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Lie algebra method in charged particle optics

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Abstrakt

Tato práce částečně pokrývá problematiku analytických poruchových metod užívaných v optice nabitých částic, důraz je kladen především na výpočet geometrických aberací optického systému. Zejména se pak práce věnuje metodě Lieových algeber, která se standardně používá ve fyzice urychlovačů, a srovnává ji s metodami, jejichž použití je v optice častější.

Ve své práci se nejprve věnuji různým přístupům při popisu optických vlastností sytému, formulacím rovnice trajektorie a vlastnostem řešení jejího lineárního přiblížení. Dále jsou zde popsány jednotlivé analytické poruchové metody a jejich aplikace na jednoduchém příkladu osově symetrické magnetické čočky. V poslední kapitole je pak popsána symplektická klasifikace aberací.

V průběhu prvních let svého studia jsem se věnoval matematickému základu metody Lieových algeber, kanonickému poruchovému počtu a jejich vzájemnému vztahu. Zjistil jsem, že existuje přímý vztah mezi kanonickým poruchovým počtem a faktorizačním teorémem. Dále jsem použitím vhodné zobecněné kanonické transformace rozšířil použití metody Lieových algeber i na případ parametrizace trajektorie polohami v rovině předmětu a apertury, která se často používá v geometrické optice. Tuto metodu jsem s ostatními metodami aplikoval na příklad magnetické osově symetrické čočky, u kterého je možné jednotlivé přístupy snadno vzájemně porovnat.

Během dalšího studia jsem narazil na problém vhodné klasifikace aberačních polynomů a jejich vztahů. Ukázalo se, že klasifikace je ovlivněna tvarem paraxiální aproximace – ovlivňuje vztahy mezi aberačními koeficienty. Protože tyto vztahy jsou velmi komplikované v obecném případě, zaměřil jsem se na případ stigmatických systémů. Klasifikaci aberačních polynomů jsem popsal jako reprezentaci Lieovy grupy asociované k Lieově algebře kvadratických polynomů, které jsou určené kvadratickou částí hamiltoniánu. Strukturu této reprezentace jsem explicitně popsal. V neposlední řadě jsem také zmínil symetrii aberačních polynomů vzhledem k zrcadlení vůči rovinám, které obsahují optickou osu.

Abstract

This work covers partly the field of analytical perturbation methods that are used in charged particle optics; the emphasis is given mainly on the calculation of geometrical aberrations of an optical system. In particular, the Lie algebra method often used in accelerator physics is described and compared with more usual methods used in charged particle optics like the trajectory method and the eikonal method.

First I describe basic approaches in the description of the optical system properties, formulations of the trajectory equation, and the properties of the paraxial approximation. The description of the most common analytical perturbation methods and their application to a simple round magnetic lens are subject of the next part. Finally, in the last part the symplectic classification of the aberration polynomials is described.

During the first two years of my PhD study I dealt with the mathematical background of the Lie algebra method, canonical perturbation theory, and its connection with the Lie algebra method. I showed that there exists a significant relationship between the factorization theorem and the canonical perturbation theory. The Lie algebra method has been extended to the case when the parameterization by position in the object and aperture plane is used.

During the next study I solved an issue of advisable classification of the aberration polynomials and their relationship. It was shown that the way of classification is connected to the form of the paraxial approximation that affects the relationship among the aberration coefficients. Because of the complexity of general system classification, the effort was aimed at the classification of stigmatic systems. The aberration polynomials were classified as a representation of the Lie group adjoint to the algebra of the quadratic polynomials that are determined by the quadratic part of Hamiltonian. This representation was explicitly described. I also discussed the symmetry of aberration coefficients according to reflection.

Obsah

1 Introduction

Calculations of electron or ion optical systems are mostly done in the approximation of geometrical optics; the quantum effects are in most cases negligible. The standard computation methods come either from the trajectory equation, which is derived from the equation of motion for a particle in electromagnetic field, or from the eikonal equation. Unfortunately, both equations are not analytically solvable for other than trivial problems.

The paraxial approximation provides the first insight into the properties of an optical system. This linear approximation of the trajectory equation is also used in the light optics. The description of the paraxial properties is essential for the basic system design. Unfortunately, the omission of higher order terms in the trajectory equation is much more problematic than in light optics. In light optics the maximal resolution is given by the wave length of light, it varies between $400 - 800$ nm. Objects of these dimensions cannot be observed with this technology. On the other hand, the wave length of electron is in the order of magnitude of pm depending on its energy. Hence, in electron optics the resolution is given mainly by the influence of the nonlinear terms in the trajectory equation.

The nonlinear terms in the trajectory equation cause that a point is not imaged on a point by the optical system. This property of optical systems is already known from the light optics, where it was described by Seidel in 1856 (Seidel aberrations). However, the systems in electron optics contain more complicated elements; therefore, the nonlinear properties of these systems are more complicated too: the elements with lower than axial symmetry are often used in electron optical systems and the magnetic field causes that the electron rays are not perpendicular to the wave surfaces. As a consequence aberrations with no analogy in light optics are present in electron optics. For these reasons it was necessary to develop new perturbation methods that are suitable for the description of nonlinear properties of electron optical systems.

These methods are represented by the trajectory method, the eikonal method, and the Lie algebra method. All methods are analytical perturbation methods, each of them is from one point of view advantageous and from the other one disadvantageous. The trajectory method is based on an iterative solution of trajectory equations, the eikonal method comes from the perturbation method for the eikonal and the Lie algebra method from the canonical perturbation method.

The Lie algebra method was developed at University of Maryland by A.J. Dragt et al. in 1980's. It was applied step by step in imaging electron optics but also in accelerator physics. The method stands out by its stability in the calculation of high-order aberrations and in the description of the periodical systems. It introduces the Lie algebra structure on the space of aberration polynomials. Thus, it is advisable for the description of structure of aberration polynomials and for the study of global properties of the system.

The aim of my PhD thesis is to describe these three methods, to solve a simple optical system by using all of them and to compare the procedures and the insight into the structure of the system that they provide.

The second chapter contains basic approaches in description of the properties of optical systems, particularly different forms of trajectory equation and its derivations. In the third chapter the basic properties of fields that are used in charged particle optics are summarized. Particular forms of series expansions of fields in the vicinity of the optical axis are also presented.

The next chapter deals with the method of solution of the trajectory equation. The lager part of the chapter describes the paraxial approximation for mono–energetic and general dispersion case. The form of the solution is described both in Lagrangian and Hamiltonian variables. At the end of the chapter a procedure for a general case is outlined.

The fifth chapter contains an overview of the perturbation methods. After a short introduction of the differential algebra method the description of the trajectory method, the eikonal method, and the Lie algebra method is presented in more details. These methods are applied to a simple but important example — a round magnetic lens.

In the sixth chapter the structure of aberration polynomials according to representation of $Sp(2,\mathbb{R})$ is described. The influence of the form of the paraxial approximation on the structure of the aberration polynomials is explained too. The last part covers the description of the symmetry of the aberration polynomials with respect to the reflection.

2 Trajectory Equations

The motion of particles in electromagnetic field is completely determined by the equations of motion. Unfortunately, their mathematical form does not describe the optical properties in a consistent way. The use of the time parameterization in case when just the trajectories of particles and their directives are relevant would lead to clumsy formulations without direct optical meaning. That is the reason why the time parameterization of trajectory is replaced by other parameterization, e.g. by the optical axis position. The equations of motion that use time derivatives are then replaced by the trajectory equation which contains derivatives with respect to the new independent variable. The solution of such equations are just particle trajectories not the motion of particles; however, if the rays are known the velocity of particle in given point can be easily calculated.

The coordinate system will be chosen so that the optical axis coincides with the coordinate axis z and coordinates x and y form the transversal space. The optical devices are constructed so that the particle with given energy that starts to move on the optical axis and along it remains on the axis. Such a particle is known as design particle and its energy as design energy. The design trajectory term is used for the trajectory of the design particle. Unless stated otherwise we will restrict ourselves to systems with straight optical axis in which case it is coincided with the design trajectory.

The treatment to the trajectory equations differs according to which formulation of mechanics is used. We will review some of them.

2.1 Newton Formulation

The relativistically modified second Newton's law for electron in electromagnetic field

$$m\frac{\mathrm{d}}{\mathrm{d}t}(\gamma\dot{\boldsymbol{r}}) = -e\boldsymbol{E} - e\dot{\boldsymbol{r}}\times\boldsymbol{B}, \tag{2.1}$$

completely describes the system evolution. The standard notation for time derivative is used, $\gamma = (1-\frac{v^2}{c^2})^{-\frac{1}{2}}$, $\boldsymbol{r} = (x,y,z)$, the electron current $e = 1.602\cdot 10^{-19}\mathrm{C}$ and mass of the electron $m = 9.109534\cdot 10^{-31}\mathrm{kg}$. However, while knowing just the particle trajectories is relevant in optics we switch to parameterization of the trajectory by the axis coordinate z. We will consider only time independent forces in next two sections.

Let us start with the time parameterized trajectory $\zeta(t) = (x(t),y(t),z(t))$, supposing it can be reparameterized by the axis coordinate z like $\zeta(z) = (x(z),y(z),z)$. The time

derivative of the trajectory is then expressed

$$\frac{\mathrm{d}\zeta}{\mathrm{d}t} = \frac{\mathrm{d}\zeta}{\mathrm{d}z}\frac{\mathrm{d}z(t)}{\mathrm{d}t} = \frac{\mathrm{d}\zeta}{\mathrm{d}z}v_z,$$

or more generally the time derivative along trajectory takes form

$$\frac{\mathrm{d}}{\mathrm{d}t} = v_z\frac{\mathrm{d}}{\mathrm{d}z}. \tag{2.2}$$

The z-component of velocity reads

$$v_z = \frac{v}{\sqrt{1+\boldsymbol{q}'^2}}$$

with notation $\boldsymbol{q} = (x,y)^T$ for the vector of transversal deviations of the trajectory from the optical axis used. The velocity v is in direct relationship with kinetic energy of the particle. It can be expressed using scalar potential Φ. If we suppose that all particles have the same energy, the additive constant in Φ can be chosen so that value $e\Phi$ coincides with kinetic energy of the particle. The relativistic factor γ then takes form

$$\gamma = 1 + \frac{e\Phi}{mc^2}. \tag{2.3}$$

We will express the velocity using the kinetic momentum

$$g = \gamma m v = \frac{e}{\eta}\Phi^{*\frac{1}{2}}, \tag{2.4}$$

where $\eta = \sqrt{e/2m}$ and the acceleration potential

$$\Phi^* = \Phi\left(1 + \frac{e}{2mc^2}\Phi\right) \tag{2.5}$$

was introduced. Then using previous equations one can find z component of velocity

$$v_z = \frac{e\Phi^{*\frac{1}{2}}}{m\eta\gamma\sqrt{(1+\boldsymbol{q}'^2)}},$$

with using of which (2) gives

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{e\Phi^{*\frac{1}{2}}}{m\eta\gamma\sqrt{1+\boldsymbol{q}'^2}}\frac{\mathrm{d}}{\mathrm{d}z} \tag{2.6}$$

Substituting into (1) one can find after some trivial calculations the trajectory equations

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\left(\frac{\Phi^*}{1+\boldsymbol{q}'^2}\right)^{\frac{1}{2}}\boldsymbol{q}'\right) = \frac{1}{2}\gamma\left(\frac{1+\boldsymbol{q}'^2}{\Phi^*}\right)^{\frac{1}{2}}\nabla\Phi + \eta\begin{pmatrix} B_y - y'B_z \\ -B_x + x'B_z \end{pmatrix}, \tag{2.7}$$

where prime denotes the derivative with respect to z. Let us note that one can use this form of trajectory equations only if the trajectory can be parameterized by the axis coordinate otherwise, as in case of electric mirror, the parameterization must be switch to some other.

For beam of particles with different energy a new quantity δ with the meaning of particle energy deviation from design particle has to be introduced. As the system is time independent, δ remains constant along each ray. For the scalar potential to be determined uniquely $e\Phi$ must coincide with kinetic energy of the particle which has design energy. The relationship between the relativistic factor γ and scalar potential Φ is then modified to

$$\gamma = 1 + \frac{e\Phi}{mc^2} + \frac{\delta}{mc^2} = \gamma_0 + \frac{\delta}{mc^2}. \tag{2.8}$$

and (4) similarly

$$g = \frac{e}{\eta}\left(\Phi^* + \frac{\gamma_0\delta}{e} + \frac{\delta^2}{2mec^2}\right)^{\frac{1}{2}}. \tag{2.9}$$

The subscript 0 denotes the value for particles with the same energy as the design particle has, i.e.

$$\gamma_0 = 1 + \frac{e\Phi}{mc^2}$$

The form of the trajectory equation (7) remains unchanged only the acceleration potential must be replaced by

$$\Phi^* + \frac{\gamma_0\delta}{e} + \frac{\delta^2}{2mec^2} \tag{2.10}$$

and relativistic factor γ by (8).

2.2 Lagrangian Approach

The particle trajectories in time parametrization are found as extremals of functional

$$S = \int_{t_1}^{t_2} L(\boldsymbol{r}(t), \dot{\boldsymbol{r}}(t), t)\mathrm{d}t \tag{2.11}$$

called action. In case of electromagnetic field the function L – Lagrangian reads [2]

$$L = mc^2\left(1 - \sqrt{1 - \frac{v^2}{c^2}}\right) - e(\boldsymbol{vA} - \Phi), \tag{2.12}$$

where $\boldsymbol{A}$ denotes the vector potential.

As we assume the Lagrangian does not explicitly depend on time, instead of direct reparameterization the Maupertius principle can be used. The trajectories are then found as the extremals of the functional

$$S = \int_{t_1}^{t_2} \boldsymbol{p}\dot{\boldsymbol{r}}\mathrm{d}t = \int_{\zeta} \boldsymbol{p}\,\mathrm{d}\boldsymbol{q} \tag{2.13}$$

where the canonical momentum is defined as

$$\boldsymbol{p} = \frac{\partial L(\boldsymbol{r},\boldsymbol{v})}{\partial \boldsymbol{v}} = \boldsymbol{g} - e\boldsymbol{A}, \tag{2.14}$$

Substituting (14) into (13) and using z-parameterization one can find

$$S = \int_{z_o}^{z_i} [\Phi^{*\frac{1}{2}}(1+\boldsymbol{q}'^2)^{\frac{1}{2}} - \eta(A_x x' + A_y y' + A_z)]\mathrm{d}z. \tag{2.15}$$

The physical interpretation of the integrand is index of refraction, let us denote it

$$M(\boldsymbol{q},\boldsymbol{q}',z) = \Phi^{*\frac{1}{2}}(1+\boldsymbol{q}'^2)^{\frac{1}{2}} - \eta(A_x x' + A_y y' + A_z) \tag{2.16}$$

which is effectively adequate to anisotropic non-homogeneous medium.

The trajectory equations found as equations for the extremals of (15)

$$\frac{\mathrm{d}}{\mathrm{d}z}\frac{\partial M}{\partial \boldsymbol{q}'} - \frac{\partial M}{\partial \boldsymbol{q}} = 0 \tag{2.17}$$

take form

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\left(\frac{\Phi^*}{1+\boldsymbol{q}'^2}\right)^{\frac{1}{2}}\boldsymbol{q}'\right) = \frac{1}{2}\gamma\left(\frac{1+\boldsymbol{q}'^2}{\Phi^*}\right)^{\frac{1}{2}}\nabla\Phi + \eta\begin{pmatrix} B_y - y'B_z \\ -B_x + x'B_z \end{pmatrix},$$

which are equivalent to (7).

Even though the final trajectory equation is identical to trajectory equation in Newtonian formulation, advantage of this approach is that it shows analogy between light optics represented by Fermat's principle and electron optics. Moreover, the Lagrangian perturbation methods can be used at the aberration computation.

The extension for case in which the particles have different energy is completely analogous with description of such systems in Newton formulation. The action to minimalize

takes form

$$S=\int_{z_o}^{z_i}\left[(\Phi^*+\frac{\gamma_0\delta}{e}+\frac{\delta^2}{2mec^2})^{\frac{1}{2}}(1+\boldsymbol{q}'^2)^{\frac{1}{2}}-\eta(A_x x'+A_y y'+A_z)\right]\mathrm{d}z \tag{2.18}$$

and its extremals are solutions of equations equivalent to trajectory equation extended to cases when the particles have different energy. Let us note that setting $\delta=0$ (18) reduces to (15).

2.3 Hamiltonian approach

We drop the assumption of time independent field in this subsection. The relativistic electron moving through electromagnetic field is described by the Hamiltonian [2]

$$H=\sqrt{m^2c^4+c^2(\boldsymbol{p}+e\boldsymbol{A})^2}-e\Phi_\infty, \tag{2.19}$$

where the scalar potential Φ_∞ is chosen to be zero in infinity. However, the choice that scalar potential expresses kinetic energy of the particle with the design energy is obvious in electron optics. Such a potential is denoted by Φ and its relationship with Φ_∞ is given by

$$e\Phi=e\Phi_\infty+E_{k\infty}\,, \tag{2.20}$$

where $E_{k\infty}$ stands for kinetic energy of the design particle in infinity.

