

Factorization of the phase-space transformation produced by an arbitrary refracting surface

Miguel Navarro-Saad

Facultad de Ciencias, Universidad Nacional Autónoma de México, 0100 México D.F., México

Kurt Bernardo Wolf*

Departamento de Física, Centro de Investigación y Estudios Avanzados, Instituto Politécnico Nacional, México 14, D.F., México

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We study the transformation produced on optical phase space by an arbitrary refracting surface. We show that this factorizes into two root canonical transformations, one representing the propagation from a reference plane to the refracting surface in the first medium, and the other, the inverse propagation back to the reference surface in the second medium. This factorization allows for a simple parameterization of the effect of a refracting surface to some aberration order, illustrated for cubic surfaces and Dragt's Lie-algebraic description of a quartic surface and its Seidel aberration coefficients.

1. INTRODUCTION

Lie-algebraic methods were recently used by Dragt¹ to describe Hamiltonian systems that aberrate. Aberration is, loosely speaking, the nonlinearity of the phase-space transformation² brought about by an optic or magnetic³ device. It is also unavoidable if the Hamiltonian is of polynomial order higher than 2 in the phase-space variables. If the Hamiltonian is strictly quadratic, we are in a Gaussian system,² and phase space will be subject only to linear transformation. This happens in quantum mechanics in its Schrödinger formulation⁴ and in wave^{5,6} and geometrical optics² in the Gaussian approximation. Lie algebra and group theory developed out of the use of quantum mechanics⁷ and are thus well adapted to Gaussian systems. The use of group theory in aberrating systems seems to require further insights.

One problem that has been present within Hamiltonian mechanics in its Lie-algebraic formulation is what to do with systems that undergo an abrupt change in their Hamiltonian through a hard refracting surface as one travels in the direction of the optical axis (or the time axis for more general systems). The process is discontinuous, and it is not clear that an infinitesimal transformation method should be the most appropriate. It seems more natural to seek the description of the discontinuity through a finite group transformation. What group? In principle, this would be the group of all canonical transformations.⁸ More practically, it can be a factor structure of the former modulo, the set of transformations that lie outside our interest. This leads to approximating the system to a given order N of aberration through a finite-parameter group of effective nonlinear transformations of phase space of N th order of nonlinearity.⁹

This paper focuses on the general canonical transformation produced by a refracting surface and applies it to two cases in which the aberration orders are 2 and 3. Section 2 is introductory: the Hamiltonian formulation of simple optics. In Section 3 we give the refracting-surface trans-

formation of phase space in implicit form. Making this form explicit is done later on for the two cases. This is aided by the main result of this paper, which is given as a theorem (proved in Appendix A) that states that the refracting-surface transformation can be factored into two root transformations that are canonical; one represents the free-space propagation from a reference plane to the surface in the first medium followed by the inverse of that root transformation in the environment of the second medium. Section 4 settles the issue of the choice for optical axis and center in a general surface. The concatenation of the root transformations is indicated in Section 5, and Sections 6 and 7 apply the method to a general cubic surface and a general quartic (axis-symmetric) lens surface, respectively. In the latter it is shown that one derives Dragt's results¹ on Seidel aberrations in a rather economical way. Section 8 offers some directions of development for the study of aberrating systems in terms of group theory.

2. THE HAMILTONIAN FORMULATION OF OPTICS

The Hamiltonian formulation of geometric optics^{2,3} describes an optical ray as a point in phase space (\mathbf{p}, \mathbf{q}) . We have a coordinate z along an axis that takes the place of time or distance along the optical axis. With reference to a given $z = 0$ plane, with coordinates q_1, q_2 , the position of an optical ray is given by a two-vector \mathbf{q} , its point of intersection with the reference plane. The canonically conjugate momentum \mathbf{p} is related to the direction of the ray projected onto the reference plane of magnitude

$$p = (p_1^2 + p_2^2)^{1/2} = n \sin \theta, \quad (2.1)$$

where n is the refractive index of the medium at \mathbf{q} and θ is the angle between the ray and the z axis.

The Hamiltonian of an optical system is given by^{2,3}

$$h(\mathbf{p}, \mathbf{q}) = -(n^2 - p^2)^{1/2} = -n \cos \theta, \quad (2.2)$$

where n may depend on \mathbf{q} and z . If the system is homogeneous along the z axis, the mapping of phase space from the $z = 0$ reference plane to a general z plane is given by the Green evolution operator

$$G_h(z) = \exp(-z\hat{h}), \quad (2.3a)$$

$$\hat{h}(\mathbf{p}, \mathbf{q}) = \sum_i \left(\frac{\partial h}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial h}{\partial p_i} \frac{\partial}{\partial q_i} \right). \quad (2.3b)$$

This operator \hat{h} acts on functions of \mathbf{p} and \mathbf{q} , in particular on the phase-space coordinates themselves, and produces functions $\mathbf{p}'(\mathbf{p}, \mathbf{q}; z)$, $\mathbf{q}'(\mathbf{p}, \mathbf{q}; z)$; the latter is the map of the original $z = 0$ phase space by the homogeneous system S of thickness z :

$$S_z: \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \rightarrow \begin{pmatrix} \mathbf{p}'(\mathbf{p}, \mathbf{q}; z) \\ \mathbf{q}'(\mathbf{p}, \mathbf{q}; z) \end{pmatrix} = G_h(z) \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}. \quad (2.4)$$

It is standard to show that a continuous transformation generated by an operator exponentiated as Eq. (2.2) is *canonical*,⁸ i.e., that the values of the *Poisson brackets* between the canonical set are preserved under S_z :

$$\{q'_i, p'_j\} = \sum_k \left(\frac{\partial q'_i}{\partial q_k} \frac{\partial p'_j}{\partial p_k} - \frac{\partial q'_i}{\partial p_k} \frac{\partial p'_j}{\partial q_k} \right) = \delta_{ij}, \quad (2.5a)$$

$$\{q'_i, q'_j\} = 0, \quad \{p'_i, p'_j\} = 0. \quad (2.5b)$$

Dependence of h on z produces a Hamiltonian flow in phase space (volume elements are preserved and flow lines do not intersect²) where the tangent vector (the Lie-algebra generator) changes direction with the parameter z .

