The general connecting formula between the monomial and symplectic polynomial aberrations is obtained from (7.5), expanding Ξ in (7.3). This yields

$${}^{2N}\chi^j_m=\sum_{n_\sigma(k)}\Gamma^{Njm}_{n_+n_0n_-}M_{n_+n_0n_-} \tag{7.9a}$$

$$n_+(k)=k+m, \qquad n_0(k)=N-2k-m, \qquad n_-(k)=k \tag{7.9b}$$

$$\Gamma^{Njm}_{n_+n_0n_-}=\frac{(j+m)!\,(j-m)!}{(2j-1)!!}\sum_s\binom{\nu}{s}\frac{(-1)^{\nu-s}2^{-\nu-n_+-n_-+2s}}{(n_+-s)!\,(n_0+2s)!\,(n_--s)!}, \tag{7.10}$$

where $\nu=(N-j)/2$ is a nonnegative integer. These coefficients in turn connect the aberration coefficients in the symplectic classification (7.7), v^{2N-1}_{jm}, as they appear in the table, and the Cartesian classification of aberration coefficients by monomials of the aberration polynomials in their form (6.2), $c^N_{n_+n_0n_-}$. They are related through

$$c^N_{n_+n_0n_-}=\sum_{j=N(-2)}^{1\text{ or }0}v^{2N-1}_{j,n_+-n_-}\Gamma^{N,j,n_+-n_-}_{n_+n_0n_-}. \tag{7.11}$$

Conversely, the monomial basis vectors can be written in terms of the symplectic basis vectors as

$$M_{n_+n_0n_-}=\sum_{j=N(-2)}^{1\text{ or }0}L^{Njm}_{n_+n_0n_-}\,{}^{2N}\chi^j_m, \tag{7.12a}$$

$$N=n_++n_0+n_-, \qquad m=n_+-n_-. \tag{7.12b}$$

We cannot offer the general closed form of $L^{Njm}_{n_+n_0n_-}$ but we can find from [13, Eq. (6.139); 23, Eq. (8.922)], the expansion of x^N in terms of Legendre polynomials $\mathscr{Y}_{j0}(\mathbf{x})$ and applying $\hat{K}_\pm$ appropriately, for the case $n_- = 0$. This corresponds to $n_+ = m$, $n_0 = N - m$, and recalling that $v = (N-j)/2$ is integer, we obtain

$$L^{Njm}_{m,N-m,0} = (-1)^v \frac{(N-m)!}{v!\,(j-m)!} \frac{(2j+1)!!}{(N+j+1)!!}. \tag{7.13}$$

Applying now $\hat{K}_\mp$ for $m \gtrless 0$, we obtain the 3-term recursion relation for k,

$$\begin{aligned}(N-2k-m)&(N-2k-m-1)\, L^{Njm}_{n_\sigma(k+1)} \\ &+ [2(N-2k-m)(2k+m+1) + 2k - (j-m)(j+m+1)]\, L^{Njm}_{n_\sigma(k)} \\ &+ 4k(k+m)\, L^{Njm}_{n_\sigma(k-1)} = 0,\end{aligned} \tag{7.14a}$$

where, as in (7.9),

$$n_+(k) = k + m, \qquad n_0(k) = N - 2k - m, \qquad n_-(k) = k, \tag{7.14b}$$

and valid for $0 \leqslant k \leqslant (N-m)/2$. With these intertwining matrix elements, the converse of (7.11) is

$$v^{2N-1}_{jm} = \sum_{k=0}^{[N-m]/2} c^N_{n_\sigma(k)} L^{Njm}_{n_\sigma(k)}, \tag{7.15}$$

with (7.14b).

The surface aberration selection rule (6.5) only elliminates the $k = 0$ summand above. It is sufficient to allow us to state, however, that *no* surface will produce by itself the two highest-m aberration terms:

$$v^{2N-1}_{NN} = 0, \qquad v^{2N-1}_{N,N-1} = 0, \tag{7.16}$$

i.e., the direct higher order analogs of sphereical aberration and coma are absent. The next two coefficients, $v^{2N-1}_{N,N-2}$ and $v^{2N-1}_{N,N-3}$ are bound to their next j-neighbors, $v^{2N-1}_{N-2,N-2}$ and $v^{2N-1}_{N-2,N-3}$ through the vanishing of $c^N_{N-2,2,0}$ and $c^N_{N-2,3,0}$. In third aberration, (7.8d) results in $v^3_{20} = c^2_{101}$ which is known from (6.7), and $v^3_{00} = \frac{4}{3} v^3_{20}$. Here the implied relations are

$$v^{2j-1}_{j,j-2} = c^j_{j-1,0,1}, \qquad v^{2j-1}_{j-2,j-2} = 4\frac{j-1}{2j-1} v^{2j-1}_{j,j-2}, \qquad v^{2j-1}_{j-2,j-3} = 4\frac{j-2}{2j-1} v^{2j-1}_{j,j-3}. \tag{7.17}$$

This we may observe in Table I. For values of m lower than $j-3$ we have in general more than two multiplets, and the surface selection rule (6.5) only imposes a condition on the sum of three or more v's, which stems from (7.11).