The transformation to Hamiltonian describing just the deviation of energy from the design energy would seem advisable. As the electrons are moving through conservative fields, such a Hamiltonian reads

$$\mathcal{H}=\sqrt{m^2c^4+c^2(\boldsymbol{p}+e\boldsymbol{A})^2}-e\Phi-mc^2. \tag{2.21}$$

Let us note that value $\mathcal{H}$ along phase space trajectory equals δ used in the previous subsections.

The phase space trajectories in time parametrization can be found as extremals of the action

$$S=\int_{t_1}^{t_2}(\boldsymbol{p}\dot{\boldsymbol{r}}-\mathcal{H}(\boldsymbol{r},\boldsymbol{p},t))\mathrm{d}t=\int_\zeta \boldsymbol{p}\mathrm{d}\boldsymbol{r}-\mathcal{H}(\boldsymbol{r},\boldsymbol{p},t)\mathrm{d}t. \tag{2.22}$$

With notation $p_t = -\mathcal{H}$ the action in z-parametrization of the trajectory reads

$$S = \int_{z_o}^{z_i} (\boldsymbol{p}\boldsymbol{q}' + p_t t' - K(\boldsymbol{q},\boldsymbol{p},p_t,t,z))\mathrm{d}z \tag{2.23}$$

where from here $\boldsymbol{p}$ and $\boldsymbol{A}$ denote transversal part of momentum $\boldsymbol{p} = (p_x, p_y)^T$ and vector potential $\boldsymbol{A} = (A_x, A_y)^T$, respectively. The function K, the solution of

$$\mathcal{H}(p_x, p_y, -K, x, y, z, t) = -p_t\,,$$

has the meaning of the Hamiltonian in z parametrization and takes form

$$K = -\sqrt{\frac{e^2}{\eta^2}\Phi^* + \frac{p_t^2}{c^2} - 2mp_t\gamma_0 - (\boldsymbol{p} + e\boldsymbol{A})^2} + eA_z\,. \tag{2.24}$$

The time and p_t play role of canonical variables in z-parametrization.

It is convenient to employ phase-space variables so that they all vanish on the design trajectory. Evidently this is true for all of them except t which must be replaced by new variable $\tau = c(t - z/v_0)$. It causes a change of the canonical conjugate variable p_t to $p_\tau = p_t/c$. This change is represented by the canonical transformation described by the generating function

$$F_2 = \boldsymbol{q}\tilde{\boldsymbol{p}} + cp_\tau t - \frac{p_\tau z}{\beta_0}\,. \tag{2.25}$$

The canonical variables $\boldsymbol{q}$ and $\boldsymbol{p}$ do not change with the transformation, and for convenience we shall drop the use of tilde. The new Hamiltonian denoted H reads

$$H = -\sqrt{\frac{e^2}{\eta^2}\Phi^* + p_\tau^2 - 2mcp_\tau\gamma_0 - (\boldsymbol{p} + e\boldsymbol{A})^2} + eA_z - \frac{p_\tau}{\beta_0}\,. \tag{2.26}$$

One can find the trajectory equations as equations for extremal of (23) which take form of standard Hamilton equations

$$\boldsymbol{q}' = \frac{\partial H}{\partial \boldsymbol{p}} \qquad\qquad \boldsymbol{p}' = -\frac{\partial H}{\partial \boldsymbol{q}} \tag{2.27a}$$

$$\tau' = \frac{\partial H}{\partial p_t} \qquad\qquad p_\tau' = -\frac{\partial H}{\partial t}\,. \tag{2.27b}$$

The case when the energy of particles does not differ and forces do not depend on time is described by the Hamiltonian with $p_\tau = 0$ substituted into (26). When Hamiltonian does not explicitly depends on time ie. $\partial H/\partial t = 0$, $p_\tau = \mathrm{const}$ results from (27b) .

2.4 Hamilton-Jacobi approach

This approach is based on the fact that motion can be described as a canonical transformation that transforms the initial state into the state with given z. Finding of such a transformation is equivalent to solving of the trajectory equations. In transformed coordinates the evolution is identity, the consequence of which is vanishing of the Hamiltonian. This leads to Hamilton-Jacobi equation

$$H\left(\boldsymbol{q}, \frac{\partial F_2}{\partial \boldsymbol{q}}, z\right) + \frac{\partial F_2(\boldsymbol{q}, \tilde{\boldsymbol{p}}, z)}{\partial z} = 0 \tag{2.28}$$

the solution of which is the generating function of the sought for canonical transformation and the trajectories we seek are solutions $\boldsymbol{q} = \boldsymbol{q}(\tilde{\boldsymbol{q}}, \tilde{\boldsymbol{p}}, z)$ of the algebraic equation

$$\tilde{\boldsymbol{q}} = \frac{\partial F_2}{\partial \tilde{\boldsymbol{p}}} \qquad\qquad \boldsymbol{p} = \frac{\partial F_2}{\partial \boldsymbol{q}} \tag{2.29}$$

where $\tilde{\boldsymbol{q}}$ and $\tilde{\boldsymbol{p}}$ play role of the initial conditions.

Generally, it is more complicated to solve the partial differential equation (28) than the trajectory equation; however the formalism of canonical transformations is very suitable for the perturbation calculus. The idea is not to compensate the whole Hamiltonian at once like in (28), but step by step only those parts that contribute to given perturbation order. Modified a little we will use this approach in Lie algebra method.

3 The Field Computation

Except some trivial assumptions we have said nothing about field the electrons are moving in wherefore we will shortly describe some methods of its calculation. Because in the vast majority of practical optical devices the applied fields are staticWe we can restrict our attention to the stationary field.

3.1 The Basic Equations

The electromagnetic field is described by the Maxwells' equations which in the case of stationary fields reduce to [2]

$$\nabla \times \boldsymbol{E} = 0 \qquad \nabla \times \boldsymbol{H} = \boldsymbol{j} \tag{3.1a}$$

$$\nabla \boldsymbol{D} = \rho \qquad \nabla \boldsymbol{B} = 0. \tag{3.1b}$$

These are to be completed by the material equations

$$\boldsymbol{D} = \epsilon \boldsymbol{E}, \qquad \boldsymbol{B} = \mu \boldsymbol{H} \quad (\boldsymbol{H} = \nu \boldsymbol{B}). \tag{3.2}$$

In ferromagnetic materials the reluctance ν is function of $B = \mid \boldsymbol{B} \mid$. The space charge density and current density are regarded as functions of position.

The source-free Maxwells' equations permit us to introduce electromagnetic potential

$$\boldsymbol{E} = -\nabla \Phi, \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{3.3}$$

The scalar potential then can be find as the solution of

$$-\nabla(\epsilon(\boldsymbol{r})\nabla\Phi) = \rho, \tag{3.4}$$

which reduces to

$$\nabla^2 \Phi = 0 \tag{3.5}$$

in domains free of space charge. Similarly one can find the equation for the vector potential

$$\nabla \times (\nu(|\nabla \times \boldsymbol{A}|)\nabla \times \boldsymbol{A}) = \boldsymbol{j}, \tag{3.6}$$

which reduces for constant ν and gauge $\nabla \boldsymbol{A} = 0$ to

$$\nabla^2 \boldsymbol{A} = \mu \boldsymbol{j}. \tag{3.7}$$

Yet another simplification is possible in vacuum current-free domain, where $\nabla \times \boldsymbol{H} = 0$. In such a case it is always permissible to write

$$\boldsymbol{B}(\boldsymbol{r}) = -\nabla W(\boldsymbol{r}). \tag{3.8}$$

$W(\boldsymbol{r})$ being the scalar magnetic potential. Since $\nabla \boldsymbol{B} = 0$ the scalar magnetic potential satisfies the Laplace equation

$$\nabla^2 W = 0 \tag{3.9}$$

The simplification achieved lies in the fact that only one scalar differential equation is to be solved instead of three coupled.

3.2 The Field in the Vicinity of the Optical Axis

The region where the field will be computed is a vacuum source free domain; hence, equations (5) and (9) can be used for the field calculation. More over it is known that the field in the vicinity of the optical axis can be obtained by the analytic continuation of the axial distribution. So the electrostatic or magnetic potentials can be express in form of Taylor polynomial in transversal coordinates x and y whose coefficients are functions of coordinate z.

The field in the vicinity of the axis can be divided according to its level of rotation symmetry. The axial symmetric electric or magnetic field is very often used as focusing field. Other important fields are dipole fields with the lowest symmetry (rotation of 360°and one plane of reflection symmetry) and quadrupole (rotation of 180°and two planes of reflection symmetry). The sextupole and octupole fields are the multipole fields of the highest order used in optical devices especially for reduction of the axial aberrations of the lenses.

The axial field distribution and all its derivatives must be known for us to be able to compute the analytic continuation. The procedure is described e.g. in [1], we will

summarise the results. For the scalar electrostatic potential one can find

$$\begin{aligned}\Phi(\boldsymbol{r}) =& \phi(z) - \frac{1}{4}(x^2+y^2)\phi''(z) + \frac{1}{64}(x^2+y^2)^2\phi^{(4)}(z) \\ & - xF_1(z) - yF_2(z) + \frac{1}{8}(x^2+y^2)(xF_1'' + yF_2'') \\ & + \frac{1}{2}(x^2-y^2)p_2(z) + xyq_2(z) - \frac{1}{24}(x^4-y^4)p_2'' - \frac{1}{12}(x^3y+xy^3)q_2'' \\ & - \frac{1}{6}p_3(z)(x^3-3xy^2) + \frac{1}{6}q_3(z)(y^3-3x^2y) \\ & + \frac{1}{24}p_4(z)(x^4-6x^2y^2+y^4) + \frac{1}{6}q_4(z)(x^3y-xy^3),\end{aligned} \tag{3.10}$$

where the first row represents the axial symmetric field, the second one the dipole field, the third one quadrupole field and the last two represent the hexupole and octupole field respectively. The meaning of z-dependent coefficients can be found as

$$\begin{aligned}&\phi = \Phi(0,0z), && F_1 = -\frac{\partial\Phi}{\partial x}\,|_{[0,0,z]} = E_x(0,0,z), && F_2 = -\frac{\partial\Phi}{\partial y}\,|_{[0,0,z]} = E_y(0,0,z) \\ &p_2 = \frac{\partial E_y}{\partial y}\,|_{[0,0,z]}, && q_2 = -\frac{\partial E_x}{\partial y}\,|_{[0,0,z]} && p_3 = \frac{\partial^2 E_x}{\partial x^2}\,|_{[0,0,z]} \\ &q_3 = -\frac{\partial^2 E_y}{\partial y^2}\,|_{[0,0,z]} && p_4 = -\frac{\partial^3 E_y}{\partial y^3}\,|_{[0,0,z]}, && q_4 = \frac{\partial^3 E_x}{\partial y^3}\,|_{[0,0,z]}\end{aligned}$$

As the magnetic scalar potential is the solution of Poisson equation as well its form will be analogous to the electric one

$$\begin{aligned}\Psi(\boldsymbol{r}) =& -\int B(z)\mathrm{d}z + \frac{1}{4}(x^2+y^2)B'(z) - \frac{1}{64}(x^2+y^2)^2B'''(z) \\ & - xB_1(z) - yB_2(z) + \frac{1}{8}(x^2+y^2)(xB_1'' + yB_2'') \\ & + \frac{1}{2}(x^2-y^2)P_2(z) + xyQ_2(z) - \frac{1}{24}(x^4-y^4)P_2'' - \frac{1}{12}(x^3y+xy^3)Q_2'' \\ & - \frac{1}{6}(x^3-3xy^2)P_3(z) + \frac{1}{6}(y^3-3x^2y)Q_3(z) \\ & + \frac{1}{24}(x^4-6x^2y^2+y^4)P_4(z) + \frac{1}{6}(x^3y-xy^3)Q_4(z)\,,\end{aligned} \tag{3.11}$$

but the meaning of the coefficients is derived from the flux density

$$\begin{aligned}&B(z) = B_z(0,0,z) && B_1(z) = B_x(0,0,z) && B_2(z) = B_y(0,0,z) \\ &P_2(z) = \frac{\partial B_y}{\partial y}\,|_{[0,0,z]} && Q_2(z) = -\frac{\partial B_x}{\partial y}\,|_{[0,0,z]} && P_3(z) = \frac{\partial^2 B_x}{\partial x^2}\,|_{[0,0,z]} \\ &Q_3(z) = \frac{\partial^2 B_y}{\partial x^2}\,|_{[0,0,z]} && P_4(z) = -\frac{\partial^3 B_x}{\partial x^3}\,|_{[0,0,z]} && Q_4(z) = \frac{\partial^3 B_x}{\partial y^3}\,|_{[0,0,z]}\end{aligned} \tag{3.12}$$

Knowing the vector potential is necessary for Lagrangian and Hamiltonian formulation. In appropriate gauge it takes form [1]

$$\begin{aligned} A_x = &-\frac{y}{2}\left(B-\frac{1}{8}(x^2+y^2)B''\right)+ \\ &+\frac{1}{4}(x^2-y^2)B_2'-\frac{1}{48}(x^4-y^4)B_2'''-\frac{xy}{2}B_1'+\frac{1}{24}(x^3y+xy^3)B_1''' \\ &-\frac{1}{12}(x^3-3xy^2)Q_2'-\frac{1}{12}(y^3-3x^2y)P_2' \\ &+\frac{1}{48}(x^4-6x^2y^2+y^4)Q_3'-\frac{1}{12}(x^3y-xy^3)P_3' \end{aligned} \tag{3.13a}$$

$$\begin{aligned} A_y = &\frac{x}{2}\left(B-\frac{1}{8}(x^2+y^2)B''\right) \\ &+\frac{1}{4}(x^2-y^2)B_1'-\frac{1}{48}(x^4-y^4)B_1'''+\frac{xy}{2}B_2'-\frac{1}{24}(x^3y+xy^3)B_2''' \\ &-\frac{1}{12}(x^3-3xy^2)P_2'+\frac{1}{12}(y^3-3x^2y)Q_2' \\ &+\frac{1}{48}(x^4-6x^2y^2+y^4)P_3'+\frac{1}{12}(x^3y-xy^3)Q_3' \end{aligned} \tag{3.13b}$$

$$\begin{aligned} A_z = &-xB_2+yB_1+\frac{1}{8}(x^2+y^2)(xB_2''-yB_1'') \\ &+\frac{1}{2}(x^2-y^2)Q_2-xyP_2-\frac{1}{24}(x^4-y^4)Q_2''+\frac{1}{12}(x^3y+xy^3)P_2'' \\ &-\frac{1}{6}(x^3-3xy^2)Q_3-\frac{1}{6}(y^3-3x^2y)P_3 \\ &+\frac{1}{24}(x^4-6x^2y^2+y^4)Q_4-\frac{1}{6}(x^3y-xy^3)P_4. \end{aligned} \tag{3.13c}$$

The results for the scalar potentials and z component of vector potential were written with the accuracy up to fourth order, for the transversal part of vector potential up to third order. The reason is to include all terms contributing to the third order aberration.

The last but not least issue relates to getting the axial field distribution. It can be obtained from numerical solution of the Maxwells' equations. There exist three common methods, the boundary elements method (BEM) [27], the finite difference method (FDM) [28] and the finite elements method (FEM) [29, 30]. All of them compute the field values in nodal points, the approximate field value in any point can then be computed using some of the spline methods [31, 32]. However, the computation of potential derivatives is more sophisticated and in fact the accuracy of the methods used is not

good. That is the reason why the raytracing as the method using only the field values is used at final computation of the system parameters.

4 Trajectory Equations – Methods of Solution

One can find out that the forms of the trajectory equations are similar independently on the way they are derived or coordinates used. From the mathematical point of view they are the set of two nonlinear ordinary differential equations of the second order with variable coefficients in case of Lagrangian coordinates which is equivalent to the set of four ordinary differential equations of first order in Hamiltonian case.

In general, the analytic form of the solution does not exist; hence, the perturbation or numerical methods have to be used. Although the numerical solution using mostly Runge-Kutta algorithm is the easiest and exact one the methods that allow finding the solution in form of polynomial in initial conditions seem to be very suitable. We will describe the features of these two classes of methods in following subsections.

4.1 Paraxial Approximation

The particles moving close to the optical axis are well described by the paraxial approximation. It is based on the fact that the particle trajectories deviation from the axis and their directives are so small that their second and higher powers can be neglected in the trajectory equation. It is the standard assumption of Gaussian optics. We will suppose that energy of particles does not differ. Similarly to the case of the trajectory equation two approaches can be used here: the direct linearization of the trajectory equation or the Hamiltonian approach. We will review both of them.