In the case of a homogeneous and isotropic medium (h is independent of \mathbf{q} and z), we have the free-propagation Hamiltonian generating $\mathbf{q} \rightarrow \mathbf{q} + z\hat{u} \tan \theta$, where \hat{u} is the unit vector in the direction of \mathbf{p} . In phase space,

$$\exp(-z\hat{h}): \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \rightarrow \begin{pmatrix} \mathbf{p}' \\ \mathbf{q}' \end{pmatrix} = \begin{bmatrix} \mathbf{p} \\ \mathbf{q} + z\mathbf{p}/(n^2 - p^2)^{1/2} \end{bmatrix}. \quad (2.6)$$

This transformation is, of course, canonical.

3. REFRACTING SURFACES

The more interesting elements of optical systems are their refracting surfaces. These are not readily found through the above formalism; it would be surprising if they were, since the process is discontinuous. We describe a hard refracting surface by an at least twice-differentiable function ζ of \mathbf{q} (and of \mathbf{q} only), at $z = \zeta(\mathbf{q})$. Before it, the refraction index is n , and after it, it is n' . Both are, from here on, explicitly assumed to be independent of \mathbf{q} or z . We may project the effect of the surface ζ to a finite canonical transformation at the $z = 0$ plane; see Fig. 1. The effect of the surface may be described by

$$S_\zeta: \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \rightarrow \begin{bmatrix} \mathbf{p}'(\mathbf{p}, \mathbf{q}; \zeta) \\ \mathbf{q}'(\mathbf{p}, \mathbf{q}; \zeta) \end{bmatrix} \quad (3.1)$$

as a single, discrete transformation due to ζ . Figure 1 seems to depict a one-dimensional optical world; what we show here is the state of affairs in the plane containing the incoming ray, the vector normal to the surface, and the outgoing ray. The incoming ray crosses $z = 0$ at \mathbf{q} (with a momentum

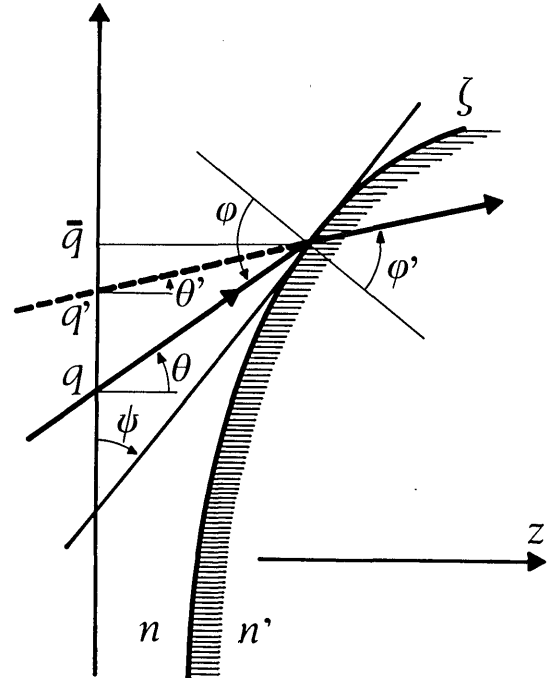


Fig. 1. Ray undergoing refraction by a surface ζ . The action of this surface is to transform the object phase-space plane $[p(\theta), q]$ to the image plane $[p'(\theta'), q']$ at the chosen $z = 0$ plane. This is determined by the surface function $\zeta(\bar{q})$ and the incidence angle ϕ at the point of refraction \bar{q} .

$\mathbf{p} \sim n \sin \theta$), strikes ζ at \bar{q} , and refracts to $\mathbf{p}' \sim n' \sin \theta'$. The continuation of the refracted ray back to the $z = 0$ plane defines \mathbf{q}' . Thus the action of ζ is projected—as for a Fresnel lens—to a single “instant,” $z = 0$. In the plane of the figure we have the following scalar trigonometric identities⁹:

$$\bar{q} - q = \zeta(\bar{q}) \tan \theta, \quad (3.2a)$$

$$\bar{q} - q' = \zeta(\bar{q}) \tan \theta', \quad (3.2b)$$

each of which represents free propagation from $z = 0$ to $z = \zeta(\bar{q})$. Since the propagations are along the lines of the respective vectors \mathbf{p} , we may write

$$\bar{\mathbf{q}} = \mathbf{q} + \zeta(\bar{\mathbf{q}})\mathbf{p}/(n^2 - p^2)^{1/2}, \quad (3.3a)$$

$$\bar{\mathbf{q}} = \mathbf{q}' + \zeta(\bar{\mathbf{q}})\mathbf{p}'/(n'^2 - p'^2)^{1/2}. \quad (3.3b)$$

Next, we use Snell's law for the ray directions, noting that the tangent to ζ at $\bar{\mathbf{q}}$ makes an angle ψ with the z -plane projection, so that $\tan \psi = d\zeta(\bar{\mathbf{q}})/d\bar{q} = \zeta'(\bar{\mathbf{q}})$. The angle of incidence ϕ is $\psi + \theta$ from Fig. 1; the refraction angle ϕ' is $\psi + \theta'$. Snell's law demands that

$$n \sin \phi = n' \sin \phi'. \quad (3.4a)$$

A bit of trigonometry now leads to

$$p + (n^2 - p^2)^{1/2} \zeta'(\bar{q}) = p' + (n'^2 - p'^2)^{1/2} \zeta'(\bar{q}). \quad (3.4b)$$

The derivative is directional along the $(\mathbf{p}, \mathbf{p}')$ plane, so this expression is also valid in its vector form with $(\nabla \zeta)(\bar{\mathbf{q}})$, where we keep in mind that it is the vector derivative with respect to $\bar{\mathbf{q}}$. We may now write Eq. (3.4b) as a pair of equations:

$$\bar{\mathbf{p}} = \mathbf{p} + (n^2 - p^2)^{1/2} (\nabla \zeta)(\bar{\mathbf{q}}), \quad (3.5a)$$

$$\bar{\mathbf{p}} = \mathbf{p}' + (n'^2 - p'^2)^{1/2} (\nabla \zeta)(\bar{\mathbf{q}}). \quad (3.5b)$$

Observing that Eqs. (3.3a), (3.4a), and (3.5a) and Eqs. (3.3b), (3.4b), and (3.5b) have the same structure, we should be interested in what follows.

