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Lie-Hamilton geometric aberration optics: symmetries and symbolic computation

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ABSTRACT. We review the Lie-Hamilton treatment of optical aberrations to highlight its algorithmic composition property for concatenation of optical elements. `mexLIE` is a set of symbolic computation functions developed by the authors which permits the fully parametric design of optical systems including free spaces, aligned radial graded-index media, and polynomial refracting surfaces between these, to seventh aberration order. We give simple examples to illustrate its use.

RESUMEN. Revisamos el tratamiento de aberraciones ópticas de Lie-Hamilton para destacar su propiedad de concatenación algorítmica de elementos ópticos. `mexLIE` es un paquete de funciones para cómputo simbólico desarrollado por los autores, que permite el diseño completamente paramétrico de sistemas ópticos, incluyendo espacios libres, medios con gradiente de índice radial alineados, y superficies refractantes de perfil polinomial entre éstos, a séptimo orden de aberración. Damos ejemplos sencillos para ilustrar su uso.

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1. OUTLINE

Symmetry is an integral part of the mathematical tools to analyze classical and quantum mechanics, and simplify the study of composite systems. Such techniques—and indeed, such point of view—also apply in geometric optics. Optical models have added advantages over mechanical ones in the use of symmetry, because:

- The basic laws of optics are known exactly and are formulated axiomatically as conservation laws.
- Whereas mechanics considers continuous evolution under a variety of potentials (corresponding to a variety of refractive-index profiles in optical waveguides), optics has at its dispositon the "potential jolts" due to refracting surfaces.

The Lie-Hamilton formulation of geometric aberration optics applies the experience on the use of symmetry gained from quantum mechanics. Both classical and wave theories are equally amenable to group-theoretical treatment; the Lie brackets are Poisson brackets in the former and commutators in the latter, but the formalisms are essentially parallel otherwise. Thus we shall see that aberrations are set in one-to-one correspondence with the eigenstates of the quantum harmonic oscillator (symmetric three-quark multiplets). They generate flows of phase space that can be used to approximate the transformation due to an optical system in a large neighborhood of the design ray.

This review is organized as follows: the basics of the Lie-Hamilton formulation of geometric optics on phase space are presented in Sect. 2. Section 3 details the structure and classification of pure aberrations. The authors have built a set of symbolic computation functions that are now formalized in a program called `mexLIE` [1]. From Sect. 3 onwards we relate the Lie-Poisson aberration operators to functions in `mexLIE`. Section 4 mentions some optical elements present in the tabular functions of `mexLIE`, and Sect. 5 offers examples of concatenation of such elements to more general optical subsystems. Section 6 comments on the extant capabilities and structure of `mexLIE`.

2. Optical phase space transformations

Lie theory works in the arena of Hamiltonian phase-space coordinates for the manifold of rays. Refered to a plane screen, the rays of geometric optics are characterized by two coordinates of *position* $\mathbf{q} = (q_x, q_y) \in \Re^2$ and two coordinates of *momentum*-ray direction $\mathbf{p} = (p_x, p_y) = n \sin\theta\,(\cos\phi, \sin\phi)$.

We use the Lie-Poisson bracket between functions on the classical phase space coordinates,

$$\{f, g\}(\mathbf{p}, \mathbf{q}) = \frac{\partial f(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}} \cdot \frac{\partial g(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}} - \frac{\partial f(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}} \cdot \frac{\partial g(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}}.$$

In particular the *basic* Heisenberg-Weyl Lie brackets are

$$\{q_i, p_j\} = \delta_{i,j}, \qquad \{q_i, q_j\} = 0 = \{p_i, p_j\}.$$

A transformation $\mathcal{A}$ is termed *canonical* when it preserves this algebraic structure, *i.e.*, when

$$\mathcal{A} : \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} = \begin{pmatrix} \mathbf{p}'(\mathbf{p}, \mathbf{q}) \\ \mathbf{q}'(\mathbf{p}, \mathbf{q}) \end{pmatrix} \to \{q'_i, p'_j\} = \delta_{i,j}, \qquad \{q'_i, q'_j\} = 0 = \{p'_i, p'_j\}.$$

Optical elements are canonical transformations which are in general nonlinear [2]. When an optical system is symmetric under rotations around (and inversions through) a common axis, the four coordinates p_i, q_i reduce to three essential ones: $p^2 = \mathbf{p} \cdot \mathbf{p}$, $\mathbf{p} \cdot \mathbf{q}$, and $q^2 = \mathbf{q} \cdot \mathbf{q}$.