Paraxial Approximation from the Trajectory Equation

The paraxial trajectory equations emerge by linearization of general trajectory equation (2.7), like

$$\frac{\mathrm{d}}{\mathrm{d}z}(\phi^{*\frac{1}{2}}x') = -\frac{\gamma E_x}{2\phi^{*\frac{1}{2}}} + \eta(B_y - y'B_z) - \frac{F_1(F_1x + F_2y)}{4\phi^{*\frac{3}{2}}} \tag{4.1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}(\phi^{*\frac{1}{2}}y') = -\frac{\gamma E_y}{2\phi^{*\frac{1}{2}}} + \eta(x'B_z - B_x) - \frac{F_2(F_1x + F_2y)}{4\phi^{*\frac{3}{2}}}, \tag{4.1b}$$

where

$$\begin{aligned} E_x &= \frac{1}{2}\phi''x + F_1 - p_2x - q_2y, \\ E_y &= \frac{1}{2}\phi''y + F_2 + p_2y - q_2x, \\ E_z &= -\phi' \end{aligned}$$

and

$$B_x = -\frac{1}{2}B'x + B_1 - Q_2 y - P_2 x,$$
$$B_y = -\frac{1}{2}B'y + B_2 - Q_2 x + P_2 y,$$
$$B_z = B.$$

Henceforward γ relates to the design particle, $\gamma = 1 + \frac{e\phi}{mc^2}$. Having the orientation of dipoles and quadrupoles selected such that $x-z$ plane is the symmetry plane of the electric dipole and quadrupole fields and the antisymmetry plane of the magnetic dipole and quadrupole fields, F_2, q_2, B_1 and P_2 vanish which reduces the paraxial approximation to

$$x'' + \frac{\gamma\phi'}{2\phi^*}x' + \left(\frac{\gamma\phi''}{4\phi^*} - \frac{\gamma p_2}{2\phi^*} + \frac{\eta Q_2}{\phi^{*\frac{1}{2}}} + \frac{F_1^2}{4\phi^{*2}}\right)x + \frac{\eta}{\phi^{*\frac{1}{2}}}\left(\frac{1}{2}B'y + y'B\right) = -\frac{\gamma F_1}{2\phi^*} + \frac{\eta B_2}{\phi^{*\frac{1}{2}}} \quad (4.2a)$$

$$y'' + \frac{\gamma\phi'}{2\phi^*}y' + \left(\frac{\gamma\phi''}{4\phi^*} + \frac{\gamma p_2}{2\phi^*} - \frac{\eta Q_2}{\phi^{*\frac{1}{2}}}\right)y - \frac{\eta}{\phi^{*\frac{1}{2}}}\left(\frac{1}{2}B'x + x'B\right) = 0. \quad (4.2b)$$

The linear differential equations of the second order (2a) and (2b) are not separated and the first order derivatives of x and y emerge which does not fit our needs. We will switch to the normal form of the equations which is more advisable for the description of the solution general properties. As the term that causes mixing of coordinates generates the rotation of particles around z axis, it can be eliminated by transition to rotation coordinates

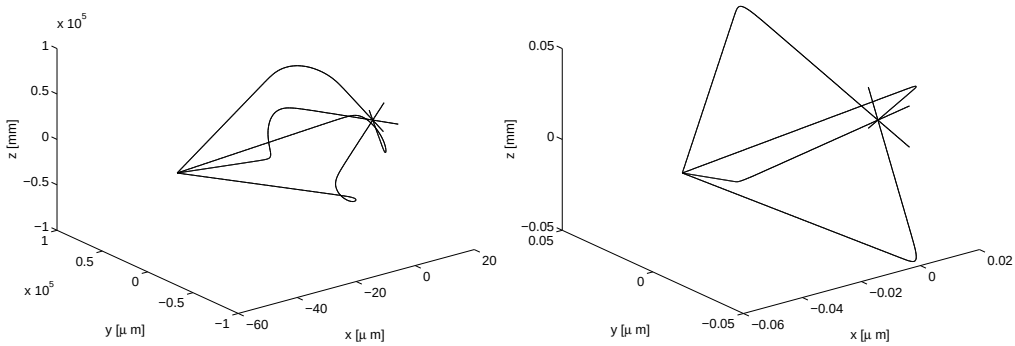
$$\begin{pmatrix} X \\ Y \end{pmatrix} = \hat{R}\begin{pmatrix} x \\ y \end{pmatrix} \quad (4.3)$$

where

$$\hat{R} = \begin{pmatrix} \cos\Theta & \sin\Theta \\ -\sin\Theta & \cos\Theta \end{pmatrix}$$

represents the rotation about angle

$$\Theta(z) = \frac{\eta}{2}\int_{z_i}^{z} \frac{B(z)}{\phi^{*\frac{1}{2}}(z)}\mathrm{d}z.$$



Obrázek 1: The paraxial rays in magnetic lens using standard and rotation coordinates

In such coordinates the paraxial trajectory equations read

$$X''+\frac{\gamma\phi'}{2\phi^*}X'+\left(\frac{\gamma\phi''}{4\phi^{*2}}+\frac{\eta^2B^2}{4\phi^*}+\frac{F_1^2}{8\phi^{*2}}\right)X+ \tag{4.4a}$$
$$+\left(\frac{F_1^2}{8\phi^{*2}}-\frac{\gamma p_2}{2\phi^*}+\frac{\eta Q_2}{\phi^{*\frac{1}{2}}}\right)(\cos(2\Theta)X-\sin(2\Theta)Y)=\left(\frac{\eta B_2}{\phi^{*\frac{1}{2}}}-\frac{\gamma F_1}{2\phi^*}\right)\cos\Theta$$
$$Y''+\frac{\gamma\phi'}{2\phi^*}Y'+\left(\frac{\gamma\phi''}{4\phi^{*2}}+\frac{\eta^2B^2}{4\phi^*}+\frac{F_1^2}{8\phi^{*2}}\right)Y- \tag{4.4b}$$
$$-\left(\frac{F_1^2}{8\phi^{*2}}-\frac{\gamma p_2}{2\phi^*}+\frac{\eta Q_2}{\phi^{*\frac{1}{2}}}\right)(\sin(2\Theta)X+\cos(2\Theta)Y)=-\left(\frac{\eta B_2}{\phi^{*\frac{1}{2}}}-\frac{\gamma F_1}{2\phi^*}\right)\sin\Theta.$$

Unfortunately the equations are still neither separated nor homogeneous. The reason is that the field considered is too general for the real optic devices which contain fields restricted by given requirements. Let us mention some of them which are used in the most of the devices. The stability condition for the design particle trajectory is the first such a requirement. It is conditioned by vanishing of the right hand sides of (4a) and (4b), i.e.

$$B_2-\frac{\gamma F_1}{2\eta\phi^{*\frac{1}{2}}}=B_2-\frac{F_1}{v_o}=0, \tag{4.5}$$

which forms a relationship between magnetic and electric dipole fields – the Wien condition.

As the paraxial trajectory equations (4a), (4b) are not separated another natural restriction is to have a field in which they would. One can find two such situations. The first one represents systems in which no axial magnetic field is present. Thus, $\Theta=0$,

which leads to the paraxial trajectory equations

$$X'' + \frac{\gamma\phi'}{2\phi^*}X' + \left(\frac{\gamma\phi''}{4\phi^*} + \frac{F_1^2}{4\phi^{*2}} - \frac{\gamma p_2}{2\phi^*} + \frac{\eta Q_2}{\phi^{*\frac{1}{2}}}\right)X = 0$$
$$Y'' + \frac{\gamma\phi'}{2\phi^*}Y' + \left(\frac{\gamma\phi''}{4\phi^*} + \frac{\gamma p_2}{\phi^*} - \frac{\eta Q_2}{2\phi^{*\frac{1}{2}}}\right)Y = 0.$$

The second and more interesting situation occurs when

$$\frac{F_1^2}{8\phi^{*2}} - \frac{\gamma p_2}{2\phi^*} + \frac{\eta Q_2}{\phi^{*\frac{1}{2}}} = 0. \tag{4.6}$$

Not only that the paraxial trajectory equations are separated but also their form is the same for X and Y coordinates:

$$\boldsymbol{Q}'' + \frac{\gamma\phi'}{2\phi^*}\boldsymbol{Q}' + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)\boldsymbol{Q} = 0, \tag{4.7}$$

where vector $\boldsymbol{Q}$ defined as $\boldsymbol{Q} = (X,Y)^T$ was used.

It causes the electron initially travelling on any surface $\alpha X + \beta Y = 0$ remains on this surface. Such types of systems are cold stigmatic and condition (6) is known as the stigmatic condition. We will describe only stigmatic systems fulfilling the Wien condition, unless stated otherwise.

This form of the paraxial equations will occur later, therefore it is suitable to define a linear operator $\hat{P}_1$:

$$\hat{P}_1(f) = f'' + \frac{\gamma\phi'}{2\phi^*}f' + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)f. \tag{4.8}$$

The equation (7) is then equivalent to $\hat{P}_1(\boldsymbol{Q}) = 0$.

The trajectory equations may be written in more compact form using Picht's transformation

$$\boldsymbol{Q}_p = \phi^{*\frac{1}{4}}\boldsymbol{Q} \tag{4.9}$$

that transforms the trajectory equations into

$$\boldsymbol{Q}_p'' + \left(\frac{(2+\gamma^2)\phi'^2}{16\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)\boldsymbol{Q}_p = 0, \tag{4.10}$$

The result is of great interest for two reasons. First it is simpler to perform numerical calculations than using (2a) and (2b). Secondly, as $\phi^* \geq 0$ the coefficient

$$G(z) = \frac{(2+\gamma^2)\phi'^2}{16\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}$$

in (10) is essentially nonnegative, which imposes an interesting restriction on stigmatic electron lenses: they always exert a converging action.

Using numerical calculations one can find the solution of (7) in form of a block matrix

$$\begin{pmatrix} \boldsymbol{Q}(z) \\ \boldsymbol{Q}'(z) \end{pmatrix} = \begin{pmatrix} g(z)\hat{1} & h(z)\hat{1} \\ g'(z)\hat{1} & h'(z)\hat{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{Q}(z_o) \\ \boldsymbol{Q}'(z_o) \end{pmatrix}, \tag{4.11}$$

where $\hat{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $g(z)$ or $h(z)$ are solutions of

$$\hat{P}_1(g) = 0, \quad g(z_o) = 1, g'(z_o) = 0$$
$$\hat{P}_1(h) = 0, \quad h(z_o) = 0, h'(z_o) = 1.$$

The solution in original coordinates then takes form

$$\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{q}' \end{pmatrix} = \begin{pmatrix} \hat{R}^{-1} & 0 \\ -\Theta' \hat{J} \hat{R}^{-1} & \hat{R}^{-1} \end{pmatrix} \begin{pmatrix} g(z)\hat{1} & h(z)\hat{1} \\ g'(z)\hat{1} & h'(z)\hat{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}_o \\ \boldsymbol{q}'_o \end{pmatrix}, \tag{4.12}$$

where $\hat{J}$ is the standard symplectic matrix

$$\hat{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.13}$$

The solution (11,12) are parameterized by position of the ray in object plane and its directives. Similarly we can parameterize the rays using the position in the object plane and the position in the aperture plane $z = z_a$. Let us choose the pair of independent solutions $c(z)$ and $s(z)$ that fulfill

$$\hat{P}_1(s) = 0, \qquad s(z_o) = 1, s(z_a) = 0 \tag{4.14}$$
$$\hat{P}_1(t) = 0, \qquad t(z_o) = 0, t(z_a) = 1. \tag{4.15}$$

The solution in rotation coordinates then reads

$$\begin{pmatrix} \boldsymbol{Q}(z) \\ \boldsymbol{Q}'(z) \end{pmatrix} = \begin{pmatrix} s(z)\hat{1} & t(z)\hat{1} \\ s'(z)\hat{1} & t'(z)\hat{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{Q}_o \\ \boldsymbol{Q}_a \end{pmatrix}, \tag{4.16}$$

and in original coordinates takes form

$$\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{q}' \end{pmatrix} = \begin{pmatrix} \hat{R}^{-1} & 0 \\ -\Theta' \hat{J} \hat{R}^{-1} & \hat{R}^{-1} \end{pmatrix} \begin{pmatrix} s(z)\hat{1} & t(z)\hat{1} \\ s'(z)\hat{1} & t'(z)\hat{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}_o \\ \boldsymbol{q}_a \end{pmatrix}. \tag{4.17}$$

The first form of solution corresponds to Cauchy initial value problem and the second to boundary value problem. In the first case we can write the Wronskian in form

$$W_g = g(z)h'(z) - h(z)g'(z) = W_g(z_o)\phi^{*-\frac{1}{2}} = \phi^{*-\frac{1}{2}}(z) \tag{4.18}$$

while in the second case the Wronskian reads

$$W = s(z)t'(z) - t(z)s'(z) = W_s(z_o)\phi^{*-\frac{1}{2}}(z) \tag{4.19}$$

In both cases there exists the invariant quality

$$\phi^{*\frac{1}{2}}(z)W(z) = \text{const.} \tag{4.20}$$

The Hamiltonian formulation of the paraxial approximation

On contrary to expansion of the trajectory equation used in the previous paragraph the Hamiltonian approach is based on the expansion of Hamiltonian into polynomial in canonical variables. The second order of the expanded Hamiltonian completely describes the system paraxial properties. As we suppose the monochromatic systems $p_\tau = 0$ is substituted into (2.26). Using the same restriction on dipole and quadrupole fields as in the previous paragraph the expansion up to the second order takes form

$$H_0 = -\frac{e}{\eta}\phi^{*\frac{1}{2}} \tag{4.21a}$$

$$H_1 = e\left(\frac{F_1}{v_0} - B_2\right)x \tag{4.21b}$$

$$H_2 = \frac{\eta}{2e\phi^{*\frac{1}{2}}}\boldsymbol{p}^2 + \frac{\eta B}{2\phi^{*\frac{1}{2}}}L_z + \frac{1}{2}\left(\frac{e\gamma_0\phi''}{4\eta\phi^{*\frac{1}{2}}} + \frac{e\eta B^2}{4\phi^{*\frac{1}{2}}} + \frac{eF_1^2}{8\eta\phi^{*\frac{3}{2}}}\right)\boldsymbol{q}^2 + \tag{4.21c}$$
$$+ \frac{1}{2}\left(\frac{eF_1^2}{8\eta\phi^{*\frac{3}{2}}} - \frac{e\gamma_0 p_2}{2\eta\phi^{*\frac{1}{2}}} + eQ_2\right)(x^2 - y^2).$$

Notation $L_z = q_x p_y - q_y p_x$ for z-component of angular momentum $\boldsymbol{L}$ was used. The zero order part of the Hamiltonian does not contribute to the equations of motion and vanishing of the H_1 is equivalent to fulfilling the Wien's condition. The transition into rotation coordinates is represented by the extended canonical transformation

$$\begin{aligned} \boldsymbol{Q} &= \hat{R}\boldsymbol{q} \\ \boldsymbol{P} &= \frac{\eta}{e}\hat{R}\boldsymbol{p} \end{aligned} \tag{4.22}$$

which transforms the Hamiltonian according

$$\tilde{H} = \frac{\eta}{e}\left(H(\boldsymbol{q}(\boldsymbol{Q},\boldsymbol{P},z),\boldsymbol{q}(\boldsymbol{Q},\boldsymbol{P},z),z) + \frac{\partial F_2}{\partial z}\right),$$

where the generation function F_2 reads

$$F_2 = (\hat{R}\boldsymbol{q})\boldsymbol{P}.$$

Applying to the quadratic part of the Hamiltonian one can find

$$\begin{aligned}\tilde{H}_2 = \frac{1}{2\phi^{*\frac{1}{2}}}\boldsymbol{P}^2 + \frac{1}{2}\left(\frac{\gamma\phi''}{4\phi^{*\frac{1}{2}}} + \frac{\eta^2 B^2}{4\phi^{*\frac{1}{2}}} + \frac{F_1^2}{8\phi^{*\frac{3}{2}}}\right)\boldsymbol{Q}^2 + \\ + \frac{1}{2}\left(\frac{F_1^2}{8\phi^{*\frac{3}{2}}} - \frac{\gamma_0 p_2}{2\phi^{*\frac{1}{2}}} + \frac{\eta Q_2}{\phi^{*\frac{1}{2}}}\right)\boldsymbol{Q}^T\begin{pmatrix}\cos(2\Theta) & \sin(2\Theta)\\ \sin(2\Theta) & -\cos(2\Theta)\end{pmatrix}\boldsymbol{Q},\end{aligned} \tag{4.23}$$

which reduces into

$$\tilde{H}_2 = \frac{1}{2\phi^{*\frac{1}{2}}}\boldsymbol{P}^2 + \frac{1}{2}\left(\frac{\gamma\phi''}{4\phi^{*\frac{1}{2}}} + \frac{\eta^2 B^2}{4\phi^{*\frac{1}{2}}} + \frac{F_1^2}{8\phi^{*\frac{3}{2}}}\right)\boldsymbol{Q}^2 \tag{4.24}$$

for stigmatic systems. The quadratic part of such a Hamiltonian is axially symmetric, which causes that L_z is the integral of motion in paraxial approximation.

Using Hamilton equations of motion one can find the paraxial trajectory equations

$$\boldsymbol{Q}' = \phi^{*-\frac{1}{2}}\boldsymbol{P} \tag{4.25a}$$

$$\boldsymbol{P}' = -\left(\frac{\gamma\phi''}{4\phi^{*\frac{1}{2}}} + \frac{\eta^2 B^2}{4\phi^{*\frac{1}{2}}} + \frac{F_1^2}{8\phi^{*\frac{3}{2}}}\right)\boldsymbol{Q}, \tag{4.25b}$$

which after eliminating $\boldsymbol{P}$ can be written in form of ordinary differential equations of the second order

$$\boldsymbol{Q}'' + \frac{\gamma\phi'}{2\phi^*}\boldsymbol{Q}' + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)\boldsymbol{Q} = 0 \tag{4.26}$$

that agrees with results of the previous paragraph.