Theorem. For every twice-differentiable surface $\zeta(\mathbf{q})$, the transformation

$$R_{\zeta,n}: \mathbf{p} \rightarrow \bar{\mathbf{p}} = \mathbf{p} + (n^2 - p^2)^{1/2}(\nabla\zeta)(\bar{\mathbf{q}}), \quad (3.6a)$$

$$R_{\zeta,n}: \mathbf{q} \rightarrow \bar{\mathbf{q}} = \mathbf{q} + \zeta(\bar{\mathbf{q}})\mathbf{p}/(n^2 - p^2)^{1/2} \quad (3.6b)$$

is locally canonical at all its nonsingular points.

The proof makes economical use of differential forms¹⁰ and is given in Appendix A. Below, we examine the singularities of Eqs. (3.6).

The transformation [Eqs. (3.6)] has the property of mapping the observable $q_1p_2 - q_2p_1$ into

$$\begin{aligned} & \bar{q}_1\bar{p}_2 - \bar{q}_2\bar{p}_1 \\ &= q_1p_2 - q_2p_1 + (n^2 - p^2)^{1/2}[\bar{q}_1\nabla_2\zeta(\bar{\mathbf{q}}) + q_2\nabla_1\zeta(\bar{\mathbf{q}})], \quad (3.7) \end{aligned}$$

as may be easily verified. If the surface $\zeta(\mathbf{q})$ has rotational symmetry around the optical axis [i.e., as $\zeta(|\mathbf{q}|)$], then the second summand is zero, and $q_1p_2 - q_2p_1$ is the skewness invariant of the ray; it is the link to angular momentum theory.

The transformation [Eqs. (3.6)] is peculiar in that it is defined *implicitly*; $\bar{\mathbf{q}}$ appears on the right-hand side of the function ζ and is not easily extractable. As is obvious from Fig. 1, the values of the incoming ray (\mathbf{p}, \mathbf{q}) could be chosen such that they are tangent to ζ at some point \mathbf{q}_0 and thereafter cross ζ at two or more points. These will be the singular points, and they will form lines in \mathbf{q} space and also in \mathbf{p} space. The implicit function theorem¹¹ allows us to have continuously differentiable functions $\bar{\mathbf{p}}(\mathbf{p}, \mathbf{q})$ and $\bar{\mathbf{q}}(\mathbf{p}, \mathbf{q})$ in a neighborhood of a regular point when the transformation Jacobian is nonsingular. The latter is easily calculated as a 4×4 matrix, reducible to a 2×2 one, which is $1 - (n^2 - p^2)^{-1/2}\mathbf{p} \cdot \nabla\zeta(\bar{\mathbf{q}})$. The regular points in phase space are those for which $(n^2 - p^2)^{-1/2}\mathbf{p} \cdot \nabla\zeta(\bar{\mathbf{q}}) \neq 1$. In terms of the angles in the figure, this says that $\tan \theta |\nabla\zeta(\bar{\mathbf{q}})| \neq 1$; when the surface is anything but a z plane, $|\nabla\zeta(\bar{\mathbf{q}})| > 0$ for some $\bar{\mathbf{q}}$, and, as θ increases from zero, a singular point must be crossed. The equality is achieved when $\theta_0 + \psi = \pi/2$, i.e., tangency indeed.

By means of collimator screens we may always stay within a region of regularity of our hard-surface root transformation $R_{\zeta,n}$. (This nonglobality may cast a spell on the possibility of quantizing the transformation.)

4. THE OPTICAL CENTER OF A SURFACE FOR A POINT

Since we are obviously interested in having a reference system in phase space with the origin as far away from singularities as possible when the coordinates are transformed under Eqs. (3.6), let us speak of an optical axis and center for our system. Actual optical lenses are built with an optical axis, usually of rotational symmetry or at least of two intersecting plane reflection symmetries. Reason dictates that we place the optical center at the origin of phase space ($\mathbf{p} = \mathbf{0}, \mathbf{q} = \mathbf{0}; z = 0$). We shall then have the function described by $\zeta(\mathbf{q})$, such that $\zeta(\mathbf{0}) = 0$ and $\nabla\zeta(\mathbf{0}) = \mathbf{0}$. The advantage of having the optical axis and center thus defined with respect to the

surface is that the ray at the origin of phase space will remain there after the surface transformation. In detail, $\zeta(\mathbf{0}) = 0 \Rightarrow \mathbf{q}(\bar{\mathbf{p}}, \mathbf{0}) = \mathbf{0}$ (any ray through the optical center is crossing the $z = 0$ surface there, so $\bar{\mathbf{q}} = \mathbf{q} = \mathbf{0}$) and $\nabla\zeta(\mathbf{0}) = \mathbf{0} \Rightarrow \mathbf{p}(\bar{\mathbf{p}}, \mathbf{0}) = \bar{\mathbf{p}}$ (the momentum of rays through the optical center is invariant, so that the angles obey Snell's law). Canonical transformations leaving the origin invariant^{1,12} are generated by second- and higher-order polynomial functions of phase space [see, for example, Eqs. (2.2)–(2.6)], and these have special Lie-algebraic properties. They have been used in current work on the group-theoretical treatment of aberrations. Here we shall not make explicit use of group-theoretical language, but, in the sections with applications, we shall translate it into order-of-approximation arguments.