An axis-symmetric canonical map of phase space can be written in the generic form

$$\mathcal{A} = \mathcal{G}\{\mathbf{A}; \mathbf{M}\} = \mathcal{G}\{\mathbf{A}; \mathbf{1}\}\mathcal{G}\{\mathbf{0}; \mathbf{M}\}, \qquad \text{where} \qquad \mathbf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad \det \mathbf{M} = 1,$$

is the *paraxial* (*linear*) *part* of the transformation,

$$\mathcal{G}\{\mathbf{0};\mathbf{M}\}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix} = \mathbf{M}^{-1}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix} = \begin{pmatrix}d\mathbf{p} - b\mathbf{q}\\ -c\mathbf{p} + a\mathbf{q}\end{pmatrix},$$

and $\mathbf{A}$ labels the *aberration (nonlinear) part.*

The aberration part can be factorized into a product of transformations generated by operators corresponding to aberrations of increasing order. In Lie-Poisson exponential form, these are

$$\mathcal{G}\{\mathbf{A};\mathbf{1}\} = \cdots \times \exp\{A_4, \circ\}\exp\{A_3, \circ\}\exp\{A_2, \circ\},$$
$$\exp\{A_k, \circ\} = 1 + \{A_k, \circ\} + \tfrac{1}{2!}\{A_k, \{A_k, \circ\}\} + \cdots,$$
$$\{A_k, \circ\} = \frac{\partial A_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{q}}\cdot\frac{\partial}{\partial \mathbf{p}} - \frac{\partial A_k(\mathbf{p},\mathbf{q})}{\partial \mathbf{p}}\cdot\frac{\partial}{\partial \mathbf{q}},$$

where $A_k(\mathbf{p},\mathbf{q})$ are *aberration polynomials* of homogeneous degree $2k$ in the phase space coordinates $(\mathbf{p},\mathbf{q})$, and of degree k in the "axis-symmetric" phase space coordinates $(p^2, \mathbf{p}\cdot\mathbf{q}, q^2)$; k is called the *rank* and the *aberration order* is $2k-1$.

3. Aberration polynomials

The aberration polynomials of rank k have the following generic expansions in two bases:

$$\begin{aligned} A_k(p^2, \mathbf{p}\cdot\mathbf{q}, q^2) &= \sum_{k_1+k_2+k_3=k} A_{k_1k_2k_3}(p^2)^{k_1}(\mathbf{p}\cdot\mathbf{q})^{k_2}(q^2)^{k_3} \\ &= \sum_{j=k(-2)}^{1 \text{ or } 0}\ \sum_{m=-j}^{j} {}^kA^j_m\, {}^k\chi^j_m(p^2, \mathbf{p}\cdot\mathbf{q}, q^2), \end{aligned}$$

where the $\frac{1}{2}(k+1)(k+2)$ coefficients $A_{k_1k_2k_3}$ and ${}^kA^j_m$ are, respectively, the *monomial* and *symplectic* aberration coefficients, and ${}^k\chi^j_m(\vec{x})$ are the *symplectic* (essentially the solid spherical) harmonics [3]. Axis-symmetric aberrations are thus in 1 : 1 correspondence with the eigenstates of the three-dimensional quantum harmonic oscillator, $|k_1, k_2, k_3\rangle$ and $|k, j, m\rangle$ respectively, classified in cartesian and spherical coordinates. The symplectic basis is preferred for symbolic computation because it is the most economic for composition of transformations [4]. In Fig. 1 we arrange the monomial and symplectic coefficients in a pattern familiar from hadron multiplets (the paraxial part is $k=1$ and corresponds to the quark triplet). Angular momentum is here the *symplectic spin* $j = k,\ k-2,\ \ldots$ 1 or 0, and its "third projection" $m = -j,\ -j+1,\ \ldots, j$ has been called the *Seidel index.*