The solution then takes form analogous to (11)

$$\begin{pmatrix}\boldsymbol{Q}\\ \boldsymbol{P}\end{pmatrix} = \begin{pmatrix} g(z)\hat{1} & \phi_o^{*-\frac{1}{2}}h(z)\hat{1}\\ \phi^{*\frac{1}{2}}g'(z)\hat{1} & \sqrt{\frac{\phi^*}{\phi_o^*}}h'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{Q}_o\\ \boldsymbol{P}_o\end{pmatrix} \tag{4.27}$$

and in original coordinates

$$\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{pmatrix} = \begin{pmatrix}\hat{R}^{-1} & 0\\ 0 & \frac{e}{\eta}\hat{R}^{-1}\end{pmatrix}\begin{pmatrix} g(z)\hat{1} & \phi_o^{*-\frac{1}{2}}h\hat{1}\\ \phi^{*\frac{1}{2}}g'(z)\hat{1} & \sqrt{\frac{\phi^*}{\phi_o^*}}h'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{q}_o\\ \boldsymbol{p}_o\end{pmatrix}, \tag{4.28}$$

In case when the position in object and aperture plane is used to parameterize the rays, the solution in rotation coordinates takes a similar form

$$\begin{pmatrix} \boldsymbol{Q} \\ \boldsymbol{P} \end{pmatrix} = \begin{pmatrix} s(z)\hat{1} & t(z)\hat{1} \\ \phi^{*\frac{1}{2}} s'(z)\hat{1} & \phi^{*\frac{1}{2}} t'(z)\hat{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{Q}_o \\ \boldsymbol{Q}_a \end{pmatrix} \tag{4.29}$$

and in original coordinates

$$\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \hat{R}^{-1} & 0 \\ 0 & \frac{e}{\eta}\hat{R}^{-1} \end{pmatrix} \begin{pmatrix} s(z)\hat{1} & t(z)\hat{1} \\ \phi^{*\frac{1}{2}} s'(z)\hat{1} & \phi^{*\frac{1}{2}} t'(z)\hat{1} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \hat{R}(z_a) \end{pmatrix} \begin{pmatrix} \boldsymbol{q}_o \\ \boldsymbol{q}_a \end{pmatrix}, \tag{4.30}$$

The Picht's transformation corresponds to canonical transformation

$$\begin{aligned} \boldsymbol{Q}_p &= \phi^{*\frac{1}{4}} \boldsymbol{Q} \\ \boldsymbol{P}_p &= \phi^{*-\frac{1}{4}} \boldsymbol{P} \end{aligned} \tag{4.31}$$

which transforms the quadratic part of Hamiltonian into form of the Hamiltonian of linear oscillator

$$\tilde{H}_2 = \frac{1}{2}\boldsymbol{P}^2 + \frac{1}{2}\left(\frac{(2+\gamma^2)\phi'^2}{16\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}} \right) \boldsymbol{Q}^2 \tag{4.32}$$

the equation of motion then agree with trajectory equation (10).

In both the approaches the paraxial approximation is presented by the linear transformation described by the transfer matrix. The main consequence is that a point in the object plane is imaged into a point in the image one. It is an important property of the paraxial monochromatic optics. For detail description of the paraxial properties, cardinal elements etc. see e.g. [1].

4.2 The Paraxial Transformation – General Dispersion Case

We abandon the assumption that all of electrons have the same energy. According the previous description in such a case the new variable δ describing the energy deviation must be introduced. Like for the space variables only the first power of δ will contribute to the paraxial approximation. The paraxial trajectory equation is then obtained by linearization of the general trajectory equation described above. If the assumptions similar to previous subsection are used for the field it reads

$$x'' + \frac{\gamma\phi'}{2\phi^*}x' + \left(\frac{\gamma\phi''}{4\phi^*} - \frac{\gamma p_2}{2\phi^*} + \frac{\eta Q_2}{\phi^{*\frac{1}{2}}} + \frac{F_1^2}{4\phi^{*2}} \right) x + \frac{\eta}{\phi^{*\frac{1}{2}}}\left(\frac{1}{2}B'y + y'B\right) = -\frac{\gamma F_1}{2\phi^*} + \frac{\eta B_2}{\phi^{*\frac{1}{2}}} + \frac{\delta F_1}{4e\phi^{*2}} \tag{4.33a}$$

$$y'' + \frac{\gamma\phi'}{2\phi^*}y' + \left(\frac{\gamma\phi''}{4\phi^*} + \frac{\gamma p_2}{2\phi^*} - \frac{\eta Q_2}{\phi^{*\frac{1}{2}}} \right) y - \frac{\eta}{\phi^{*\frac{1}{2}}}\left(\frac{1}{2}B'x + x'B\right) = 0. \tag{4.33b}$$

The equations must be completed by equation $\delta' = 0$. In the rotation coordinates for the stigmatic systems fulfilling the Wien condition the equations read

$$X'' + \frac{\gamma\phi'}{2\phi^*}X' + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)X = \frac{\delta F_1}{4e\phi^{*2}}\cos(\Theta) \tag{4.34a}$$

$$Y'' + \frac{\gamma\phi'}{2\phi^*}Y' + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{F_1^2}{8\phi^{*2}}\right)Y = -\frac{\delta F_1}{4e\phi^{*2}}\sin(\Theta). \tag{4.34b}$$

These are two separated differential equations but unlike previous chapter they are inhomogeneous. Using the variation of parameter one can find the general solution

$$\begin{pmatrix} X \\ X' \\ \delta \end{pmatrix} = \begin{pmatrix} g(z) & h(z) & -g(z)\hat{\mu}(h) + h(z)\hat{\mu}(g) \\ g'(z) & h'(z) & -g'(z)\hat{\mu}(h) + h'(z)\hat{\mu}(g) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} X_o \\ X_o' \\ \delta \end{pmatrix} \tag{4.35}$$

$$\begin{pmatrix} Y \\ Y' \\ \delta \end{pmatrix} = \begin{pmatrix} g(z) & h(z) & -g(z)\hat{\nu}(h) + h(z)\hat{\nu}(g) \\ g'(z) & h'(z) & -g'(z)\hat{\nu}(h) + h'(z)\hat{\nu}(g) \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y_o \\ Y_o' \\ \delta \end{pmatrix}. \tag{4.36}$$

where the functionals

$$\hat{\mu}(f) = \frac{1}{4e\phi_o^{*\frac{1}{2}}}\int \frac{F_1 f\cos\Theta}{\phi^{*\frac{3}{2}}}\,\mathrm{d}z \qquad \hat{\nu}(f) = -\frac{1}{4e\phi_o^{*\frac{1}{2}}}\int \frac{F_1 f\sin\Theta}{\phi^{*\frac{3}{2}}}\,\mathrm{d}z \tag{4.37}$$

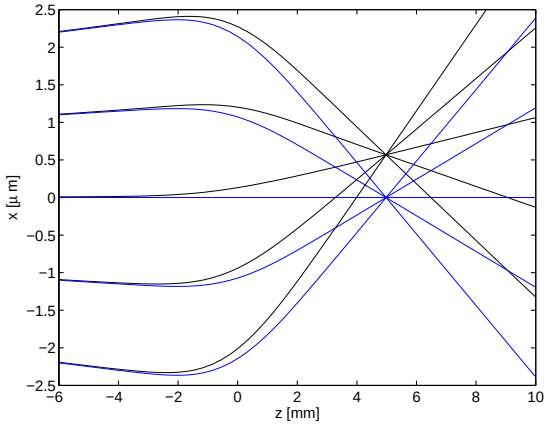
were defined. Finding the solution in original coordinates x, y is trivial.

In Hamiltonian approach the dispersion case is described by the quadratic part of the Hamiltonian (2.26) in which on contrary to (22) p_τ is not neglected. If the stigmatic systems in which the Wien's condition is fulfilled are considered the quadratic part of the Hamiltonian reads

$$\begin{aligned} H_2 = &\frac{\eta}{2e\phi^{*\frac{1}{2}}}\boldsymbol{p}^2 + \frac{\eta B}{2\phi^{*\frac{1}{2}}}L_z + \frac{1}{2}\left(\frac{e\gamma_0\phi''}{4\eta\phi^{*\frac{1}{2}}} + \frac{e\eta B^2}{4\phi^{*\frac{1}{2}}} + \frac{eF_1^2}{8\eta\phi^{*\frac{3}{2}}}\right)\boldsymbol{q}^2 + \\ &+ \frac{\eta mc^2}{4e^2\phi^{*\frac{3}{2}}}p_\tau^2 + \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}xp_\tau. \end{aligned} \tag{4.38}$$

The transition into rotation coordinates and using $P_\tau = \frac{\eta}{e}p_\tau$ transforms the Hamiltonian into

$$\begin{aligned} \tilde{H}_2 = &\frac{1}{2\phi^{*\frac{1}{2}}}\boldsymbol{P}^2 + \frac{1}{2}\left(\frac{\gamma\phi''}{4\phi^{*\frac{1}{2}}} + \frac{\eta^2 B^2}{4\phi^{*\frac{1}{2}}} + \frac{F_1^2}{8\phi^{*\frac{3}{2}}}\right)\boldsymbol{Q}^2 + \\ &+ \frac{mc^2}{4e\phi^{*\frac{3}{2}}}P_\tau^2 + \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}\cos\Theta X P_\tau - \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}\sin\Theta Y P_\tau. \end{aligned} \tag{4.39}$$



Obrázek 2: Focus of the rays with different energy

The computation of the trajectory determined by such an extended Hamiltonian we start from results of the previous subsection. We apply a canonical transformation which compensates the geometrical part of (39). It coincides with (27) and the transformed Hamiltonian takes form

$$\begin{aligned}\bar{H}_2 = &\frac{mc^2}{4e\phi^{*\frac{3}{2}}}\tilde{P}_\tau^2 + \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}\cos\Theta\tilde{P}_\tau(g(z)\tilde{X} + h(z)\phi_o^{*-\frac{1}{2}}\tilde{P}_x) \\ &- \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}\sin\Theta\tilde{P}_\tau(g(z)\tilde{Y} + h(z)\phi_o^{*-\frac{1}{2}}\tilde{P}_y).\end{aligned} \tag{4.40}$$

In this coordinates the trajectory equations are trivial

$$\tilde{X}' = \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}\phi_o^{*\frac{1}{2}}}h(z)\cos\Theta\tilde{P}_\tau \qquad \tilde{Y}' = -\frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}\phi_o^{*\frac{1}{2}}}h(z)\sin\Theta\tilde{P}_\tau \tag{4.41a}$$

$$\tilde{P}_x' = -\frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}g(z)\cos\Theta\tilde{P}_\tau \qquad \tilde{P}_y' = \frac{F_1 mc\eta}{2e\phi^{*\frac{3}{2}}}g(z)\sin\Theta\tilde{P}_\tau \tag{4.41b}$$

$$\tilde{P}_\tau' = 0, \tag{4.41c}$$

after short integration one can find the solution

$$\begin{pmatrix}\tilde{X}\\ \tilde{Y}\\ \tilde{P}_x\\ \tilde{P}_y\\ \tilde{P}_\tau\end{pmatrix} = \begin{pmatrix}1 & 0 & 0 & 0 & 2mc\eta\hat{\mu}(h)\\ 0 & 1 & 0 & 0 & 2mc\eta\hat{\nu}(h)\\ 0 & 0 & 1 & 0 & -2mc\eta\phi_o^{*\frac{1}{2}}\hat{\mu}(g)\\ 0 & 0 & 0 & 1 & -2mc\eta\phi_o^{*\frac{1}{2}}\hat{\nu}(g)\\ 0 & 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\tilde{X}_o\\ \tilde{Y}_o\\ \tilde{P}_{xo}\\ \tilde{P}_{yo}\\ \tilde{P}_{\tau o}\end{pmatrix}. \tag{4.42}$$

Transforming to rotation coordinates and using $P_\tau = \frac{\eta}{ec}\delta$ one can verify that the result is in agreement with (35) and (36).

Similarly to monochromatic case the dispersion paraxial approximation is described by the linear transformation. But on contrary to monochromatic one the added dimension causes that a point in the object plane is not imaged into point in the image plane. In fact the image plane intersection of the electron trajectory with energy about δ higher than the design energy is shifted about value proportional to δ. In the rotation coordinates it reads $-g(z_i)\hat{\mu}(h)(z_i)\delta$ in X direction and $g(z_i)\hat{\nu}(h)(z_i)\delta$ in Y direction. The example of imaging with three different energies of electrons can be seen in the picture.

4.3 Polynomial Form of Solution

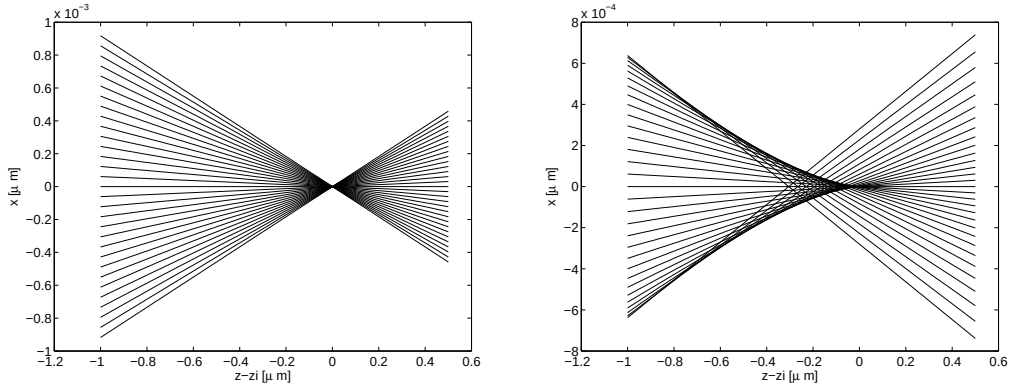
As a direct extension of the paraxial approximation in which the second and higher powers of the trajectory deviations and directives are neglected there appear the methods in which only powers of higher order than a given one can be neglected. The solution computed is then in form of the k-order polynomial, where k is the highest power which can not be neglected. Unfortunately this extension leads to great difficulties during solving of the trajectory equation. Adding of the higher orders terms causes the equations solved become nonlinear. Namely the trajectory equations in rotation coordinates read

$$\hat{P}_1(X) - \frac{\delta F_1}{4e\phi^{*2}}\cos\Theta = f_2(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z) + \cdots + f_k(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z) \tag{4.43a}$$

$$\hat{P}_1(Y) + \frac{\delta F_1}{4e\phi^{*2}}\sin\Theta = g_2(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z) + \cdots + g_k(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z) \tag{4.43b}$$

where $f_l(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z)$ and $g_l(\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',\delta,z)$ are homogeneous polynomials of l-th order in variables $\boldsymbol{Q}$, $\boldsymbol{Q}'$, $\boldsymbol{Q}''$ and δ with z-dependent coefficients. These equations can not be solved analytically. Fortunately we do not need the exact solution, but only its part up to k-th order polynomial in variables mentioned. There exists a number of perturbation methods used for the computation of such a form of solution. They are based on an interactive solution of the trajectory equations, Lagrangian or Hamiltonian perturbation method or on the solution of the trajectory equations in the higher degree polynomial space where they become linear. We will describe some of the methods in the next section.

Well, what the higher order terms cause from a physical point of view? They change the image properties rapidly. In brief they cause an object plane point not to be imaged into the image plane point, the focusing is perturbed. We observe it as image



Obrázek 3: Paraxial beam focus and focus of the same beam influenced by the spherical aberration. z_i is the position of the Gaussian image.

imperfection. The benefits of this solution form compared to direct numerical solution of the equations of motion lie in the possibility of the qualitative description of the imperfection, for each coefficient of the polynomial represents an aberration, the basic optical characteristic of the devices. Such coefficients are known as aberration coefficients. Knowledge of the aberration coefficients is sufficient to classify the imperfections and to find the way how to compensate them.

The perturbation methods compute the coefficients of the polynomial solution either in analytical or in numerical form. The analytical form of the coefficients includes the most of information about the optical elements the electron was going through, e.g. the spherical aberration coefficient of the axial symmetric magnetic lens reads [3]

$$C_S = M\phi_o^{*-\frac{1}{2}} \int_{z_o}^{z_i} (L_1 h^4 + 2L_2 h^2 h'^2 + L_3 h'^4)\mathrm{d}z \tag{4.44}$$

where

$$L_1 = \frac{\eta^2 B'' B}{8\phi^{*\frac{1}{2}}} + \frac{\eta^4 B^4}{32\phi^{*\frac{3}{2}}} \tag{4.45}$$

$$L_2 = \frac{\eta^2 B^2}{8\phi^{*\frac{1}{2}}} \tag{4.46}$$

$$L_3 = \frac{1}{2}\phi^{*\frac{1}{2}} \tag{4.47}$$

and M is magnification in image plane. It is easy to see the influence of the field from this form of solution, but the mathematical form of the term is complicated even if the system is very simple. In fact the complexity of such terms increases with the polynomial order and number of elements in the device. In general its use for higher order aberrations is very difficult. On the other hand there are the numerical methods which allow expressing the numerical solution in polynomial form. The aberration coefficients are then computed numerically. They do not include so much information about the system, but the method can be used for the higher orders aberrations easily.

4.4 Numerical Methods

The numerical methods mostly based on the standard Runge-Kutta numerical algorithm compute the ray from its position and directive in the object plane. The methods do not use the Taylor expansion of the field in the vicinity of the optical axis, but the values in an arbitrary point are calculated by a spline method [32, 33] from the values of the field in nodal points computed by (FEM, BEM, FDM). The advantage of this approach is that the field derivatives need not be computed by which we avoid the accuracy errors.