The surface $\zeta(\mathbf{q})$ in Eqs. (3.6) may be quite arbitrary, so the origin of coordinates may not be a natural optical center for the system. Any point C on the surface ζ may be chosen to be an optical center through translation and rotation of the coordinates. In Fig. 1 we may choose a certain point C = $[q_0, \zeta(q_0)]$ on ζ to be the new origin of phase space through translation in z and \mathbf{q} so that, at the point C, the new coordinates be $\mathbf{q}' = \mathbf{0}, z' = 0$; rotation around C will finally make the new \mathbf{q}' plane tangent to ζ at C, and $\mathbf{p}' = \mathbf{0}$ will denote the direction of the optical axis. Each one of these operators is a canonical transformation of phase space that we shall now examine in turn.

z Translation

Suppose that, at C, $\zeta(\mathbf{q}_0) = c$. We perform the canonical transformation [Eq. (2.6)] by $z = c$ so as to shift the $z = 0$ plane to C:

$$\mathbf{p}' = \mathbf{p}, \quad \mathbf{q}' = \mathbf{q} + c\mathbf{p}/(n^2 - p^2)^{1/2}, \quad (4.1a)$$

$$\bar{\mathbf{p}}' = \bar{\mathbf{p}}, \quad \bar{\mathbf{q}}' = \bar{\mathbf{q}}. \quad (4.1b)$$

The new phase-space coordinates $(\mathbf{p}', \mathbf{q}')$ will transform under the refracting surface through Eqs. (3.6) but see the surface as described by $\chi(\mathbf{q}) = \zeta(\mathbf{q}) - c$ and $\chi(\mathbf{q}_0) = 0$. This will be the new ζ , and we may drop primes for the next operation.

q Translation

The point C chosen on ζ to be the optical center may be at $\mathbf{q}_0 \neq \mathbf{0}$. It is canonical simply to translate

$$\mathbf{p}' = \mathbf{p}, \quad \mathbf{q}' = \mathbf{q} - \mathbf{q}_0, \quad (4.2a)$$

$$\bar{\mathbf{p}} = \bar{\mathbf{p}}, \quad \bar{\mathbf{q}}' = \bar{\mathbf{q}} - \mathbf{q}_0. \quad (4.2b)$$

The surface transformation [Eqs. (3.6)] keeps its form but under a function $\chi(\mathbf{q}') = \zeta(\mathbf{q})$. The origin of phase space is now on C, and at C, $\chi(\mathbf{0}) = 0$. The optical axis is still tilted with respect to the surface normal at C. Again we label the surface ζ and drop primes.

p Translation

Suppose that the surface tilt is $\zeta'(0) = \tan \psi_0$. We must rotate the coordinate axes (q, z) by ψ_0 in the plane of Fig. 1 to new ones (q', z') ; the chosen optical center is at the origin, and the surface ζ is held fixed, as are the ray paths with $\theta' = \theta + \psi_0$ and $\psi' = \psi - \psi_0$. Geometry and Eq. (2.1) lead to the following relations for the coordinates in the plane of rotation:

$$\begin{aligned}
 p' &= \sin \psi_0 (n^2 - p^2)^{1/2} + \cos \psi_0 p, \\
 q' &= q [\cos \psi_0 - \sin \psi_0 p / (n^2 - p^2)^{-1/2}], \quad (4.3a)
 \end{aligned}$$

$$\begin{aligned}
 \bar{p}' &= \bar{p} [\cos \psi_0 + \zeta'(\bar{q}) \sin \psi_0]^{-1}, \\
 \bar{q}' &= \cos \psi_0 \bar{q} + \sin \psi_0 \zeta(\bar{q}). \quad (4.3b)
 \end{aligned}$$

These transformations are canonical. The new phase-space coordinates undergo the surface transformation [Eq. (3.6a)] but see it as described by the surface $\chi(\bar{q}') = -\sin \psi_0 \bar{q}' + \cos \psi_0 \zeta(\bar{q})$, which now satisfies $\nabla \chi(\mathbf{0}) = \mathbf{0}$. In dropping primes, we have related Eqs. (3.6) to the coordinates where the optical center is C. In this frame, the origin of phase space is mapped on itself.

Rotation to Principal Axes

At this point $\zeta(\mathbf{0}) = 0, \nabla \zeta(\mathbf{0}) = \mathbf{0}$ implies that the Taylor series of ζ in the components of \mathbf{q} has only second- and higher-order terms. The *quadratic* terms (if any) will have the form $a q_1^2 + b q_1 q_2 + c q_2^2$. Through a rotation of the coordinate system around the optical axis, we can always bring this form to principal axes, i.e., $a' q_1'^2 + c' q_2'^2$. Most surfaces of optical interest are axisymmetric, but magnetic devices³ in general are not.

Through these four transformations we may turn any point on the refracting surface into its optical center where the transformation $R_{\zeta,n}$ takes its simplest form; the surface function $\zeta(\mathbf{q})$ is not less than quadratic. This may be seen in the context of the result¹² that any optical path can be taken as an optical axis³ or design orbit¹² for the system. The concatenated mapping is then that of neighborhoods in object and image phase spaces around the reference ray.

5. CONCATENATION TO THE SURFACE TRANSFORMATION

The refracting-surface transformation will map incoming rays (\mathbf{p}, \mathbf{q}) onto outgoing rays (\mathbf{p}', \mathbf{q}'), mediated by the quantities $(\bar{\mathbf{p}}, \bar{\mathbf{q}})$. (Primes refer hereafter, as in Section 3, to image coordinates on the $z = 0$ plane.) The meaning of $\bar{\mathbf{q}}$ is that of point of contact with the surface; the meaning of $\bar{\mathbf{p}}$ is less evident, but from Snell's law [Eqs. (3.4)] it appears to be $\cos \psi$ times the momentum taken with respect to the surface normal as an axis. In terms of $R_{\zeta,n}$, Eqs. (3.3) and (3.5) read as

$$(R_{\zeta,n} f)(\mathbf{p}, \mathbf{q}) = f(\bar{\mathbf{p}}, \bar{\mathbf{q}}) = (R_{\zeta,n} f)(\mathbf{p}', \mathbf{q}') \quad (5.1)$$

on any function of phase space f , understanding that $(R_{\zeta,n} f)(\mathbf{p}, \mathbf{q}) = f(R_{\zeta,n} \mathbf{p}, R_{\zeta,n} \mathbf{q})$. Since the $R_{\zeta,n}$ are canonical, their inverse $R_{\zeta,n}^{-1}$ exists at all regular points, and thus we may write the surface transformation

$$\begin{aligned}
 f(\mathbf{p}', \mathbf{q}') &= (S_{\zeta,n \rightarrow n'} f)(\mathbf{p}, \mathbf{q}) \\
 &= (R_{\zeta,n'}^{-1} f)(\bar{\mathbf{p}}, \bar{\mathbf{q}}) \\
 &= [R_{\zeta,n} (R_{\zeta,n'}^{-1} f)](\mathbf{p}, \mathbf{q}) \quad (5.2)
 \end{aligned}$$

on any function, i.e.,

$$S_{\zeta,n \rightarrow n'} = R_{\zeta,n} R_{\zeta,n'}^{-1}. \quad (5.3)$$

Since the root transformations $R_{\zeta,n}$ are canonical, so is⁸ the composition $S_{\zeta,n \rightarrow n'}$.