The aberration coefficients of free propagation by z are those of Eq. (2.1), times $-z$.

TABLE I

Aberration Coefficients (in the Symplectic Basis) of a Spherical Refracting Surface, to Ninth Order

Third order:

$$v^3_{22} = v^3_{21} = 0$$
$$v^3_{20} = (m-n)/4rmn$$
$$v^3_{2-1} = (m-n)/2r^2m$$
$$v^3_{2-2} = (-m^2+3mn-2n^2)/8r^3m$$
$$v^3_{00} = (m-n)/3rmn$$

Fifth order:

$$v^5_{33} = v^5_{32} = 0$$
$$v^5_{31} = (m^3-n^3)/16rm^3n^3$$
$$v^5_{30} = (m^3+mn^2-2n^3)/8r^2m^3n^2$$
$$v^5_{3-1} = (5m^3-5m^2n+6mn^2-6n^3)/16r^3m^3n$$
$$v^5_{3-2} = (-m^4+4m^3n-4m^2n^2+3mn^3-2n^4)/8r^4m^3n$$
$$v^5_{3-3} = (-m^4+3m^3n-3m^2n^2+2mn^3-n^4)/16r^5m^3$$

$$v^5_{11} = (m^3-n^3)/10rm^3n^3$$
$$v^5_{10} = (m^3+mn^2-2n^3)/10r^2m^3n^2$$
$$v^5_{1-1} = (mn-n^2)/10r^3m^3$$

Seventh order:

$$v^7_{44} = v^7_{43} = 0$$
$$v^7_{42} = (m^5-n^5)/32rm^5n^5$$
$$v^7_{41} = (m^5+m^2n^3+mn^4-3n^5)/16r^2m^5n^4$$
$$v^7_{40} = (23m^5+7m^2n^3+60mn^4-90n^5)/192r^3m^5n^3$$
$$v^7_{4-1} = (14m^5-15m^4n+18m^3n^2-17m^2n^3+30mn^4-30n^5)/48r^4m^5n^2$$
$$v^7_{4-2} = (-16m^6+75m^5n-93m^4n^2+82m^3n^3-63m^2n^4+60mn^5-45n^6)/96r^5m^5n^2$$
$$v^7_{4-3} = (-7m^6+26m^5n-33m^4n^2+28m^3n^3-20m^2n^4+15mn^5-9n^6)/48r^6m^5n$$
$$v^7_{4-4} = (-8m^7+17m^6n+m^5n^2-28m^4n^3+40m^3n^4-34m^2n^5+24mn^6-12n^7)/384r^7m^5n$$

$$v^7_{22} = 3(m^5-n^5)/56rm^5n^5$$
$$v^7_{21} = (m^5+m^2n^3+mn^4-3n^5)/14r^2m^5n^4$$
$$v^7_{20} = 3(m^5+2mn^4-3n^5)/28r^3m^5n^3$$
$$v^7_{2-1} = (2m^4-m^3n-m^2n^2+3mn^3-3n^4)/14r^4m^5n$$
$$v^7_{2-2} = (8m^6-27m^5n+36m^4n^2-20m^3n^3+12mn^5-9n^6)/168r^5m^5n^2$$

$$v^7_{00} = (m^3-n^3)/30r^3m^3n^3$$

Ninth order:

$$v^9_{55} = v^9_{54} = 0$$
$$v^9_{53} = 5(m^7-n^7)/256rm^7n^7$$
$$v^9_{52} = (3m^7+4m^2n^5+3mn^6-10n^7)/64r^2m^7n^6$$
$$v^9_{51} = (14m^7+3m^5n^2-7m^4n^3-8m^3n^4+26m^2n^5+42mn^6-70n^7)/128r^3m^7n^5$$
$$v^9_{50} = (35m^7-15m^6n+18m^5n^2-27m^4n^3+3m^3n^4+126mn^6-140n^7)/128r^4m^7n^4$$

For passage from a medium of refraction index n to a medium of refraction index m; r is the sperical radius.

Table continued

TABLE I—*Continued*

$$v^9_{5-1} = (-9m^8 + 82m^7n - 71m^6n^2 + 87m^5n^3 - 120m^4n^4 + 106m^3n^5 - 110m^2n^6 + 210mn^7 - 175n^8)/128r^5m^7n^4$$

$$v^9_{5-2} = (-17m^8 + 80m^7n - 99m^6n^2 + 118m^5n^3 - 134m^4n^4 + 117m^3n^5 - 100m^2n^6 + 105mn^7 - 70n^8)/64r^6m^7n^3$$

$$v^9_{5-3} = (-72m^8 + 281m^7n - 393m^6n^2 + 486m^5n^3 - 522m^4n^4 + 432m^3n^5 - 324m^2n^6 + 252mn^7 - 140n^8)/256r^7m^7n^2$$

$$v^9_{5-4} = (-8m^9 + 21m^8n - 12m^7n^2 - 19m^6n^3 + 74m^5n^4 - 105m^4n^5 + 91m^3n^6 - 64m^2n^7 + 42mn^8 - 20n^9)/128r^8m^7n^2$$