The computation mostly does not use the trajectory equations but it is based on the solution of the equation of motion in time parameterization

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\gamma\dot{\boldsymbol{r}}) = -e\boldsymbol{E} - e\dot{\boldsymbol{r}}\times\boldsymbol{B}, \tag{4.48}$$

where on contrary to analytical methods the values of γ, $\boldsymbol{E}$ and $\boldsymbol{B}$ are given in every point in the way mentioned above. The accuracy of such methods is given by numerical algorithm, generally it is very high especially for small z. Nevertheless, they have two disadvantages.

The first restriction comes from using any numerical method. As the computation of one ray does not include any information about rays close to it, each ray we are interested in must be computed separately. It means that we can not qualitatively describe the relationship between object ray conditions and the image properties – the aberrations coefficients – like from the polynomial form of solutions. Although the polynomial regression of numerical results is the method used for such a kind of problems, it is advisable for low orders of aberrations only [1].

Let us further note that the second disadvantage lies in the fact that the method forms only a relationship between initial and final coordinates without any parameter adopted. This after all means that the solution itself does not include any information

about the system; hence, it is not possible to recognize which elements have to be changed to make it better.

In spite of the issues mentioned the method can be used for the exact rays computation when the field distribution is known. Moreover, they are used at comparing the accuracy of polynomial form of solution as well but its use in designing of optical devices is restricted.

5 The Analytic Perturbation Method

The analytical perturbation methods are used for description of nonlinear properties of the electron optical systems. They are represented by the trajectory method, the eikonal method, and the Lie algebra method. The differential algebra method can be also used for calculation of aberration integrals but it is more used for numerical evaluation of the aberration coefficients.

The first calculation of aberration was done in the early 1930s by Scherzer [8], who used the trajectory method and by Glaser [9], who introduced the eikonal method. The other methods were introduced much later: the Lie algebra method by Dragt [3] in 1980s and the differential algebra method by Berz [7] in the late 1990s.

In this part we will shortly describe each of the perturbation method and show the application of the trajectory method, the eikonal method, and the Lie algebra method on the simple system of the round magnetic lens.

5.1 The Differential Algebra Method

It might at least seem courageous to start the introduction to perturbation methods used in the electron optics with the differential algebra method [7], which is not as familiar in electron optics community as methods described in following subsections. However, the features of the polynomial form of the solution straightly lead to the usage the method. Even though the polynomial form of the solution is not the exact, it is exact up to order of the solution polynomial, e.g. the polynomial solution

$$x = x_o - \frac{1}{2} f^2(z) x_o^2 + g(z) x_o' \tag{5.1}$$

is second order approximation of the exact solution

$$x = x_o + \cos(f(z)x_o) - 1 + \sin(g(z)x_o') \,.$$

The principle of the differential algebra method resides in the observation that the nonlinear approximated solution (1) in coordinates x_o, x_o' corresponds to the linear approximation of the map in coordinates x_o, x_o' extended by the polynomial coordinates

x_o^2, $x_o x_o'$ and $(x_o')^2$,

$$\begin{pmatrix} x \\ x' \\ x^2 \\ xx' \\ (x')^2 \end{pmatrix} = \begin{pmatrix} 1 & g(z) & -\frac{1}{2}f^2(z) & 0 & 0 \\ 0 & g'(z) & -f(z)f'(z) & 0 & 0 \\ 0 & 0 & 1 & 2g(z) & g^2(z) \\ 0 & 0 & 0 & g'(z) & g'g \\ 0 & 0 & 0 & 0 & g'^2 \end{pmatrix} \begin{pmatrix} x_o \\ x_o' \\ x_o^2 \\ x_o x_o' \\ (x_o')^2 \end{pmatrix} \tag{5.2}$$

which is the solution of some linear differential equation in the polynomial space of the second order. Thus if one finds such equations from the nonlinear differential equations in coordinates x and x', just the set of the linear differential equations will be solved, the result of which can be written in matrix form similar to (2). The coefficients in the polynomial solution will be represented by the matrix elements present in first two rows. Now let us apply it to the trajectory equation.

The trajectory equations in accuracy up to k-th order read

$$\boldsymbol{q}' = \frac{\partial H_2(\boldsymbol{q},\boldsymbol{p},z)}{\partial p} + \cdots + \frac{\partial H_{k+1}(\boldsymbol{q},\boldsymbol{p},z)}{\partial p} \tag{5.3a}$$

$$\boldsymbol{p}' = -\frac{\partial H_2(\boldsymbol{q},\boldsymbol{p},z)}{\partial q} - \cdots - \frac{\partial H_{k+1}(\boldsymbol{q},\boldsymbol{p},z)}{\partial q}\,, \tag{5.3b}$$

Now we will find the linear approximation of these equations in the polynomial space of the k-th order in variables $\boldsymbol{q}$, $\boldsymbol{p}$. The derivative of the differential algebraic basis element $|l_1,l_2,l_3,l_4\rangle = x^{l_1} y^{l_2} p_x^{l_3} p_y^{l_4}$ in such a space reads [10]

$$\frac{\mathrm{d}}{\mathrm{d}z}|l_1,l_2,l_3,l_4\rangle = [\,|l_1,l_2,l_3,l_4\rangle, H_2 + \cdots + H_l] \tag{5.4}$$

where the Poisson bracket are defined as

$$[g,h] = \frac{\partial g}{\partial \boldsymbol{q}}\frac{\partial f}{\partial \boldsymbol{p}} - \frac{\partial g}{\partial \boldsymbol{p}}\frac{\partial f}{\partial \boldsymbol{q}} \tag{5.5}$$

and $l = k - l_1 - l_2 - l_3 - l_4 + 2$, which is enough for us to describe the k^{th} aberration order, as $\text{degree}([g,h]) = \text{degree}(g) + \text{degree}(h) - 2$.

Using this procedure one can find the set of $\binom{4+k}{k} - 1$ linear differential equations of the first order which determines the solution up to k-th order. Generally it takes form

$$\boldsymbol{w}' + \hat{A}(z)\boldsymbol{w} = 0\,, \tag{5.6}$$

where

$$\boldsymbol{w}^T = (x, y, p_x, p_y, x^2, xy, \ldots, p_y^2, \ldots, x^k, \ldots, p_y^k). \tag{5.7}$$

The evolution operator of which can be formally written

$$\mathcal{M}(z,z_o)=\mathcal{T}\exp\left(-\int_{z_o}^{z}\hat{A}(t)\mathrm{d}t\right), \tag{5.8}$$

where $\mathcal{T}$ represents the time ordering. The usual way of practical computation is based on iteration method, but unfortunately the matrix $\hat{A}$ with block structure

$$\hat{A}=\begin{pmatrix} 4\times 4 & 4\times 20 & \cdots & 4\times\binom{3+k}{k} \\ 0 & 20\times 20 & \cdots & 20\times\binom{3+k}{k} \\ 0 & 0 & \cdot & \cdot \\ 0 & 0 & \cdots & \binom{3+k}{k}\times\binom{3+k}{k} \end{pmatrix} \tag{5.9}$$

is not nilpotent which causes that $\hat{A}^n\neq 0$ for any n; hence, the iteration method will not converge. The standard way of calculation used in differential algebra method is to solve the equation numerically using eg. Runge—Kutta method. It causes that the method is not analytical but it combines approaches of analytical and numerical methods.

This difficulty is surpassed by the use of interaction coordinates

$$\begin{pmatrix}\tilde{\boldsymbol{Q}}\\ \tilde{\boldsymbol{P}}\end{pmatrix}=\mathcal{M}_1^{-1}\begin{pmatrix}\boldsymbol{q}\\ \boldsymbol{p}\end{pmatrix}, \tag{5.10}$$

in which the quadratic part of Hamiltonian vanishes and the trajectory equations read

$$\tilde{\boldsymbol{Q}}'=\frac{\partial H_3^{\mathrm{int}}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}},z)}{\partial\tilde{\boldsymbol{P}}}+\cdots+\frac{\partial H_{k+1}^{\mathrm{int}}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}},z)}{\partial\tilde{\boldsymbol{P}}} \tag{5.11a}$$

$$\tilde{\boldsymbol{P}}'=-\frac{\partial H_3^{\mathrm{int}}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}},z)}{\partial\tilde{\boldsymbol{Q}}}-\cdots-\frac{\partial H_{k+1}^{\mathrm{int}}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}},z)}{\partial\tilde{\boldsymbol{Q}}}, \tag{5.11b}$$

where the H^{int} is transformed Hamiltonian – interaction Hamiltonian. We will discuss it more particularly in the Lie algebra method. The linear extension of the trajectory equation in k-th order polynomial space takes form

$$\tilde{\boldsymbol{W}}'+\hat{A}^{\mathrm{int}}(z)\tilde{\boldsymbol{W}}=0 \tag{5.12}$$

where the matrix $\hat{A}^{\mathsf{int}}$ with structure

$$\hat{A}^{\mathsf{int}} = \left(\begin{array}{c|c|c|c} 0 & 4\times 20 & \cdots & 4\times\binom{3+k}{k} \\ \hline 0 & 0 & \cdots & 20\times\binom{3+k}{k} \\ \hline 0 & 0 & \cdot & \cdot \\ \hline 0 & 0 & \cdots & 0 \end{array}\right) \tag{5.13}$$

is nilpotent – $(\hat{A}^{\mathsf{int}})^{k+1} = 0$ – which causes the iteration method to converge in k steps. One can then express the transfer map

$$\tilde{M} = \hat{1} - \int_{z_o}^{z} \hat{A}(t)\mathrm{d}t + \int_{z_o}^{z}\mathrm{d}t_1 \int_{z_o}^{t_1}\mathrm{d}t_2 \hat{A}(t_1)\hat{A}(t_2) + \cdots + (-1)^k \int_{z_o}^{z}\mathrm{d}t_1 \cdots \int_{z_o}^{t_{k-1}}\mathrm{d}t_k \hat{A}(t_1)\cdots\hat{A}(t_k)\,. \tag{5.14}$$

In original coordinates the solution reads

$$\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} = \mathcal{M}_1 \begin{pmatrix} \tilde{\boldsymbol{Q}}(z) \\ \tilde{\boldsymbol{P}}(z) \end{pmatrix} \tag{5.15}$$

Previous text was only short description of principles of the method. More information can be found in [7]. The method was implemented into computer code [24] and it is often used for numerical calculation of higher order aberration [26]. Such calculation is based on equation (6). The result is not the formula for the aberration coefficient like the formula (4.44) but only the numerical value. The form of the method is independent from the order of aberration. Thus, having exact axial potential and their derivatives we can compute aberrations of any order. But the use of the method is limited by inaccuracy of the higher order derivatives of axial potential in real optical systems.

5.2 The Trajectory Method

Although the differential algebra method allows us to compute the polynomial form of solution in a really representative way, finding the analytical form of differential equations in higher polynomial space might grow too lengthy. In the trajectory method the polynomial form of solution is computed directly from the trajectory equations, but on the other hand it loses the transparency of the differential algebra method.

The computation is commonly based on the iterative solution of the trajectory equation (2.7), in which the linear approximation is taken as a initial assumption [1]. The equation for the k-th iteration in the rotation coordinates then takes form

$$\hat{P}_1(\boldsymbol{Q}^{[k]}) = \boldsymbol{f}_2(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},z) + \boldsymbol{f}_3(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},z) + \cdots, \qquad (5.16)$$

where $\boldsymbol{Q}^{[0]} = \boldsymbol{Q}^{[0]}(\boldsymbol{Q}_o,\boldsymbol{Q}'_o,z)$ is the solution of the paraxial equation in rotation coordinates. The highest order of the terms considered on the right hand side coincides with the order of the aberrations computed. The equations (16) form a set of two linear inhomogeneous differential equations of the second order, the solution of which can be found using parameter variation method in case of parameterization by object position and directives

$$\begin{aligned}\boldsymbol{Q}^{[k]} = &\frac{h(z)}{\phi_o^{*\frac{1}{2}}}\int_{z_o}^{z} g(t)\phi^{*\frac{1}{2}}\left(\boldsymbol{f}_2(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},t) + \boldsymbol{f}_3(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},t) + \cdots\right)\mathrm{d}t \qquad (5.17)\\ &- \frac{g(z)}{\phi_o^{*\frac{1}{2}}}\int_{z_o}^{z} h(t)\phi^{*\frac{1}{2}}\left(\boldsymbol{f}_2(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},t) + \boldsymbol{f}_3(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},t) + \cdots\right)\mathrm{d}t.\end{aligned}$$

where $\boldsymbol{Q}^{[k-1]} = \boldsymbol{Q}^{[k-1]}(\boldsymbol{q}_o,\boldsymbol{q}'_o,z)$. In case of parameterization by position in the object and aperture plane

$$\begin{aligned}\boldsymbol{Q}^{[k]} = &\frac{1}{W_{so}\phi_o^{*\frac{1}{2}}}\left(t(z)\int_{z_o}^{z} s\phi^{*\frac{1}{2}}\left(\boldsymbol{f}_2(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},\alpha) + \boldsymbol{f}_3(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},\alpha) + \cdots\right)\mathrm{d}\alpha\right. \qquad (5.18)\\ &\left. - s(z)\int_{z_o}^{z} t\phi^{*\frac{1}{2}}\left(\boldsymbol{f}_2(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},\alpha) + \boldsymbol{f}_3(\boldsymbol{Q}^{[k-1]},\boldsymbol{Q}^{[k-1]\prime},\boldsymbol{Q}^{[k-1]\prime\prime},\alpha) + \cdots\right)\mathrm{d}\alpha\right).\end{aligned}$$

where $\boldsymbol{Q}^{[k-1]} = \boldsymbol{Q}^{[k-1]}(\boldsymbol{Q}_o,\boldsymbol{Q}_a,z)$

The procedure presented is commonly used; however, it is not easy to see which terms on the right hand side have to be included and how many iteration steps must be done to evaluate the solution exact up to k-th order. For this purposes we must handle with trajectory equations more carefully. The best choice seems to introduce the perturbation parameter λ using which the comparison of perturbation orders become more transparent.

Let us suppose the solution in polynomial form

$$\boldsymbol{Q} = \boldsymbol{Q}_1(\boldsymbol{Q}_o,\boldsymbol{Q}'_o,z) + \boldsymbol{Q}_2(\boldsymbol{Q}_o,\boldsymbol{Q}'_o,z) + \boldsymbol{Q}_3(\boldsymbol{Q}_o,\boldsymbol{Q}'_o,z) + \cdots \qquad (5.19)$$

where $\boldsymbol{Q}_k(\boldsymbol{Q}_o,\boldsymbol{Q}'_o,z)$ is k-th order homogeneous polynomial in $\boldsymbol{Q}_o$ and $\boldsymbol{Q}'_o$. Similarly when the parameterization by position in the object and aperture plane is used the solution will be in form

$$\boldsymbol{Q} = \boldsymbol{Q}_1(\boldsymbol{Q}_o,\boldsymbol{Q}_a,z) + \boldsymbol{Q}_2(\boldsymbol{Q}_o,\boldsymbol{Q}_a,z) + \boldsymbol{Q}_3(\boldsymbol{Q}_o,\boldsymbol{Q}_a,z) + \cdots \tag{5.20}$$

and $\boldsymbol{Q}_k(\boldsymbol{Q}_o,\boldsymbol{Q}_a,z)$ is k-th order homogeneous polynomial in $\boldsymbol{Q}_o$ and $\boldsymbol{Q}_a$. Using the perturbation parameter it can be rewritten into

$$\boldsymbol{Q}(\lambda) = \boldsymbol{Q}_1 + \lambda\boldsymbol{Q}_2 + \lambda^2\boldsymbol{Q}_3 + \cdots, \tag{5.21}$$

which would be used in perturbation procedure. Comparing (19) and (21) one can easily see that $\boldsymbol{Q}(\lambda=1) = \boldsymbol{Q}$. Similarly to (19) the right hand side of equation (2.7) must be rewritten such that trajectory equation takes form

$$\hat{P}_1(\boldsymbol{Q}(\lambda)) = \lambda\boldsymbol{f}_2 + \lambda^2\boldsymbol{f}_3 + \cdots \tag{5.22}$$

where $\boldsymbol{f}_k$ is k^{th} order homogeneous polynomial in $\boldsymbol{Q}_o$ and $\boldsymbol{Q}'_o$ or $\boldsymbol{Q}_o$ and $\boldsymbol{Q}_a$.