Whether this result is useful should be judged by the ease

with which we may apply the root transformations to calculate $\bar{\mathbf{p}}, \bar{\mathbf{q}}$ in explicit form up to a given aberration order and concatenate the result to produce the refracting-surface transformation. This we do in detail in Sections 6 and 7 for cubic surfaces and quartic lenses.

6. SECOND-ORDER ABERRATIONS IN GENERAL CUBIC SURFACES

As we saw in Section 4, we may orient our phase-space axes so that a cubic surface ζ be such that $\zeta(\mathbf{0}) = 0$ and $\nabla \zeta(\mathbf{0}) = \mathbf{0}$; through rotation around the optical axis, we may bring the quadratic part to its principal axes, so that the most general cubic surface is

$$\begin{aligned}
 \zeta(\mathbf{q}) &= \beta_1 q_1^2 + \beta_2 q_2^2 + \gamma_0 q_1^3 \\
 &\quad + \gamma_1 q_1^2 q_2 + \gamma_2 q_1 q_2^2 + \gamma_3 q_2^3 \quad (6.1a)
 \end{aligned}$$

and thus

$$\begin{aligned}
 \nabla_1 \zeta(\mathbf{q}) &= 2\beta_1 q_1 + 3\gamma_0 q_1^2 \\
 &\quad + 2\gamma_1 q_1 q_2 + \gamma_2 q_2^2, \quad (6.1b)
 \end{aligned}$$

$$\begin{aligned}
 \nabla_2 \zeta(\mathbf{q}) &= 2\beta_2 q_2 + \gamma_1 q_1^2 \\
 &\quad + 2\gamma_2 q_1 q_2 + 3\gamma_3 q_2^2. \quad (6.1c)
 \end{aligned}$$

We may calculate the effect on phase space of this refracting surface through calculation of the root transformations [Eqs. (3.6)] to second order in the components of \mathbf{p} and \mathbf{q} , the aberration order. Whatever higher orders are calculated, the essential part of the transformation, i.e., the effective action of the surface as a finite canonical transformation, is contained in the second approximation, as we shall see below. All higher-order approximations may be obtained in terms of the set of parameters β_1, \dots, γ_3 , all of which already appear in second order. The information relevant for the concatenation of optical elements is contained maximally at that aberration order, for surfaces of the aberration order plus 1.

We recall, from well-known expansion series, that

$$\sqrt{n^2 - p^2} = n - \frac{p^2}{2n} - \frac{p^4}{8n^3} - \dots, \quad (6.2a)$$

$$\frac{1}{\sqrt{n^2 - p^2}} \mathbf{p} = \frac{1}{n} \mathbf{p} + \frac{p^2}{2n^3} \mathbf{p} + \frac{3p^4}{8n^5} \mathbf{p} + \dots \quad (6.2b)$$

Now, substituting Eqs. (6.1a) and (6.2b) into Eq. (3.6b), we obtain

$$\begin{aligned}
 \bar{\mathbf{q}} &= \mathbf{q} + (\beta_1 q_1^2 + \beta_2 q_2^2 + \dots) \left(\frac{1}{n} \mathbf{p} + \dots \right) \\
 &= \mathbf{q} + O_3(\mathbf{p}, \bar{\mathbf{q}}). \quad (6.3a)
 \end{aligned}$$

So, up to second order, $\bar{\mathbf{q}} = \mathbf{q}$. We use this information to replace Eqs. (6.1a), (6.1b), and (6.2a) in Eq. (3.6a) to find

$$\begin{aligned}
 \bar{\mathbf{p}} &= \mathbf{p} + \left(n - \frac{1}{2n} p^2 - \dots \right) (\nabla \zeta)(\bar{\mathbf{q}}) \\
 &= \mathbf{p} + n(\nabla \zeta)(\mathbf{q}) + O_5(\mathbf{p}, \bar{\mathbf{q}}). \quad (6.3b)
 \end{aligned}$$

These expressions for $\bar{\mathbf{p}}$ and $\bar{\mathbf{q}}$ in terms of \mathbf{p} and \mathbf{q} are now completely explicit through Eqs. (6.1) and constitute the

root transformation $R_{\zeta,n}$. The inverse root transformation is simply

$$\mathbf{q} = \bar{\mathbf{q}}, \quad \mathbf{p} = \bar{\mathbf{p}} - n(\nabla\zeta)(\bar{\mathbf{q}}). \quad (6.4)$$

The final point in the program is to concatenate Eqs. (6.3) and (6.4) to the surface transformation $S_{\zeta,n \rightarrow n'}$ through their composition [Eq. (5.3)]. This we may do explicitly on the position coordinates:

$$S_{\zeta,n \rightarrow n'}: \mathbf{q} = \mathbf{q}' = \bar{\mathbf{q}} = \mathbf{q}. \quad (6.5a)$$

Cubic surfaces may thus be replaced by planes in configuration space to second approximation, as one does in Gaussian optics when introducing "plane" lenses. The effect of the surface transformation is felt only in the ray directions:

$$\begin{aligned} S_{\zeta,n \rightarrow n'}: \mathbf{p} = \mathbf{p}' = \mathbf{p} - n'(\nabla\zeta)(\bar{\mathbf{q}}) \\ = \mathbf{p} + (n - n')(\nabla\zeta)(\mathbf{q}). \end{aligned} \quad (6.5b)$$