$$v^9_{5-5} = (-35m^8 + 133m^7n - 245m^6n^2 + 340m^5n^3 - 364m^4n^4 + 302m^3n^5 - 190m^2n^6 + 84mn^7 - 25n^8)/1280r^9m^7$$

$$v^9_{33} = 5(m^7 - n^7)/144rm^7n^7$$

$$v^9_{32} = (3m^7 + 4m^2n^5 + 3mn^6 - 10n^7)/48r^2m^7n^6$$

$$v^9_{31} = (13m^7 + 3m^5n^2 - 5m^4n^3 - 4m^3n^4 + 13m^2n^5 + 30mn^6 - 50n^7)/96r^3m^7n^5$$

$$v^9_{30} = (17m^7 - 6m^6n + 9m^5n^2 - 9m^4n^3 + 3m^3n^4 - 9m^2n^5 + 45mn^6 - 50n^7)/72r^4m^7n^4$$

$$v^9_{3-1} = (-6m^8 + 29m^7n - 7m^6n^2 + 3m^5n^3 - 9m^4n^4 + 14m^3n^5 - 34m^2n^6 + 60mn^7 - 50n^8)/96r^5m^7n^4$$

$$v^9_{3-2} = (m^8 - 7m^7n + 21m^6n^2 - 20m^5n^3 + 10m^4n^4 - 10m^2n^6 + 15mn^7 - 10n^8)/48r^6m^7n^3$$

$$v^9_{3-3} = (9m^8 - 41m^7n + 78m^6n^2 - 81m^5n^3 + 54m^4n^4 - 18m^3n^5 - 9m^2n^6 + 18mn^7 - 10n^8)/288r^7m^7n^2$$

$$v^9_{11} = (7m^5 + 2m^3n^2 + 4mn^4 - 13n^5)/140r^3m^5n^5$$

$$v^9_{10} = (7m^5 - m^4n + 4m^3n^2 + m^2n^3 + 3mn^4 - 14n^5)/140r^4m^5n^4$$

$$v^9_{1-1} = (m^6 + m^5n - 3m^4n^2 + 2m^3n^3 + 4m^2n^4 - 4mn^5 - n^6)/140r^5m^5n^4$$

8. CONCLUDING REMARKS

We have tabulated the Gaussian and aberration coefficients to order nine for the transformation of optical phase space due to the spherical refracting surface. Although the treatment of refracting surfaces is in itself an interesting endeavor and much of the global properties remains to be studied, our final objective is to describe optical *systems*. For this, we must *concatenate* transformations described by Gaussian part an aberration coefficients. This was done explicitly for the case of third-order aberrations in [6, 24], since it involves only a 9-parameter inhomogeneous symplectic group $(I_5 \otimes I_1) \otimes \mathrm{Sp}(2, R)$. There, $\mathrm{Sp}(2, R)$ acts on aberrations in I_5 through a 5-dimensional representation which is simple enough to write explicitly [6, Eqs. (4.5) and (4.6)], and aberrations only sum, since they constitute an abelian ideal.

For aberrations of order higher than third, the action of $\mathrm{Sp}(2, R)$ on them is also through finite representation matrices; however, aberrations not only sum, but *compose* into aberrations of higher order. Computationally, this has been solved in MARYLIE [20] through the use of Baker–Campbell–Hausdorff relations in a program which works with non-axially symmetric systems. (We should note carefully that Lie maps differ from optical ray-tracing algorithms in that the Lie map is, in principle, given analytically, and the concatenation or integration need be performed *once* for the system. Thereafter, the mapping of individual rays is more economic.) Work in progress indicates that the necessary expressions for the Poisson brackets $\{{}^{2N}\chi^{j}_{m}, {}^{2N'}\chi^{j'}_{m'}\}$ involve Clebsch–Gordan coefficients (without square roots). This Raccah-type algebra is under development [15].

The "merely" group-theoretical aspects of our construction should not be slighted, however, as certain other common refracting surfaces may yield to the same methods. Spherical surfaces are special in that the surface *root* transformations (3.3) solve exactly as a second-order equation. This is a property shared by planes, revolution ellipsoids, paraboloids, and hyperboloids. In terms of canonical representations of algebras [25], the Poisson brackets between functions of p^2, $\mathbf{p}\cdot\mathbf{q}$, and q^2, are actually the Berezin brackets [26] for $sp(2, R)$. The problem thus turns into that of exploitation of the covering algebra of the symplectic algebra, rather than the Heisenberg–Weyl algebra, as is usually done in mechanics. The homogeneous space on which the corresponding Lie group acts is the optical phase space. There, we have $\mathbf{p}$ and $\mathbf{q}$ again, in addition to functions of the $sp(2, R)$ generators, leading to half-integral spin ${}^{2N}\chi^{j}_{m}$'s. For aberration order three, see [5, 24].

Finally, the "wavization" of these systems replaces the Sp(2, R), 2×2 matrices, by canonical integral-transforms [27]. There, $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ are the Schrödinger operators and the representation of Sp(2, R) is the metaplectic one on the space of phase functions. The lens transformations beyond Gaussian order also integral transforms in general. This is presently under development too.

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