Let us now substitute (21) into the trajectory equation

$$\begin{aligned}\hat{P}_1(\boldsymbol{Q}_1 + \lambda\boldsymbol{Q}_2 + \lambda^2\boldsymbol{Q}_3 + \cdots) = \\ = \lambda\boldsymbol{f}_2(\boldsymbol{Q}_1 + \lambda\boldsymbol{Q}_2 + \cdots, \boldsymbol{Q}'_1 + \lambda\boldsymbol{Q}'_2 + \cdots, \boldsymbol{Q}''_1 + \lambda\boldsymbol{Q}''_2 + \cdots, z) + \lambda^2\boldsymbol{f}_3(\boldsymbol{Q}_1 + \cdots, \boldsymbol{Q}'_1 + \cdots, \boldsymbol{Q}''_1 + \cdots, z) + \cdots.\end{aligned} \tag{5.23}$$

Comparing zero-th order terms in λ one can find the paraxial trajectory equations

$$\hat{P}_1(\boldsymbol{Q}_1) = \boldsymbol{Q}''_1 + \frac{\gamma\phi'}{2\phi^*}\boldsymbol{Q}'_1 + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{\gamma^2 F_1^2}{8\phi^{*2}}\right)\boldsymbol{Q}_1 = 0, \tag{5.24}$$

while comparing the first order terms leads to equations determinating the second aberration order

$$\boldsymbol{Q}''_2 + \frac{\gamma\phi'}{2\phi^*}\boldsymbol{Q}'_2 + \left(\frac{\gamma\phi''}{4\phi^{*2}} + \frac{\eta^2 B^2}{4\phi^*} + \frac{\gamma^2 F_1^2}{8\phi^{*2}}\right)\boldsymbol{Q}_2 = \boldsymbol{f}_2(\boldsymbol{Q}_1, \boldsymbol{Q}'_1, \boldsymbol{Q}''_1, z)\,. \tag{5.25}$$

As on the right hand side there is only function of z ($\boldsymbol{Q}_1$ is the solution of the paraxial approximation) the solution of (25) can be by parameter variation method evaluated for case of parameterization by object position and directives in form

$$\boldsymbol{Q}_2 = h(z)\phi_o^{*-\frac{1}{2}}\int_{z_o}^{z}\phi^{*\frac{1}{2}}g(t)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}'_1,\boldsymbol{Q}''_1,t)\mathrm{d}t - g(z)\phi_o^{*-\frac{1}{2}}\int_{z_o}^{z}\phi^{*\frac{1}{2}}h(t)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}'_1,\boldsymbol{Q}''_1,t)\mathrm{d}t. \tag{5.26}$$

or in case of parameterization by position in the object object and aperture planes

$$\boldsymbol{Q}_2 = \frac{1}{W_{so}\phi_o^{*\frac{1}{2}}}\left(t(z)\int_{z_o}^{z}\phi^{*\frac{1}{2}}s(\alpha)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',\alpha)\mathrm{d}t - s(z)\int_{z_o}^{z}\phi^{*\frac{1}{2}}t(\alpha)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1''\alpha)\mathrm{d}\alpha\right) \tag{5.27}$$

For computing of higher aberration orders one must compare the higher orders of λ, e.g. the third aberration order is determined by the equations

$$\hat{P}_1(\boldsymbol{Q}_3) = \sum_{i=1}^{2}\left(\frac{\partial \boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z)}{\partial Q_i}Q_{2i} + \frac{\partial \boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z)}{\partial Q_i'}Q_{2i}' + \frac{\partial \boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z)}{\partial Q_i''}Q_{2i}''\right) + \tag{5.28}$$
$$+\boldsymbol{f}_3(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z)$$

The solution of the previous equations found by the trajectory method takes form similar to (26) or (27).

Let us note that (26) and (27) comes more simply when the aberrations are expressed in image plane, where $g(z_i) = M$ and $h(z_i) = 0$, or $s(z_i) = M$ and $t(z_i) = 0$. In such a case they are simplified to

$$\boldsymbol{Q}_2 = -M\phi_o^{*-\frac{1}{2}}\int_{z_o}^{z}\phi^{*\frac{1}{2}}h(t)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1\prime,\boldsymbol{Q}_1'',t)\mathrm{d}t \tag{5.29}$$

or

$$\boldsymbol{Q}_2 = -\frac{M}{W_{so}\phi_o^{*\frac{1}{2}}}\int_{z_o}^{z}\phi^{*\frac{1}{2}}t(\alpha)\boldsymbol{f}_2(\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1''\alpha)\mathrm{d}\alpha \tag{5.30}$$

Using the previous procedure it is possible to compute the aberrations of any order; moreover, by introducing the perturbation parameter the calculation becomes more transparent compared to procedure based on (16).

5.3 The Eikonal Method

Introducing this method we get into the class of perturbation methods based on the variational principles. In particular the eikonal method is special case of the Lagrangian perturbation calculus. Thanks to its use in [1] the method is very familiar in electron optics community. Let us start from Lagrangian formulation of the trajectory equations,

namely from (2.15) where from here we will denote the integrand by M, i.e.

$$M = \Phi^{*\frac{1}{2}}(1+\boldsymbol{q}'^2)^{\frac{1}{2}} - \eta(A_x x' + A_y y' + A_z). \tag{5.31}$$

The paraxial approximation is described by action

$$S_{12}^{(0)} = \int_{z_1}^{z_2} M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}'^{(0)}, z)\mathrm{d}z \tag{5.32}$$

where M_2 is the quadratic part of the Lagrangian (31). Varying such an action one can find

$$\delta S_{12}^{(0)} = \int_{z_1}^{z_2} \left(\frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}^{(0)}} - \frac{\mathrm{d}}{\mathrm{d}z} \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'^{(0)}} \right) \delta \boldsymbol{q}^{(0)} \mathrm{d}z + \boldsymbol{p}_{\underline{2}}^{(0)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{p}_{\underline{1}}^{(0)} \delta \boldsymbol{q}_{\underline{1}}^{(0)} \tag{5.33}$$

where $\boldsymbol{p}^{(0)} = \partial M_2 / \partial \boldsymbol{q}'$. When we assume that $\boldsymbol{q}^{(0)}$ fulfils the paraxial equation of motion

$$\frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}} - \frac{\mathrm{d}}{\mathrm{d}z} \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'} = 0\,, \tag{5.34}$$

the equation reduces to

$$\delta S_{12}^{(0)} = \boldsymbol{p}_{\underline{2}}^{(0)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{p}_{\underline{1}}^{(0)} \delta \boldsymbol{q}_{\underline{1}}^{(0)}. \tag{5.35}$$

However the intention here is to describe the situation when higher terms of the Lagrangian are assumed. Let us consider that (31) can be expanded

$$M(\boldsymbol{q}, \boldsymbol{q}', z) = M_2(\boldsymbol{q}, \boldsymbol{q}', z) + \lambda M^I(\boldsymbol{q}, \boldsymbol{q}', z) + \lambda^2 M^{II}(\boldsymbol{q}, \boldsymbol{q}', z) + \cdots \tag{5.36}$$

and the paraxial trajectory is changed to

$$\boldsymbol{q} = \boldsymbol{q}^{(0)} + \lambda \boldsymbol{q}^{(1)} + \lambda^2 \boldsymbol{q}^{(2)} + \cdots, \tag{5.37}$$

where parameter λ is perturbation parameter. One can find the variation of the action

$$S_{12} = \int_{z_1}^{z_2} M(\boldsymbol{q}, \boldsymbol{q}', z)\mathrm{d}z \tag{5.38}$$

either using method similar to deriving (35)

$$\begin{aligned} \delta S = {} & \boldsymbol{p}_{\underline{2}} \delta \boldsymbol{q}_{\underline{2}} - \boldsymbol{p}_{\underline{1}} \delta \boldsymbol{q}_{\underline{1}} = (\boldsymbol{p}_{\underline{2}}^{(0)} + \lambda \boldsymbol{p}_{\underline{2}}^{(1)} + \lambda^2 \boldsymbol{p}_{\underline{2}}^{(2)} + \cdots)\, \delta(\boldsymbol{q}_{\underline{2}}^{(0)} + \lambda \boldsymbol{q}_{\underline{2}}^{(1)} + \lambda^2 \boldsymbol{q}_{\underline{2}}^{(2)} + \cdots) - \\ & - (\boldsymbol{p}_{\underline{1}}^{(0)} + \lambda \boldsymbol{p}_{\underline{1}}^{(1)} + \lambda^2 \boldsymbol{p}_{\underline{1}}^{(2)} + \cdots)\, \delta(\boldsymbol{q}_{\underline{1}}^{(0)} + \lambda \boldsymbol{q}_{\underline{1}}^{(1)} + \lambda^2 \boldsymbol{q}_{\underline{1}}^{(2)} + \cdots) \end{aligned} \tag{5.39}$$

with $\boldsymbol{p}^{(1)} = \partial M^I/\partial \boldsymbol{q}'$, $\boldsymbol{p}^{(2)} = \partial M^{II}/\partial \boldsymbol{q}'$ etc., or varying the action (38) into which (36) and (37) were substituted

$$\begin{aligned} S = \int_{z_1}^{z_2} \{ & M_2(\boldsymbol{q}^{(0)} + \lambda \boldsymbol{q}^{(1)} + \lambda^2 \boldsymbol{q}^{(2)} + \cdots, \boldsymbol{q}^{(0)\prime} + \lambda \boldsymbol{q}^{(1)\prime} + \lambda^2 \boldsymbol{q}^{(2)\prime} + \cdots, z) + \\ & + \lambda M^I(\boldsymbol{q}^{(0)} + \lambda \boldsymbol{q}^{(1)} + \lambda^2 \boldsymbol{q}^{(2)} + \cdots, \boldsymbol{q}^{(0)\prime} + \lambda \boldsymbol{q}^{(1)\prime} + \lambda^2 \boldsymbol{q}^{(2)\prime} + \cdots, z) + \\ & + \lambda^2 M^{II}(\boldsymbol{q}^{(0)} + \lambda \boldsymbol{q}^{(1)} + \lambda^2 \boldsymbol{q}^{(2)} + \cdots, \boldsymbol{q}^{(0)\prime} + \lambda \boldsymbol{q}^{(1)\prime} + \lambda^2 \boldsymbol{q}^{(2)\prime} + \cdots, z) + \cdots \} \mathrm{d}z, \end{aligned} \tag{5.40}$$

Let us note that from optical point of view S coincides with eikonal; hence, the name of method.

The idea is to expand both (39) and (40) into powers of λ

$$S_{12} = S_{12}^{(0)} + \lambda S_{12}^{(1)} + \lambda^2 S_{12}^{(2)} + \cdots \tag{5.41a}$$

$$\delta S_{12} = \delta S_{12}^{(0)} + \lambda \delta S_{12}^{(1)} + \lambda^2 \delta S_{12}^{(2)} + \cdots. \tag{5.41b}$$

and from a comparison to find the $\boldsymbol{q}^{(i)}$ and $\boldsymbol{p}^{(i)}$. We will show the procedure on perturbation of the first and second orders.

The First Order Perturbation

This perturbation is described by

$$S_{12}^{(1)} = \int_{z_1}^{z_2} \left(M^I(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z) + \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}} \boldsymbol{q}^{(1)} + \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'} \boldsymbol{q}^{(1)\prime} \right) \tag{5.42}$$

which using the per-partes integration and paraxial equations of motion is reduced into

$$S_{12}^{(1)} = S_{12}^I(\boldsymbol{q}_{\underline{1}}^{(0)}, \boldsymbol{q}_{\underline{1}}^{\prime(0)}, z) + \boldsymbol{p}_{\underline{2}}^{(0)} \boldsymbol{q}_{\underline{2}}^{(1)} - \boldsymbol{p}_{\underline{1}}^{(0)} \boldsymbol{q}_{\underline{1}}^{(1)} \tag{5.43}$$

where

$$S_{12}^I = \int_{z_1}^{z_2} M^I(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z) \mathrm{d}z \tag{5.44}$$

is given function of $\boldsymbol{q}_1$, $\boldsymbol{p}_1$ and z. The variation of (43) reads

$$\delta S_{12}^{(1)} = \delta S_{12}^I + \delta \boldsymbol{p}_{\underline{2}}^{(0)} \boldsymbol{q}_{\underline{2}}^{(1)} + \boldsymbol{p}_{\underline{2}}^{(0)} \delta \boldsymbol{q}_{\underline{2}}^{(1)} - \delta \boldsymbol{p}_{\underline{1}}^{(0)} \boldsymbol{q}_{\underline{1}}^{(1)} - \boldsymbol{p}_{\underline{1}}^{(0)} \delta \boldsymbol{q}_{\underline{1}}^{(1)}, \tag{5.45}$$

on the other hand we can express the variation from (39)

$$\delta S_{12}^{(1)} = \boldsymbol{p}_{\underline{2}}^{(0)} \delta \boldsymbol{q}_{\underline{2}}^{(1)} + \boldsymbol{p}_{\underline{2}}^{(1)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{p}_{\underline{1}}^{(0)} \delta \boldsymbol{q}_{\underline{1}}^{(1)} - \boldsymbol{p}_{\underline{1}}^{(1)} \delta \boldsymbol{q}_{\underline{1}}^{(0)} \tag{5.46}$$

and comparing the two previous equations one can find the first order perturbation relation,

$$\delta S_{12}^I = \boldsymbol{p}_{\underline{2}}^{(1)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{p}_{\underline{1}}^{(1)} \delta \boldsymbol{q}_{\underline{1}}^{(0)} - \delta \boldsymbol{p}_{\underline{2}}^{(0)} \boldsymbol{q}_{\underline{2}}^{(1)} + \delta \boldsymbol{p}_{\underline{1}}^{(0)} \boldsymbol{q}_{\underline{1}}^{(1)} . \tag{5.47}$$

The relation is more general than we commonly need; hence, we may require for the perturbed rays to fulfil some constraints. Two such cases are relevant. The first one

$$\boldsymbol{q}_{\underline{1}}^{(1)} = \boldsymbol{p}_{\underline{1}}^{(1)} = 0 \tag{5.48}$$

constrains the start position and impulses of perturbed rays with unperturbed ones. The perturbed ray is then determined by its position and directives in z_1. The first order perturbation relation then reads

$$\delta S_{12}^I = \boldsymbol{p}_{\underline{2}}^{(1)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{2}}^{(1)} \delta \boldsymbol{p}_{\underline{2}}^{(0)}, \tag{5.49}$$

which leads to the set of equations

$$\frac{\partial S_{12}^I}{\partial \boldsymbol{q}_{\underline{1}}} = \sum_{k=1}^{2} p_{\underline{2}k}^{(1)} \frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_{\underline{1}}} - q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_{\underline{1}}} \tag{5.50a}$$

$$\frac{\partial S_{12}^I}{\partial \boldsymbol{p}_{\underline{1}}} = \sum_{k=1}^{2} p_{\underline{2}k}^{(1)} \frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{p}_{\underline{1}}} - q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{p}_{\underline{1}}} , \tag{5.50b}$$

which can be write in form

$$\begin{pmatrix} \frac{\partial S_{12}^I}{\partial \boldsymbol{q}_{\underline{1}}} \\ \frac{\partial S_{12}^I}{\partial \boldsymbol{p}_{\underline{1}}} \end{pmatrix} = \mathcal{M}_1^T \begin{pmatrix} \boldsymbol{p}_{\underline{2}}^{(1)} \\ -\boldsymbol{q}_{\underline{2}}^{(1)} \end{pmatrix} \tag{5.51}$$

where $\mathcal{M}_1$ is a paraxial matrix in parameterization by $\boldsymbol{q}_o$ and $\boldsymbol{p}_o$. The coordinates $\boldsymbol{q}_{\underline{2}}^{(1)}$ and $\boldsymbol{p}_{\underline{2}}^{(1)}$ are easy to calculate,

$$\begin{pmatrix} \boldsymbol{p}_{\underline{2}}^{(1)} \\ -\boldsymbol{q}_{\underline{2}}^{(1)} \end{pmatrix} = (\mathcal{M}_1^T)^{-1} \begin{pmatrix} \frac{\partial S_{12}^I}{\partial \boldsymbol{q}_{\underline{1}}} \\ \frac{\partial S_{12}^I}{\partial \boldsymbol{p}_{\underline{1}}} \end{pmatrix} \tag{5.52}$$

When the rotation coordinates are used at calculation the previous result can be simplified for stigmatic system to

$$\begin{pmatrix} \boldsymbol{P}_{\underline{2}}^{(1)} \\ -\boldsymbol{Q}_{\underline{2}}^{(1)} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{\phi^*}{\phi_o^*}} h' \hat{1} & -\phi^{*\frac{1}{2}} g' \hat{1} \\ -\phi_o^{*-\frac{1}{2}} h \hat{1} & g \hat{1} \end{pmatrix} \begin{pmatrix} \frac{\partial S_{12}^I}{\partial \boldsymbol{Q}_{\underline{1}}} \\ \frac{\partial S_{12}^I}{\partial \boldsymbol{P}_{\underline{1}}} \end{pmatrix} \tag{5.53}$$

Thus, in image plane, where $h(z_i)=0$ and $g(z_i)=M$, we can write

$$\boldsymbol{Q}_i^{(1)} = -M\frac{\partial S_{12}^I}{\partial \boldsymbol{P}_o} \tag{5.54}$$

The second reasonable choice of constraint reads

$$\boldsymbol{q}_{\underline{1}}^{(1)} = \boldsymbol{q}_{\underline{2}}^{(1)} = 0 \tag{5.55}$$

which means that the perturbed ray is determined by its positions in z_1 and z_2. The first order perturbation relation then takes form

$$\delta S_{12}^I = \boldsymbol{p}_{\underline{2}}^{(1)}\delta\boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{p}_{\underline{1}}^{(1)}\delta\boldsymbol{q}_{\underline{1}}^{(0)}. \tag{5.56}$$

In practical computation the rays are determined by their position in the object and aperture planes which means that the constraints take form

$$\boldsymbol{q}_o^{(1)} = \boldsymbol{q}_a^{(1)} = 0 \tag{5.57}$$

and the first order perturbation relations read

$$\delta S_{o2}^I = \boldsymbol{p}_{\underline{2}}^{(1)}\delta\boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{2}}^{(1)}\delta\boldsymbol{p}_{\underline{2}}^{(0)} - \boldsymbol{p}_o^{(1)}\delta\boldsymbol{q}_o^{(0)} \tag{5.58}$$

$$\delta S_{a2}^I = \boldsymbol{p}_{\underline{2}}^{(1)}\delta\boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{2}}^{(1)}\delta\boldsymbol{p}_{\underline{2}}^{(0)} - \boldsymbol{p}_a^{(1)}\delta\boldsymbol{q}_a^{(0)}. \tag{5.59}$$