Thus, in coordinates, the effect of ζ is

$$q'_1 = q_1, \quad q'_2 = q_2, \quad (6.6a)$$

$$p'_1 = p_1 + (n - n')(2\beta_1 q_1 + 3\gamma_0 q_1^2 + 2\gamma_1 q_1 q_2 + \gamma_2 q_2^2), \quad (6.6b)$$

$$p'_2 = p_2 + (n - n')(2\beta_2 q_2 + \gamma_1 q_1^2 + 2\gamma_2 q_1 q_2 + 3\gamma_3 q_2^2), \quad (6.6c)$$

In particular, we may calculate, to third order,

$$\begin{aligned} q'_1 p'_2 - q'_2 p'_1 = q_1 p_2 - q_2 p_1 \\ + 2(n - n')(\beta_2 - \beta_1)q_1 q_2 \\ + (n - n')[\gamma_1 q_1^3 + (2\gamma_2 - 3\gamma_0)q_1^2 q_2 \\ + (3\gamma_3 - 2\gamma_1)q_1 q_2^2 - \gamma_2 q_2^3]. \end{aligned} \quad (6.7)$$

Thus no cubic surface will leave the quadratic function $q_1 p_2 - q_2 p_1$ invariant. Also, in this approximation, the transformation is canonical to all orders, and there are no finite singular points of the transformation.

We have developed the last equations explicitly in two-dimensional Cartesian coordinates, but even if we have the vector expressions (6.5), this may not be the best account of the general situation. In three-dimensional configuration space (to describe, for instance, chromatic dispersion in magnetic-lens accelerators³), we may use a spherical-harmonic type of expansion of the aberration terms over configuration space (the operator associated with $\mathbf{q} \times \mathbf{p}$ being the familiar angular momentum operator). The same classification of terms serves to specify the transformation properties under the symplectic group of Gaussian linear transformations. Symplectic matrices may be inverted easily and the same program followed once the N th-order aberrations are classified into multiplets under the Gaussian symplectic group.

7. THIRD-ORDER ABERRATIONS IN QUARTIC LENS SURFACES

In this section we examine the third-order aberrations produced by the axisymmetric surface of a quartic lens:

$$\zeta(\mathbf{q}) = \beta q^2 + \delta(q^2)^2, \quad (7.1a)$$

$$(\nabla\zeta)(\mathbf{q}) = 2\beta\mathbf{q} + 4\delta q^2\mathbf{q}. \quad (7.1b)$$

The root transformations [Eqs. (3.6)] may be easily expanded to third order in the phase-space variables by using Eq. (6.2b):

$$\begin{aligned} \bar{\mathbf{q}} &= \mathbf{q} + (\beta\bar{q}^2 + \dots)\left(\frac{1}{n} + \dots\right)\mathbf{p} \\ &= \mathbf{q} + \frac{\beta}{n}q^2\mathbf{p}. \end{aligned} \quad (7.2a)$$

Using this result, we expand for the conjugate momentum:

$$\begin{aligned} \bar{\mathbf{p}} &= \mathbf{p} + (2\beta\bar{\mathbf{q}} + 4\delta\bar{q}^2\bar{\mathbf{q}})\left(n - \frac{1}{2n}p^2 - \dots\right) \\ &= \mathbf{p} + 2n\beta\left(\mathbf{q} + \frac{\beta}{n}q^2\mathbf{p}\right) - \frac{\beta}{n}p^2\mathbf{q} + 4n\delta q^2\mathbf{q} \\ &= \mathbf{p} + 2n\beta\mathbf{q} - \frac{\beta}{n}p^2\mathbf{q} + 2\beta^2 q^2\mathbf{p} + 4n\delta q^2\mathbf{q}. \end{aligned} \quad (7.2b)$$

Next, we need to know the transformation inverse to Eqs. (7.2) to third order in the phase-space variables, i.e., we need the coefficients in

$$\begin{aligned} \mathbf{p} &= a\bar{\mathbf{p}} + b\bar{\mathbf{q}} + G\bar{p}^2\bar{\mathbf{p}} + H\bar{p} \cdot \bar{q}\bar{\mathbf{p}} \\ &\quad + J\bar{p}^2\bar{\mathbf{q}} + K\bar{p} \cdot \bar{q}\bar{\mathbf{q}} + L\bar{q}^2\bar{\mathbf{p}} + F\bar{q}^2\bar{\mathbf{q}}, \end{aligned} \quad (7.3a)$$

$$\begin{aligned} \bar{\mathbf{q}} &= c\bar{\mathbf{p}} + d\bar{\mathbf{q}} + U\bar{p}^2\bar{\mathbf{p}} + V\bar{p} \cdot \bar{q}\bar{\mathbf{p}} + W\bar{p}^2\bar{\mathbf{q}} \\ &\quad + X\bar{p} \cdot \bar{q}\bar{\mathbf{q}} + Y\bar{q}^2\bar{\mathbf{p}} + Z\bar{q}^2\bar{\mathbf{q}}. \end{aligned} \quad (7.3b)$$

We replace Eqs. (7.3) into Eq. (7.2a), keeping terms of up to third order, and find that $c = 0$, $d = 1$, $U = V = W = X = 0$, $Y = -\beta a/n$, $Z = -\beta b/n$ for Eq. (7.3b); this new result and Eq. (7.3a) replaced into Eq. (7.2b) lead us to find $a = 1$, $b = -2n\beta$, $G = H = L = 0$, $J = \beta/n$, $K = -4\beta^2$, $M = 4n(\beta^3 - \delta)$. The cubic transformation inverse to Eqs. (7.2) is thus

$$\mathbf{q} = \bar{\mathbf{q}} - \frac{\beta}{n}\bar{q}^2\bar{\mathbf{p}} + 2\beta^2\bar{q}^2\bar{\mathbf{q}}, \quad (7.4a)$$

$$\mathbf{p} = \bar{\mathbf{p}} - 2n\beta\bar{\mathbf{q}} + \frac{\beta}{n}\bar{p}^2\bar{\mathbf{q}} - 4\beta^2\bar{p} \cdot \bar{q}\bar{\mathbf{q}} + 4n(\beta^3 - \delta)\bar{q}^2\bar{\mathbf{q}}. \quad (7.4b)$$

An equivalent method may be used to invert the transformation: We rewrite Eqs. (3.6), pulling out \mathbf{p} and \mathbf{q} in terms of $\bar{\mathbf{p}}$, $\bar{\mathbf{p}}$, and $\bar{\mathbf{q}}$. Now we replace Eq. (3.6a) into itself to obtain Eq. (7.4b) and substitute this information into Eq. (3.6b) to obtain Eq. (7.4a). Note that the order of replacement is now inverted.