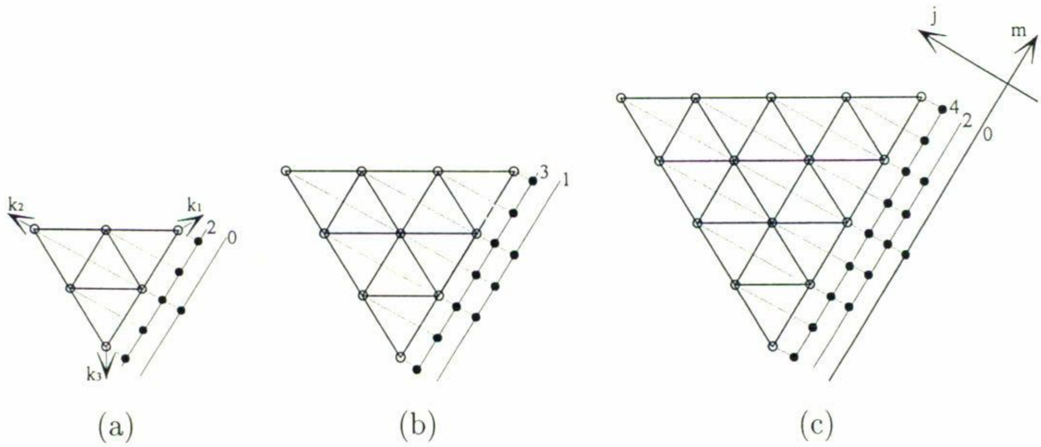

FIGURE 1. Aberration multiplets of orders 3 ($k = 2$, left), 5 ($k = 3$, mid) and 7 ($k = 4$, right). The open circles represent distinct aberrations classified by the 'number of quanta' k_1, k_2, k_3 (summing to k), as states of the 3-D quantum oscillator in the cartesian basis. The black circles represent their classification into symplectic spin multiplets j, m, as oscillator states in the angular momentum basis.

An axis-symmetric geometrical optical system will transform a ray $(\mathbf{p}, \mathbf{q})$ to

$$\begin{aligned}\mathcal{G}\{\mathbf{A}; \mathbf{1}\}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix} &= \cdots \times (1 + \{A_4, \circ\} + \cdots)(1 + \{A_3, \circ\} + \cdots)\\ &\qquad \times (1 + \{A_2, \circ\} + \tfrac{1}{2!}\{A_2, \{A_2, \circ\}\} + \tfrac{1}{3!}\{A_2, \{A_2, \{A_2, \circ\}\}\} + \cdots)\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix}\\ &= \big(1 + \{A_2, \circ\} + A_3, o + \tfrac{1}{2!}\{A_2, \{A_2, \circ\}\}\\ &\qquad + \{A_4, \circ\} + \{A_3, \{A_2, \circ\}\} + \tfrac{1}{3!}\{A_2, \{A_2, \{A_2, \circ\}\}\} + \cdots\big)\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix}\\ &= \begin{pmatrix}\mathbf{p}_A(\mathbf{p}, \mathbf{q})\\ \mathbf{q}_A(\mathbf{p}, \mathbf{q})\end{pmatrix}.\end{aligned}$$

One can consistently truncate the order of the polynomials and drop the ellipses. Thus in seventh aberration order, one needs to work only with up-to-eight degree polynomials; the canonicity of the transformation is then guaranteed up to eight-degree terms, *i.e.*, $\{q_{Ai}, p_{Aj}\} = \delta_{i,j}$ plus terms of order ten or higher.

In `mexLIE` [1], all functions $f(\mathbf{p}, \mathbf{q})$, $g(\mathbf{p}, \mathbf{q})$ of the phase space coordinates are Taylor-expanded and then truncated to rank k. This is the *aberration expansion*, structured and classified with quantum harmonic oscillator labels [3]. Finite optical transformations are thus characterized by the (matrix) parameters of the paraxial part, and a nested tower of aberration coefficients which describe the nonlinearity. The symplectic classification reduces aberrations to irreducible diagonal blocks under the paraxial part; it is used by `mexLIE` to format its tables optimally (of course, `mexLIE` can also use the monomial basis) for aberration orders $A = 2k - 1 = 3$, 5 and 7.