The quantities $\boldsymbol{p}_2^{(1)}$ and $\boldsymbol{q}_2^{(1)}$ can be evaluated from the equations

$$\frac{\partial S_{o2}^I}{\partial \boldsymbol{q}_a} = \sum_{k=1}^{2} p_{\underline{2}k}^{(1)}\frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a} - q_{\underline{2}k}^{(1)}\frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a} \tag{5.60a}$$

$$\frac{\partial S_{a2}^I}{\partial \boldsymbol{q}_o} = \sum_{k=1}^{2} p_{2k}^{(1)}\frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_o} - q_{2k}^{(1)}\frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_o}, \tag{5.60b}$$

where the functions S_{o2}^I and S_{a2}^I were parameterized by positions in the object and aperture plane $S_{o2}^I(\boldsymbol{q}_o,\boldsymbol{q}_a,z)$ and $S_{a2}^I(\boldsymbol{q}_o,\boldsymbol{q}_a,z)$. Similarly as in previous case

$$\begin{pmatrix} \frac{\partial S_{a2}^I}{\partial \boldsymbol{q}_o} \\ \frac{\partial S_{12}^I}{\partial \boldsymbol{q}_a} \end{pmatrix} = \mathcal{M}_1^T \begin{pmatrix} \boldsymbol{p}_{\underline{2}}^{(1)} \\ -\boldsymbol{q}_{\underline{2}}^{(1)} \end{pmatrix} \tag{5.61}$$

where $\mathcal{M}_1$ is a paraxial matrix in parameterization by $\boldsymbol{q}_o$ and $\boldsymbol{q}_a$. For stigmatic system in rotation coordinates one can find

$$\begin{pmatrix} \boldsymbol{P}_{\underline{2}}^{(1)} \\ -\boldsymbol{Q}_{\underline{2}}^{(1)} \end{pmatrix} = \frac{1}{W_{so}\phi_o^{*\frac{1}{2}}} \begin{pmatrix} \phi^{*\frac{1}{2}}t'\hat{1} & -\phi^{*\frac{1}{2}}s'\hat{1} \\ -t\hat{1} & s\hat{1} \end{pmatrix} \begin{pmatrix} \frac{\partial S_{a2}^I}{\partial \boldsymbol{Q}_o} \\ \frac{\partial S_{12}^I}{\partial \boldsymbol{Q}_a} \end{pmatrix} \tag{5.62}$$

where $W_s = st' - s't$ is Wronskian (4.19). Thus, in image plane, where $t(z_i) = 0$ and $s(z_i) = M$, we can write

$$\boldsymbol{Q}_i^{(1)} = -\frac{M}{\phi_o^{*\frac{1}{2}} W_{so}} \frac{\partial S_{o2}^I}{\partial \boldsymbol{Q}_a}. \tag{5.63}$$

The Second Order Perturbation

This perturbation order is described by the part of the action

$$S_{12}^{(2)} = \int_{z_1}^{z_2} \Bigg\{ M^{II}(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)}, z) + \frac{\partial M^I(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}} \boldsymbol{q}^{(1)} + \frac{\partial M^I(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'} \boldsymbol{q}^{(1)\prime} +$$
$$+ \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}} \boldsymbol{q}^{(2)} + \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'} \boldsymbol{q}^{(2)\prime} + \frac{1}{2} \sum_{i,j} \Bigg(\frac{\partial^2 M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial q_i \partial q_i} q_i^{(1)} q_j^{(1)}$$
$$+ 2 \frac{\partial^2 M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial q_i \partial q_j'} q_i^{(1)} q_j^{(1)\prime} + \frac{\partial^2 M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial q_i' \partial q_j'} q_i^{(1)\prime} q_j^{(1)\prime} \Bigg) \Bigg\} \mathrm{d}z \,. \tag{5.64}$$

Similarly to the first order perturbation by use of equation of motion we can write

$$\int_{z_1}^{z_2} \left(\frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}} \boldsymbol{q}^{(2)} + \frac{\partial M_2(\boldsymbol{q}^{(0)}, \boldsymbol{q}^{(0)\prime}, z)}{\partial \boldsymbol{q}'} \boldsymbol{q}^{(2)\prime} \right) \mathrm{d}z = \boldsymbol{p}_{\underline{2}}^{(0)} \boldsymbol{q}_{\underline{2}}^{(2)} - \boldsymbol{p}_{\underline{1}}^{(0)} \boldsymbol{q}_{\underline{1}}^{(2)} \,. \tag{5.65}$$

$S_{12}^{(2)}$ can be also simplified using

$$\int_{z_1}^{z_2} \left(\boldsymbol{q}^{(1)} \frac{\partial M}{\partial \boldsymbol{q}} + \boldsymbol{q}^{(1)\prime} \frac{\partial M}{\partial \boldsymbol{q}'} \right) \mathrm{d}z = \boldsymbol{q}_{\underline{2}}^{(1)} \boldsymbol{p}_{\underline{2}} - \boldsymbol{q}_{\underline{1}}^{(1)} \boldsymbol{p}_{\underline{1}} \tag{5.66}$$

where the left hand side can be expanded into powers of the perturbation parameter λ

$$\int_{z_1}^{z_2} \left(\boldsymbol{q}^{(1)} \frac{\partial M_2}{\partial \boldsymbol{q}} + \boldsymbol{q}^{(1)\prime} \frac{\partial M_2}{\partial \boldsymbol{q}'} \right) \mathrm{d}z + \lambda \left(\int_{z_1}^{z_2} \left(\boldsymbol{q}^{I} \frac{\partial M^I}{\partial \boldsymbol{q}} + \boldsymbol{q}^{(1)\prime} \frac{\partial M^I}{\partial \boldsymbol{q}'} \right) \mathrm{d}z + \right. \tag{5.67}$$
$$\left. + \int_{z_1}^{z_2} \sum_{i,j} \left(q_i^{(1)} q_j^{(1)} \frac{\partial^2 M_2}{\partial q_i \partial q_j} + 2 q_i^{(1)} q_j^{(1)\prime} \frac{\partial^2 M_2}{\partial q_i \partial q_j'} + q_i^{(1)\prime} q_j^{(1)\prime} \frac{\partial^2 M_2}{\partial q_i' \partial q_j'} \right) \mathrm{d}z \right) + o(\lambda^2)$$

and the right hand side to

$$\boldsymbol{q}_{\underline{2}}^{(1)} \boldsymbol{p}_{\underline{2}} - \boldsymbol{q}_{\underline{1}}^{(1)} \boldsymbol{p}_{\underline{1}} = \boldsymbol{q}_{\underline{2}}^{(1)} \boldsymbol{p}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{1}}^{(1)} \boldsymbol{p}_{\underline{1}}^{(0)} + \lambda (\boldsymbol{q}_{\underline{2}}^{(1)} \boldsymbol{p}_{\underline{2}}^{(1)} - \boldsymbol{q}_{\underline{1}}^{(1)} \boldsymbol{p}_{\underline{1}}^{(1)}) + o(\lambda^2) \tag{5.68}$$

When we compare linear terms in λ we get

$$\int_{z_1}^{z_2}\left(\boldsymbol{q}^{(1)}\frac{\partial M_2}{\partial \boldsymbol{q}}+\boldsymbol{q}^{(1)\prime}\frac{\partial M_2}{\partial \boldsymbol{q}'}\right)\mathrm{d}z= \tag{5.69}$$

$$-\int_{z_1}^{z_2}\sum_{i,j}\left(q_i^{(1)}q_j^{(1)}\frac{\partial^2 M_2}{\partial q_i\partial q_j}+2q_i^{(1)}q_j^{(1)\prime}\frac{\partial^2 M_2}{\partial q_i\partial q_j'}+q_i^{(1)\prime}q_j^{(1)\prime}\frac{\partial^2 M_2}{\partial q_i'\partial q_j'}\right)\mathrm{d}z+\boldsymbol{q}_{\underline{2}}^{(1)}\boldsymbol{p}_{\underline{2}}^{(1)}-\boldsymbol{q}_{\underline{1}}^{(1)}\boldsymbol{p}_{\underline{1}}^{(1)}$$

Hence,

$$S_{12}^{(2)}=S_{12}^{II}+\boldsymbol{p}_{\underline{2}}^{(0)}\boldsymbol{q}_{\underline{2}}^{(2)}-\boldsymbol{p}_{\underline{1}}^{(0)}\boldsymbol{q}_{\underline{1}}^{(2)}+\boldsymbol{p}_{\underline{2}}^{(1)}\boldsymbol{q}_{\underline{2}}^{(1)}-\boldsymbol{p}_{\underline{1}}^{(1)}\boldsymbol{q}_{\underline{1}}^{(1)} \tag{5.70}$$

where the second order characteristic function

$$S_{12}^{II}=\int_{z_1}^{z_2}\left\{M^{II}(\boldsymbol{q}^{(0)},\boldsymbol{q}^{(0)},z)-\frac{1}{2}\sum_{i,j}\left(\frac{\partial^2 M_2(\boldsymbol{q}^{(0)},\boldsymbol{q}^{(0)\prime},z)}{\partial q_i\partial q_j}q_i^{(1)}q_j^{(1)}+\right.\right. \tag{5.71}$$

$$\left.\left.+2\frac{\partial^2 M_2(\boldsymbol{q}^{(0)},\boldsymbol{q}^{(0)\prime},z)}{\partial q_i\partial q_j'}q_i^{(1)}q_j^{(1)\prime}+\frac{\partial^2 M_2(\boldsymbol{q}^{(0)},\boldsymbol{q}^{(0)\prime},z)}{\partial q_i'\partial q_j'}\boldsymbol{q}_i^{(1)\prime}\boldsymbol{q}_j^{(1)\prime}\right)\right\}\mathrm{d}z$$

depends either on z and values of $\boldsymbol{q}$ and $\boldsymbol{q}'$ in z_1, or on z and positions of ray in the object and aperture planes similarly to the second and third term on the left hand side while on the right hand side one can find the qualities which have to be computed.

Varying (64) and comparing with the expansion of (39) one can find the second order perturbation relation

$$\delta S_{12}^{II}-\boldsymbol{q}_{\underline{2}}^{(1)}\delta\boldsymbol{p}_{\underline{2}}^{(1)}+\boldsymbol{q}_{\underline{1}}^{(1)}\delta\boldsymbol{p}_{\underline{1}}^{(1)}=\boldsymbol{p}_{\underline{2}}^{(2)}\delta\boldsymbol{q}_{\underline{2}}^{(0)}-\boldsymbol{p}_{\underline{1}}^{(2)}\delta\boldsymbol{q}_{\underline{1}}^{(0)}-\boldsymbol{q}_{\underline{2}}^{(2)}\delta\boldsymbol{p}_{\underline{2}}^{(0)}+\boldsymbol{q}_{\underline{1}}^{(2)}\delta\boldsymbol{p}_{\underline{1}}^{(0)} \tag{5.72}$$

Using procedure similar to the first order perturbation two perturbation relations can be found. The first one for rays determined by the position and directives in the object plane

$$\delta S_{12}^{II}-\boldsymbol{q}_{\underline{2}}^{(1)}\delta\boldsymbol{p}_{\underline{2}}^{(1)}=\boldsymbol{p}_{\underline{2}}^{(2)}\delta\boldsymbol{q}_{\underline{2}}^{(0)}-\boldsymbol{q}_{\underline{2}}^{(2)}\delta\boldsymbol{p}_{\underline{2}}^{(0)} \tag{5.73}$$

which leads to the set of the equations

$$\frac{\partial S_{12}^{II}}{\partial \boldsymbol{q}_{\underline{1}}}-\sum_{k=1}^{2}q_{\underline{2}k}^{(1)}\frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{q}_{\underline{1}}}=\sum_{k=1}^{2}p_{\underline{2}k}^{(2)}\frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_{\underline{1}}}-q_{\underline{2}k}^{(2)}\frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_{\underline{1}}} \tag{5.74a}$$

$$\frac{\partial S_{12}^{II}}{\partial \boldsymbol{p}_{\underline{1}}}-\sum_{k=1}^{2}q_{\underline{2}k}^{(1)}\frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{p}_{\underline{1}}}=\sum_{k=1}^{2}p_{\underline{2}k}^{(2)}\frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{p}_{\underline{1}}}-q_{\underline{2}k}^{(2)}\frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{p}_{\underline{1}}}. \tag{5.74b}$$

Similarly as in the first order perturbation it takes form

$$\begin{pmatrix} \frac{\partial S_{12}^{II}}{\partial \boldsymbol{q}_{\underline{1}}} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{q}_{\underline{1}}} \\ \frac{\partial S_{12}^{II}}{\partial \boldsymbol{p}_{\underline{1}}} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{p}_{\underline{1}}} \end{pmatrix} = \mathcal{M}_1^T \begin{pmatrix} \boldsymbol{p}_{\underline{2}}^{(2)} \\ -\boldsymbol{q}_{\underline{2}}^{(2)} \end{pmatrix} \tag{5.75}$$

hence,

$$\begin{pmatrix} \boldsymbol{p}_{\underline{2}}^{(2)} \\ -\boldsymbol{q}_{\underline{2}}^{(2)} \end{pmatrix} = (\mathcal{M}_1^{-1})^T \begin{pmatrix} \frac{\partial S_{12}^{II}}{\partial \boldsymbol{q}_{\underline{1}}} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{q}_{\underline{1}}} \\ \frac{\partial S_{12}^{II}}{\partial \boldsymbol{p}_{\underline{1}}} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{p}_{\underline{1}}} \end{pmatrix} \tag{5.76}$$

and for stigmatic system in rotation coordinates in the image plane one can write

$$\boldsymbol{Q}_i^{(2)} = -M \left(\frac{\partial S_{oi}^{II}}{\partial \boldsymbol{P}_o} - \sum_{k=1}^{2} Q_{ik}^{(1)} \frac{\partial P_{ik}^{(1)}}{\partial \boldsymbol{P}_o} \right) \tag{5.77}$$

The second perturbation relation for rays determined by the positions in the object and aperture planes reads

$$\delta S_{o2}^{II} - \boldsymbol{q}_{\underline{2}}^{(1)} \delta \boldsymbol{p}_{\underline{2}}^{(1)} = \boldsymbol{p}_{\underline{2}}^{(2)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{2}}^{(2)} \delta \boldsymbol{p}_{\underline{2}}^{(0)} - \boldsymbol{p}_o^{(2)} \delta \boldsymbol{p}_o^{(0)} \tag{5.78a}$$

$$\delta S_{a2}^{II} - \boldsymbol{q}_{\underline{2}}^{(1)} \delta \boldsymbol{p}_{\underline{2}}^{(1)} = \boldsymbol{p}_{\underline{2}}^{(2)} \delta \boldsymbol{q}_{\underline{2}}^{(0)} - \boldsymbol{q}_{\underline{2}}^{(2)} \delta \boldsymbol{p}_{\underline{2}}^{(0)} + \boldsymbol{q}_a^{(2)} \delta \boldsymbol{p}_a^{(0)} \tag{5.78b}$$

which leads to the set of equations

$$\frac{\partial S_{o2}^{II}}{\partial \boldsymbol{q}_a} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{q}_a} = \sum_{k=1}^{2} p_{\underline{2}k}^{(2)} \frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a} - q_{\underline{2}k}^{(2)} \frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a} \tag{5.79a}$$

$$\frac{\partial S_{a2}^{I}}{\partial \boldsymbol{q}_a} - \sum_{k=1}^{2} q_{\underline{2}k}^{(1)} \frac{\partial p_{\underline{2}k}^{(1)}}{\partial \boldsymbol{q}_a} = \sum_{k=1}^{2} p_{\underline{2}k}^{(2)} \frac{\partial q_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a} - q_{\underline{2}k}^{(2)} \frac{\partial p_{\underline{2}k}^{(0)}}{\partial \boldsymbol{q}_a}. \tag{5.79b}$$

Using the similar procedure as in previous case we can find for aberration in image plane

$$\boldsymbol{Q}_i^{(2)} = -\frac{M}{\phi_o^{*\frac{1}{2}} W_{so}} \left(\frac{\partial S_{oi}^{II}}{\partial \boldsymbol{Q}_a} - \sum_{k=1}^{2} Q_{ik}^{(1)} \frac{\partial P_{ik}^{(1)}}{\partial \boldsymbol{Q}_a} \right) \tag{5.80}$$

5.4 The Lie Algebra Method

The name of the method comes from the mathematical structure used. It is based on the Poisson brackets which form the Lie algebra structure on the phase space and canonical perturbation theory [13]. It is used in electron optics [3] and beam dynamics [5, 14, 18, 25]. The great advance of the method was found at description of stability of Hamiltonian systems [19, 20, 6].