Finally, we concatenate the two root transformations to the surface transformation through Eq. (5.3). This entails placing Eqs. (7.2) (with a refractive index n) into Eqs. (7.4) (with \mathbf{q}' and \mathbf{p}' on the left-hand side and n' for refractive index) and keeping up to third-order terms. This leads quickly to

$$\mathbf{q}' = \mathbf{q} + \beta\left(\frac{1}{n} - \frac{1}{n'}\right)q^2\mathbf{p} + 2\beta^2\left(1 - \frac{n}{n'}\right)q^2\mathbf{q}, \quad (7.5a)$$

$$\begin{aligned} \mathbf{p}' &= \mathbf{p} + 2\beta(n - n')\mathbf{q} - \beta\left(\frac{1}{n} - \frac{1}{n'}\right)p^2\mathbf{q} \\ &+ 2\beta\left(1 - \frac{n'}{n}\right)q^2\mathbf{p} - 4\beta^2\left(1 - \frac{n'}{n}\right)p \cdot \mathbf{q}\mathbf{q} \\ &+ 4(n - n')\left(\delta + \beta^3\frac{n - n'}{n'}\right)q^2\mathbf{q}. \end{aligned} \quad (7.5b)$$

This is the linear + third-order phase-space transformation produced by the refracting surface ζ in Eq. (7.1a).

We will now relate the refracting-surface transformation [Eqs. (7.5)] to the third-order Seidel aberrations obtained from the Lie-algebraic methods followed by Dragt for quartic lenses.¹ The latter methods use the Lie series¹³ derived from the action of an operator associated with a function of phase space \mathbf{p}, \mathbf{q} though Eq. (2.3b), on phase itself, through explicit evaluation of the exponential series [Eqs. (2.3a)–(2.4)]. The full exponential-series transformation is canonical, whereas any truncated series such as Eqs. (7.5) is canonical only up to the order of truncation. Equations (7.5), nevertheless, contain all the information needed to obtain the Seidel coefficients of the surface.

It is known^{1-3,5} that the Gaussian lens-surface transformation is generated by the exponentiation of the quadratic function

$$g(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \nu q^2 \quad (7.6a)$$

and is a linear transformation of phase space:

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \rightarrow \begin{pmatrix} \mathbf{p}_g \\ \mathbf{q}_g \end{pmatrix} = e^{\hat{g}} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \begin{pmatrix} \mathbf{p} + \nu\mathbf{q} \\ \mathbf{q} \end{pmatrix}, \quad (7.6b)$$

for $\nu = 2\beta(n - n')$. Dragt¹ has used the phase-space transformation generated by polynomial functions $f(\mathbf{p}, \mathbf{q})$ of order 4 to define six Seidel aberration coefficients $A, B, C, D, E,$ and F . They appear in the quartic function f as

$$\begin{aligned} f(\mathbf{p}, \mathbf{q}) &= A(p^2)^2 + Bp^2p \cdot \mathbf{q} + C(p \cdot \mathbf{q})^2 \\ &+ Dp^2q^2 + Ep \cdot \mathbf{q}q^2 + F(q^2)^2. \end{aligned} \quad (7.7a)$$

The generated transformation, to third order, is

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \rightarrow \begin{pmatrix} \mathbf{p}_f \\ \mathbf{q}_f \end{pmatrix} = e^{\hat{f}} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \begin{pmatrix} \mathbf{p} + Bp^2\mathbf{p} + 2Cp \cdot \mathbf{q}\mathbf{p} + 2Dp^2\mathbf{q} + 2Ep \cdot \mathbf{q}\mathbf{q} + Eq^2\mathbf{p} + 4Fq^2\mathbf{q} \\ \mathbf{q} - 4Ap^2\mathbf{p} - 2Bp \cdot \mathbf{q}\mathbf{p} - Bp^2\mathbf{q} - 2Cp \cdot \mathbf{q}\mathbf{q} - 2Dq^2\mathbf{p} - Eq^2\mathbf{q} \end{pmatrix}. \quad (7.7b)$$

This result uses only the first term in the exponential series of \hat{f} .

The definition of A, \dots, F as aberration coefficients (independent of the relative size or Gaussian transformation between object and image phase-space planes) and based on the concept of aberration as a purely cubic transformation of phase space may be proposed. The six coefficients are named by the type of lens aberrations that they generate. These are A , spherical aberration; B , coma; C , astigmatism; D , curvature of field; E , distortion; and F , "pocus." The quartic surface [Eq. (7.1a)] may be found to be generated as¹⁴

$$\begin{aligned} e^{\hat{g}} e^{\hat{f}} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} &= e^{\hat{g}} \begin{pmatrix} \mathbf{p}_f(\mathbf{p}, \mathbf{q}) \\ \mathbf{q}_f(\mathbf{p}, \mathbf{q}) \end{pmatrix} \\ &= \begin{bmatrix} \mathbf{p}_f(e^{\hat{g}}\mathbf{p}, e^{\hat{g}}\mathbf{q}) \\ \mathbf{q}_f(e^{\hat{g}}\mathbf{p}, e^{\hat{g}}\mathbf{q}) \end{bmatrix} = \begin{pmatrix} \mathbf{p}' \\ \mathbf{q}' \end{pmatrix}. \end{aligned} \quad (7.8)$$

Now, substituting Eq. (7.6b) into Eq. (7.7b) as required by Eq. (7.8), we can compare this with the phase-space transformation found above in Eqs. (7.5) through the coefficients of the linear and cubic terms. In this way we find the six aberration coefficients to be

$$\begin{aligned} A &= 0, & B &= 0, & C &= 0, \\ D &= \frac{\beta}{2} \left(\frac{1}{n'} - \frac{1}{n} \right), & E &= 2\beta^2 \left(1 - \frac{n'}{n} \right), \\ F &= \delta(n - n') - 2\beta^3 \frac{(n - n')^2}{n}. \end{aligned} \quad (7.9)$$

These match the values found by Dragt¹⁵ and express the refracting-surface transformation as a product $e^{\hat{g}}e^{\hat{f}}$ with g quadratic and f quartic in phase space.