4. OPTICAL ELEMENTS

We have taken the task to determine the aberration coefficients of the basic elements of axis-symmetric optical systems to seventh aberration order. The basic elements include free flight in homogeneous and radial graded-index media and polynomial-shaped refracting surfaces of revolution between them. They are incorporated in `mexLIE` through tables. Below we offer two examples.

Free flight by z (along the optical axis) in a homogeneous medium of refractive index n is obtained, up to seventh aberration order (ranks $k = 1, 2, 3, 4$) by typing (with a numerical value for `K`)

? `THICK: FREEFLIGHT (Z, N, K)`

The answer given by the machine is the transformation `THICK` $= \mathcal{F}^{[k]}_{z,n}$, characterized by the "paraxial part" matrix $\mathbf{F} = \begin{pmatrix} 1 & 0 \\ -z/n & 1 \end{pmatrix}$ and a list of its Lie aberration coefficients. The six third-order coefficients are

$$F_{2,0,0} = -z/8n^3, \quad F_{1,1,0} = 0, \quad F_{1,0,1} = 0, \quad F_{0,2,0} = 0, \quad F_{0,1,1} = 0, \quad F_{0,0,2} = 0.$$

Only *spherical aberrations* $(k,0,0)$, $k = 2, 3, \ldots$ are different from zero.

A **refracting surface** of eighth-degree polynomial shape $z = \zeta(\mathbf{q}) = \zeta_2|\mathbf{q}|^2 + \zeta_4|\mathbf{q}|^4 + \zeta_6|\mathbf{q}|^6 + \zeta_8|\mathbf{q}|^8$ between two aligned radial graded-index media of the form $n(q)^2 = \nu^2 - \mu^2|\mathbf{q}|^2$ and $n'(q)^2 = \nu'^2 - \mu'^2|\mathbf{q}|^2$ is obtained from `mexLIE 2.0` by typing (for a definite numerical value of the rank `K`)

? `INTER: EFIBSURFACE (NU, MU, NUP, MUP, [Z2, Z4, Z6, Z8], K);`

The transformation (aberration group element) `INTER` $= \mathcal{S}^{[k]}_{n,n';\zeta}$ has the paraxial matrix $\mathbf{S} = \begin{pmatrix} 1 & 2(\nu' - \nu)\zeta_2 \\ 0 & 1 \end{pmatrix}$ and the following third-order aberration coefficients [5] (here in monomial basis)

a) astigmatism, $S_{1,0,1} = \zeta_2/2\nu' - \zeta_2/2\nu$,
b) coma, $S_{1,1,0} = 0$,
c) spherical aberration, $S_{2,0,0} = 0$
d) distorsion, $S_{0,1,1} = 2\zeta_2^2(\nu/\nu' - 1)$,
e) curvature of field, $S_{0,2,0} = 0$,
f) pocus, $S_{0,0,2} = \zeta_2(\mu' 2/2\nu' - \mu^2/2\nu) + \zeta_2^3(2\nu^2/\nu' - 4\nu + 2\nu') + \zeta_4(\nu - \nu')$

5. CONCATENATION OF OPTICAL ELEMENTS

We stress the fact that group elements (transformations) *multiply* as their optical counterparts concatenate—from left to right, along the z-axis. Whereas the linear part composes simply by matrix multiplication, the aberration part has a more complicated composition formula.

The *gato* composition $\sharp$ of two *pure* aberrations (*i.e.*, with unit paraxial matrix) is $\mathbf{C} = \mathbf{A} \sharp \mathbf{B}$. It stems from the Baker-Campbell-Hausdorff formula of the factored-product forms

$$\cdots \times \exp\{C_4, \circ\} \exp\{C_3, \circ\} \exp\{C_2, \circ\} = \cdots \times \exp\{A_4, \circ\} \exp\{A_3, \circ\} \exp\{A_2, \circ\} \\ \times \cdots \times \exp\{B_4, \circ\} \exp\{B_3, \circ\} \exp\{B_2, \circ\},$$

and is given explicitly, to seventh aberration order, by

$$C_2 = A_2 + B_2,$$
$$C_3 = A_3 + B_3 + \tfrac{1}{2}\{A_2, B_2\},$$
$$C_4 = A_4 + B_4 + \{A_2, B_3\} + \tfrac{1}{3}\{A_2, \{A_2, B_2\}\} - \tfrac{1}{6}\{\{A_2, B_2\}, B_2\}.$$

We may consistently truncate to rank k with group elements (transformations) $\mathcal{G}_k\{\mathbf{A}; \mathbf{M}\}$. The composition of two transformations of rank k involves the action of the paraxial part of left factor on the aberration part of the right factor:

$$\begin{aligned} \mathcal{G}_k\{\mathbf{A}; \mathbf{M}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{B}; \mathbf{N}\} &= \mathcal{G}_k\{\mathbf{A}; \mathbf{1}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{M}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{B}; \mathbf{1}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{N}\}, \\ &= \mathcal{G}_k\{\mathbf{A}; \mathbf{1}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{M}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{B}; \mathbf{1}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{M}\}^{-1} \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{M}\} \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{N}\}, \\ &= \mathcal{G}_k\{\mathbf{A}; \mathbf{1}\}\, \mathcal{G}_{\mathbf{k}}\{\mathbf{D}(\mathbf{M}, \mathbf{B}); \mathbf{1}\} \mathcal{G}_{\mathbf{k}}\{\mathbf{0}; \mathbf{MN}\}, \\ &= \mathcal{G}_k\{\mathbf{A} \sharp \mathbf{D}(\mathbf{M}, \mathbf{B}); \mathbf{MN}\}, \end{aligned}$$

where

$$\mathbf{D}(\mathbf{M}, \mathbf{B}) = \{\mathbf{D}^{(k)}(\mathbf{M}, B_k), \ \ldots\ , \mathbf{D}^{(3)}(\mathbf{M}, B_3), \mathbf{D}^{(2)}(\mathbf{M}, B_2)\}$$

is the adjoint action of the linear transformation $\mathbf{M}$ on the polynomial $B_k(\mathbf{p}, \mathbf{q})$, reduced by rank k. When we use the symplectic basis, then $\mathbf{D}^{(j)}(\mathbf{M}, B_k)$ is *completely* reduced by symplectic spin $j = k,\ k-2,\ \ldots\ \{^0_1$ into irreducible diagonal blocks. Herein lies the efficiency of this basis. `mexLIE` contains the function `COMPOSE (A, B, K)` which performs the above composition for the two (symbolic) transformations `A` and `B` to rank `K`.

For example, a singlet lens in air ($n = 1$), of thickenss t and homogeneous refractive index n, with faces ζ and ζ' as in Fig. 2a, is the composition

$$\texttt{SINGLET} = \mathcal{S}_{1,n;\zeta}\, \mathcal{F}_{t,n}\, \mathcal{S}_{n,1;\zeta'}.$$

It is obtained in `mexLIE` through

```
? SINGLET: COMPOSE (COMPOSE (INTER, THICK, K), INTER', K).
```

This singlet, when placed between an object at a distance z_0 to the left and a screen at a distance z_1 to the right, will produce a (generally unfocused) image, as in Fig. 2b. This *imager* system is obtained by composing

$$\texttt{IMAGER} = \mathcal{F}_{z_0,1}\ \texttt{SINGLET}\ \mathcal{F}_{z_1,1}.$$