On the basis of work in Ref. 9 and that in progress, we can offer an expression of the refracting-surface transformation $S_{\zeta, n \rightarrow n'}$ as a single exponential $e^{\hat{k}}$, with¹⁶

$$\begin{aligned} k(\mathbf{p}, \mathbf{q}) &= (n - n')\beta q^2 + \frac{\beta(n - n')}{2nn'} p^2 q^2 + \beta^2 \frac{n^2 - n'^2}{nn'} p \cdot \mathbf{q}q^2 \\ &+ (n - n') \left[\delta + \frac{\beta^3 [n - n']^2}{3nn'} \right] (q^2)^2. \end{aligned} \quad (7.10)$$

A pure refracting-surface transformation has no spherical aberration, coma, or astigmatism. Its concatenation with free-space propagation will generate them, however. The operator associated with Eq. (7.10) qualifies as the *logarithm* of the surface transformation $S_{\zeta, n \rightarrow n'}$ in Eq. (5.3). The logarithm of the root transformation $R_{\zeta, n} = e^{\hat{r}}$ in Eqs. (3.6) is the operator associated with

$$r(\mathbf{p}, \mathbf{q}) = n\beta q^2 - \frac{\beta}{n} p^2 q^2 + 2\beta^2 p \cdot \mathbf{q}q^2 + n \left(\delta - \frac{2}{3} \beta^3 \right) (q^2)^2. \quad (7.11)$$

It has a structure that seems to be rather simple.

8. CONCLUSION

Lie-algebraic methods for the treatment of optical systems may benefit from the consideration of finite group transformations. For free transit in a homogeneous medium the two are equivalent: The finite group element is simply generated by the optical Hamiltonian. For refracting surfaces, finite group transformations seem to be more natural than infinitesimally generated ones. Of course, the two methods continue to be equivalent, as exemplified in Eqs. (7.6)–(7.9). The simplicity of the geometric construction presented in Fig. 1 should be compelling. In his work in Ref. 1, Dragt does not detail the construction of $f(\mathbf{p}, \mathbf{q})$ in Eqs. (7.7a)–(7.9), which follows from rather laborious ray tracing in a compound system. Ray tracing is also involved in treating the refracting surface through the total transformation $(\mathbf{p}, \mathbf{q}) \rightarrow (\mathbf{p}', \mathbf{q}')$ when both sides of Eqs. (3.3)–(3.4) are

expanded to third order; this method was followed in Ref. 9, leading to Eqs. (7.9) after about a page of algebra.

The factorization theorem presented in this paper, however, simplifies the latter method considerably since in $R_{\zeta,n}$ the implicit relations in the root transformations [Eqs. (3.6)] take a form close to total explicitness. The self-replacement of \bar{q} into $\zeta(\bar{q})$ may be done efficiently in symbolic computational languages. To third order, it was done in the five lines of Eqs. (7.2). One still has to invert the transformation to $R_{\zeta,n}^{-1}$ and concatenate as $R_{\zeta,n}R_{\zeta,n}^{-1}$ to obtain the resulting action on phase space to aberration order and from there define appropriate aberration coefficients. This was done here longhand, without recourse to further group theory. In Chap. 4 of Ref. 17 we indicate how we may proceed for simple aberrations in a two-dimensional object plane so as to use the fact that axisymmetric lens aberrations transform as finite-dimensional bases for (nonunitary) irreducible representations of the Gaussian group $Sp(2, R)$ (equivalent to that of 2×2 matrices). They behave almost exactly as multipole expansions in angular momentum theory. This leads one to represent this group in a matrix *cum* vector form. From this realization one may invert and concatenate transformations rather easily. A computer program has been prepared using this method.

APPENDIX A: PROOF OF THE THEOREM

Writing $\rho = (n^2 - p^2)^{1/2}$ we put Eqs. (3.6) as

$$\bar{q}_i = q_i + \zeta \rho^{-1} p_i, \quad (A1a)$$

$$\bar{p}_i = p_i + \zeta_i \rho \quad (A1b)$$

for every regular point of the transformation. Since ζ possesses a differentiable derivative, we have a neighborhood of regularity. We note that, since ζ depends only on \bar{q} , then $d\zeta = \sum \zeta_i d\bar{q}_i$. Also, $d\rho^{-1} = \frac{1}{2} \rho^{-3} dp^2$ and $dp^2 = 2\sum p_i dp_i$. Applying external differentiation to Eq. (A1a),

$$d\bar{q}_i = dq_i + \rho^{-1} p_i d\zeta + \zeta p_i d\rho^{-1} + \zeta \rho^{-1} dp_i. \quad (A2)$$

This we use in building the Pfaffian one-form (see Ref. 10, Sec. 10.5):

$$\begin{aligned} \bar{\alpha} &= \sum \bar{p}_i d\bar{q}_i \\ &= \sum p_i dq_i + \rho d\zeta \\ &= \sum p_i dq_i + \rho^{-1} p^2 d\zeta + \zeta p^2 d\rho^{-1} + \frac{1}{2} \zeta \rho^{-1} dp^2 + \rho d\zeta \\ &= \alpha + (\rho^{-1} p^2 + \rho) d\zeta + \zeta (p^2 + \rho^2) d\rho^{-1} \\ &= \alpha + n^2 \rho^{-1} d\zeta + n^2 \zeta d\rho^{-1} \\ &= \alpha + n^2 d(\zeta \rho^{-1}). \end{aligned} \quad (A3)$$

Hence, by Poincaré's lemma, $d\bar{\alpha} = d\alpha$. In coordinates,

$$\sum d\bar{p}_i \wedge d\bar{q}_i = \sum dp_i \wedge dq_i. \quad (A4)$$

Expanding the first member in $dp_j \wedge dq_k$, the coefficients tell us that \bar{p}_j, \bar{q}_k obey a fundamental set of Lagrange

brackets and thus (see Ref. 8, Sec. 8.4) also of Poisson brackets. These coordinates of phase space are thus a canonical set. Notice that there is no restriction on the dimension of the optical object space.

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