In `mexLIE` this product of transformations is found by typing

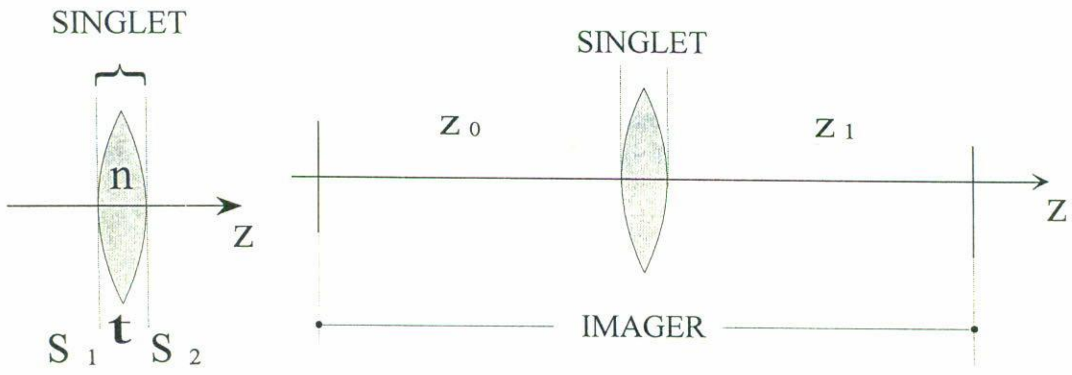

FIGURE 2. (a) Composition of $\mathcal{S}\ \mathcal{F}\ \mathcal{S}$: free flight between two surfaces to produce SINGLET. (b) Composition of $\mathcal{F}$ SINGLET $\mathcal{F}$ to IMAGER.

```
? IMAGER: COMPOSE ( COMPOSE (
FREEFLIGHT (Z0,1,K), SINGLET, K), FREEFLIGHT (Z1,1,K), K);
```

Finally, the action of IMAGER on the position coordinate of optical phase space, $\mathbf{q} \to \mathbf{q}'(\mathbf{p}, \mathbf{q})$, is obtained through the mexLIE function

```
? QPR: ACTONQ (IMAGER, K) $  PPR: ACTONP (IMAGER, K);
```

where all parameters of the system may appear with symbolic values. A similar function ACTONP (IMAGER, K) will yield the transformation of the momentum coordinates $\mathbf{p}$. Please note carefully that the classification and action of aberrations described with Lie-Hamilton methods is different from the traditional Seidel classification and action, which is based on the Lagrangian formulation of optics and the cross-variable point-angle Hamiltonian characteristic function [6]. The two approaches can be compared (and should agree) when the phase space transformations due to the optical system, $\mathbf{p}'(\mathbf{p}, \mathbf{q})$, and $\mathbf{q}'(\mathbf{p}, \mathbf{q})$, are written out explicitly.

As an example on the use of mexLIE, in reference [7] we proposed the following problem: suppose a generic optical system $\mathcal{A}$ is built to paraxial focus, so that its matrix part is upper-triangular and $\mathbf{q}'$ is function of $\mathbf{q}$ only (independent of the arriving ray directions $\mathbf{p}$). But of course the system also aberrates from third order on. The questions we posed was: through warping the screen (into a revolution surface with polynomial parameters), which aberrations are correctable, which *cannot* be corrected, and which are *immaterial* for point-image formation? The last part of the question can be answered immediately: distorsion and pocus [$m = -j$ and $-j+1$ in the symplectic basis or $(0, 1, k-1)$ and $(0, 0, k)$ in the monomial basis] are immaterial because they only produce $\mathbf{q}'(\mathbf{q})$, independent of $\mathbf{p}$. The solution to the first two questions is also well known to third aberration order: only curvature of field is corrected on a paraboloidal screen. (Notice again the *difference* between Seidel and Lie-Hamilton formulations: in the latter we correct the system through free flight to a warped surface; in the former we must recalculate the system to allow for the extra free flight that, by itself, does not "aberrate".)

It is perhaps surprising that, to aberration orders 5, 7, and 9, only *three* aberrations of each rank are correctable: in the monomial basis $(0, 2, k-2)$, $(1, 1, k-2)$, and $(1, 0, k-1)$. Linear optimization strategies can be set up once a cost function on the aberration set is agreed upon. (After all, there are more aberrations than polynomial parameters.) This is a stimulating analogue in optics of the Raccah algebra used in nuclear physics for mathematically similar problems.

6. STRUCTURE OF `mexLIE` [1]

`mexLIE` is a product of academic research that purports to be useful for parametric design of metaxial optical systems. It should also apply to any higher-order perturbation scheme which factors phase space transformations into a linear part and a nonlinear polynomial-based expansion. `mexLIE` has been published by `iimas-unam` and can be obtained from the authors; it includes a (103-page) manual and one high-density diskette.

`mexLIE` is written in `muSIMP`, a low-level list-handling derivate of `LISP` distributed by the Soft Warehouse since the mid-80s. The graphical display of aberration phenomena through their spot diagrams is accomplished through a `.COM` file of the program `SPOT_D` [8], which exists as an interactive program in `PASCAL` in the same diskette. The diskette will run *ab initio* on any good `pc`. A `MACSYMA` version is being prepared with essentially the same commands, that will run on larger machines without the limitation of infinite-precision representation of quotients and the 640 kb `RAM` memory restriction of `muSIMP`.

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