We use the standard notation

$$[f,g] = \frac{\partial f}{\partial \boldsymbol{q}}\frac{\partial g}{\partial \boldsymbol{p}} - \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{q}} \tag{5.81}$$

for the Poisson brackets of two functions. It is easy to see that the equations of motion can be written consistently in form

$$\boldsymbol{w}' = [\boldsymbol{w}, H] \tag{5.82}$$

where $\boldsymbol{w}$ is vector in the phase space

$$\boldsymbol{w} = \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} \tag{5.83}$$

By direct calculation one can easily proof the Lie algebra structure of the phase space generated by the Poisson bracket,

$$[f,\alpha g+\beta h] = \alpha[f,g]+\beta[g,h] \qquad \text{– linearity} \tag{5.84a}$$

$$[f,g] = -[g,f] \qquad \text{– antisymmetry} \tag{5.84b}$$

$$[f,[g,h]]+[h,[f,g]]+[g,[h,f]] = 0 \qquad \text{– Jacobi identity} \tag{5.84c}$$

As the Poisson brackets exist for all differentiable functions, using this operation it is possible to assign the linear operator to every such a function,

$$f \rightarrow :f:, \quad :f:g = [f,g], \tag{5.85}$$

let as call it Lie operator. The linearity is the direct consequence of (84a)

$$:f:(\alpha g+\beta h) = \alpha :f:g+\beta :f:h \tag{5.86}$$

and the Lie identity causes that it acts as derivative on the algebra of functions with product represented by the Poisson brackets,

$$:f:[g,h] = [:f:g,h]+[g,:f:h]. \tag{5.87}$$

The similar property also can be found for the algebra of functions where the product is represented by the standard product of function [11],

$$:f:gh = (:f:g)h+g:f:h\,. \tag{5.88}$$

All of these properties have great consequences mentioned later.

The Lie algebra method is based on the canonical transformations. The standard description of canonical transformation uses the generating function in which the new and original coordinates are mixed [10], i.e.

$$\tilde{\boldsymbol{q}} = \frac{\partial F(\tilde{\boldsymbol{p}},\boldsymbol{q},z)}{\partial \tilde{\boldsymbol{p}}}\,, \qquad \boldsymbol{p} = \frac{\partial F(\tilde{\boldsymbol{p}},\boldsymbol{q},z)}{\partial \boldsymbol{q}}\,. \tag{5.89}$$

But for the purposes of the perturbation theory the description via transformation using only original coordinates is more advisable. It is possible to do so by use of the Lie transformations which are defined as the exponential of the Lie operator, ie.

$$\boldsymbol{w}(\tilde{\boldsymbol{w}},z) = e^{:g(\tilde{\boldsymbol{w}},z):}\tilde{\boldsymbol{w}} \tag{5.90}$$

where

$$e^{:g:} = \hat{1} + :g: + \frac{1}{2}:g:^2 + \frac{1}{3!}:g:^3 + \cdots\,. \tag{5.91}$$

It can be shown [11] that validity of (87) provides such a transformation canonical i.e.

$$e^{:g:}[f,h] = [e^{:g:}f, e^{:g:}h]\,. \tag{5.92}$$

Moreover, (88) causes that all analytical functions are transformed via

$$\tilde{f}(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z) = f(\boldsymbol{q}(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z),\boldsymbol{p}(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z),z) = e^{:g(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z):}f(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z) \tag{5.93}$$

Unfortunately the situation for the Hamiltonian differs a little because the transformation rule for Hamiltonian differs from the transformation rule of functions [10], one can find its form for the Lie transformation [12], see also appendix,

$$\tilde{H}(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z) = e^{:g(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z):}H(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z) + \int_0^1 e^{\theta:g(\tilde{\boldsymbol{q}},\tilde{\boldsymbol{p}},z):}\frac{\partial g}{\partial z}\mathrm{d}\theta \tag{5.94}$$

The knowledge extent introduced suffices to explain the Lie algebra method.

In fact this method is just modification of the canonical perturbation methods used in the classical mechanics [15]. Similarly to the Hamilton – Jacobi theory it is based on the fact that the motion is the canonical transformation which compensates the Hamiltonian. But on contrary to the Hamilton – Jacobi theory the Hamiltonian is not

compensated using one transformation but it is compensated term by term. Four our case, when the Hamiltonian is easily expanded into polynomial in canonical variables

$$H = H_2 + H_3 + H_4 + \cdots , \tag{5.95}$$

it is natural to find such a sequence of the canonical transformations which compensate the Hamiltonian order by order. Let us say that the canonical transformation $\mathcal{M}_k$ transforms the system with Hamiltonian (95) into system with Hamiltonian

$$H = H_{k+2} + H_{k+3} + \cdots \tag{5.96}$$

the equations of motion then takes form

$$\frac{\mathrm{d}}{\mathrm{d}z}\tilde{\boldsymbol{w}} = [\tilde{\boldsymbol{w}}, H] = \boldsymbol{f}_{k+1} + \boldsymbol{f}_{k+2} + \cdots , \tag{5.97}$$

i.e. the lowest order of terms on the right hand side is $k+1$. The physical meaning of $\mathcal{M}_k$ rises from the fact that the solution of such equations can be evaluated in form

$$\tilde{\boldsymbol{w}} = \tilde{\boldsymbol{w}}_o + \boldsymbol{g}_{k+1}(\tilde{\boldsymbol{w}}_o, z) + \boldsymbol{g}_{k+2}(\tilde{\boldsymbol{w}}_o, z) + \cdots \tag{5.98}$$

hence, there is no evolution up to k-th order present. If we do not include terms of higher orders then k into calculations, the evolution described in the previous equation is approximated by identity, ie. $\tilde{\boldsymbol{w}} = \tilde{\boldsymbol{w}}_o$ and the canonical transformation $\tilde{\boldsymbol{w}} = \mathcal{M}_k \tilde{\boldsymbol{w}}_o$ completely describes the evolution up to k-th order. Before we present the procedure for finding such a transformation let us mention a property advisable at comparing of polynomial orders.

If one evaluates the Poisson bracket of two homogeneous polynomials of k-th and l-th order respectively the result emerges as the homogeneous polynomial of $(k+l-2)-th$ order, i.e.

$$[g_k, g_l] = h_{k+l-2} . \tag{5.99}$$

The proof directly raises from the definition of Poisson bracket which consists from multiplication and two derivatives.

The procedure starts by compensation of the quadratic part of the Hamiltonian, it is equivalent to solution of the paraxial approximation. We can use two approaches here, the first is to use parameterization with initial position and momentum. The canonical

transformation representing such a transformation is described by the linear map (4.28)

$$\boldsymbol{w} = \mathcal{M}_1 \tilde{\boldsymbol{w}} = \begin{pmatrix} \hat{R}^{-1} & 0 \\ 0 & \frac{e}{\eta}\hat{R}^{-1} \end{pmatrix} \begin{pmatrix} g(z)\hat{1} & \phi_o^{*-\frac{1}{2}} h(z)\hat{1} \\ \phi^{*\frac{1}{2}} g'(z)\hat{1} & \sqrt{\frac{\phi^*}{\phi_o^*}} h'(z)\hat{1} \end{pmatrix} \tilde{\boldsymbol{w}} \tag{5.100}$$

and the new Hamiltonian – the interaction Hamiltonian – reads

$$H^{\mathsf{int}} = \frac{\eta}{e}(H_3(\boldsymbol{w}(\tilde{\boldsymbol{w}},z),z) + H_4(\boldsymbol{w}(\tilde{\boldsymbol{w}},z),z) + \cdots) = H_3^{\mathsf{int}}(\tilde{\boldsymbol{w}},z) + H_4^{\mathsf{int}}(\tilde{\boldsymbol{w}},z) + \cdots . \tag{5.101}$$

In the second approach we determine the rays by their position in the object and aperture plane. Such a transformation is the extended canonical transformation expressed in the rotation coordinates

$$\begin{pmatrix} \boldsymbol{Q} \\ \boldsymbol{P} \end{pmatrix} = \begin{pmatrix} s\hat{1} & t\hat{1} \\ s'\phi^{*\frac{1}{2}}\hat{1} & t'\phi^{*\frac{1}{2}}\hat{1} \end{pmatrix} \begin{pmatrix} \tilde{\boldsymbol{Q}} \\ \tilde{\boldsymbol{P}} \end{pmatrix} \tag{5.102}$$

where $\tilde{\boldsymbol{P}}$ corresponds to $\boldsymbol{Q}_a$, which represent the generalized momentum. The interaction Hamiltonian in this case reads

$$H^{\mathsf{int}} = \frac{\eta}{e\phi_o^{*\frac{1}{2}} W_{so}}(H_3(\boldsymbol{w}(\tilde{\boldsymbol{w}},z),z) + H_4(\boldsymbol{w}(\tilde{\boldsymbol{w}},z),z) + \cdots) = H_3^{\mathsf{int}}(\tilde{\boldsymbol{w}},z) + H_4^{\mathsf{int}}(\tilde{\boldsymbol{w}},z) + \cdots . \tag{5.103}$$

where $W_s = s(z_o)t'(z_o) - t(z_o)s'(z_o)$ is the Wronskian (4.19) The following procedure does not depend on the type of paraxial approximation used; therefore we will use the same notation for both approaches.

Now we will find the canonical transformation compensating the third order part of interaction Hamiltonian. Let us assume that it takes form $\tilde{\boldsymbol{w}} = e^{:g_3(\boldsymbol{w}^{[1]},z):}\boldsymbol{w}^{[1]}$ which transforms the Hamiltonian into

$$H^{[1]}(\boldsymbol{w}^{[1]},z) = e^{:g_3(\boldsymbol{w}^{[1]},z):} H^{\mathsf{int}}(\boldsymbol{w}^{[1]},z) + \int_0^1 e^{\theta:g_3(\boldsymbol{w}^{(1)},z):} \frac{\partial g_3}{\partial z} \mathrm{d}\theta \tag{5.104}$$

Moreover, we require for the transformed Hamiltonian not to include the third order part, i.e.

$$H^{[1]}(\boldsymbol{w}^{[1]},z) = H_4^{[1]}(\boldsymbol{w}^{[1]},z) + H_5^{[1]}(\boldsymbol{w}^{[1]},z) + \cdots . \tag{5.105}$$

Comparing terms of the third order on the right hand side of (104) and (105) one can find

$$H_3^{\mathsf{int}} + \frac{\partial g_3}{\partial z} = 0 , \tag{5.106}$$

the solution of which

$$g_3 = -\int_{z_o}^{z} H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},z)\mathrm{d}z\,. \tag{5.107}$$

completely describes the sought for canonical transformation. Such a transformation together with $\mathcal{M}_1$ describe the system up to the second aberration order

$$\boldsymbol{w}_{(2)}(z) = \mathcal{M}_2\boldsymbol{w}^{[1]} = \mathcal{M}_1 e^{:g_3(\boldsymbol{w}^{[1]},z):}\boldsymbol{w}^{[1]}\,. \tag{5.108}$$

and when we neglect the evolution of the third and higher orders $\boldsymbol{w}^{[1]} = \boldsymbol{w}_o$ we can write

$$\boldsymbol{w}_{(2)}(z) = \mathcal{M}_2\boldsymbol{w}_o = \mathcal{M}_1 e^{:g_3(\boldsymbol{w}_o,z):}\boldsymbol{w}_o\,. \tag{5.109}$$

Explicitly for stigmatic system in rotation coordinates it takes form

$$\begin{pmatrix}\boldsymbol{Q}_{(2)}\\ \boldsymbol{P}_{(2)}\end{pmatrix} = \begin{pmatrix} g(z)\hat{1} & \phi_o^{*-\frac{1}{2}}h(z)\hat{1}\\ \phi^{*\frac{1}{2}}g'(z)\hat{1} & \sqrt{\frac{\phi^*}{\phi_o^*}}h'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{Q}_o - \frac{\partial g_3}{\partial \boldsymbol{P}_o}\\ \boldsymbol{P}_o + \frac{\partial g_3}{\partial \boldsymbol{Q}_o}\end{pmatrix} \tag{5.110}$$

and in the image plane one can write

$$\boldsymbol{Q}_{(2)} = M\left(\boldsymbol{Q}_o - \frac{\partial g_3}{\partial \boldsymbol{P}_o}\right) \tag{5.111}$$

When we use aperture position instead of initial momentum

$$\begin{pmatrix}\boldsymbol{Q}_{(2)}\\ \boldsymbol{P}_{(2)}\end{pmatrix} = \begin{pmatrix} s(z)\hat{1} & t(z)\hat{1}\\ \phi^{*\frac{1}{2}}s'(z)\hat{1} & \phi^{*\frac{1}{2}}t'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{Q}_o - \frac{\partial g_3}{\partial \boldsymbol{Q}_a}\\ \boldsymbol{Q}_a + \frac{\partial g_3}{\partial \boldsymbol{Q}_o}\end{pmatrix} \tag{5.112}$$

which reduces to

$$\boldsymbol{Q}_{(2)} = M\left(\boldsymbol{Q}_o - \frac{\partial g_3}{\partial \boldsymbol{Q}_a}\right) \tag{5.113}$$

in the image plane.

Using (104) one can evaluate the transformed Hamiltonian

$$H_4^{[1]} = H_4^{\mathsf{int}} - \frac{1}{2}\int_{z_o}^{z}\mathrm{d}z_1[H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},z_1),H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},z)] \tag{5.114}$$

$$H_5^{[1]} = H_5^{\mathsf{int}} - \int_{z_o}^{z}\mathrm{d}z_1[H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},z_1),H_4^{\mathsf{int}}(\boldsymbol{w}^{[1]},z)] + \tag{5.115}$$

$$+\frac{1}{3}\int_{z_o}^{z}\int_{z_o}^{z}[H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},t),[H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},s),H_3^{\mathsf{int}}(\boldsymbol{w}^{[1]},z)]]$$

The previous procedure can be used to find the canonical transformation

$$\boldsymbol{w}^{[1]}\big(\boldsymbol{w}^{[2]},z\big)=e^{:g_4(\boldsymbol{w}^{[2]},z):}\boldsymbol{w}^{[2]}$$

that compensates the fourth order part of the Hamiltonian,

$$H^{[2]}=e^{:g_4(\boldsymbol{w}^{[2]},z):}H^{[1]}(\boldsymbol{w}^{[2]},z)+\int_0^1 e^{\theta:g_4(\boldsymbol{w}^{[2]},z):}\frac{\partial g_4(\boldsymbol{w}^{[2]},z)}{\partial z}\mathrm{d}\theta \tag{5.116a}$$

$$H^{[2]}=H_5^{[2]}+H_6^{[2]}+\cdots . \tag{5.116b}$$

Comparing terms of the fourth order and solving differential equation one can find

$$\begin{aligned} g_4&=-\int_{z_o}^{z}H_4^{[1]}(\boldsymbol{w}^{[2]},z)\mathrm{d}z \\ &=-\int_{z_o}^{z}H_4^{\mathsf{int}}(\boldsymbol{w}^{[2]},z)\mathrm{d}z+\frac{1}{2}\int_{z_o}^{z}\mathrm{d}z_1\int_{z_o}^{z_2}\mathrm{d}z_1[H_3^{\mathsf{int}}(\boldsymbol{w}^{[2]},z_1),H_3^{\mathsf{int}}(\boldsymbol{w}^{[2]},z_2)]\,. \end{aligned} \tag{5.117}$$

The transformed Hamiltonian is determined by (116a) and the canonical transformation to interaction coordinates $\tilde{\boldsymbol{w}}=\tilde{\mathcal{M}}_3\boldsymbol{w}^{[2]}$ reads

$$\tilde{\mathcal{M}}_3=e^{:g_3(\boldsymbol{w}^{[1]},z):}e^{:g_4(\boldsymbol{w}^{[2]},z):}=e^{:g_4(\boldsymbol{w}^{[2]},z):}e^{:g_3(\boldsymbol{w}^{[2]},z):} \tag{5.118}$$

The rays are then described up to the third aberration order by canonical transformation

$$\boldsymbol{w}_{(3)}=\mathcal{M}_1e^{:g_4:}e^{:g_3:}\boldsymbol{w}_o\,. \tag{5.119}$$

which for stigmatic systems in rotation coordinates takes

$$\begin{pmatrix}\boldsymbol{Q}_{(3)}\\ \boldsymbol{P}_{(3)}\end{pmatrix}=\begin{pmatrix}g(z)\hat{1} & \phi_o^{*-\frac{1}{2}}h(z)\hat{1}\\ \phi^{*\frac{1}{2}}(z)g'\hat{1} & \sqrt{\frac{\phi^*}{\phi_o^*}}h'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{Q}_o-\frac{\partial g_3}{\partial \boldsymbol{P}_o}-\frac{\partial g_4}{\partial \boldsymbol{P}_o}-[g_3,\frac{\partial g_3}{\partial \boldsymbol{P}_o}]\\ \boldsymbol{P}_o+\frac{\partial g_3}{\partial \boldsymbol{Q}_o}+\frac{\partial g_4}{\partial \boldsymbol{Q}_o}+[g_3,\frac{\partial g_3}{\partial \boldsymbol{Q}_o}]\end{pmatrix} \tag{5.120}$$

and when the aperture position instead o initial momentum is used

$$\begin{pmatrix}\boldsymbol{Q}_{(3)}\\ \boldsymbol{P}_{(3)}\end{pmatrix}=\begin{pmatrix}s(z)\hat{1} & t(z)\hat{1}\\ \phi^{*\frac{1}{2}}s'(z)\hat{1} & \phi^{*\frac{1}{2}}t'(z)\hat{1}\end{pmatrix}\begin{pmatrix}\boldsymbol{Q}_o-\frac{\partial g_3}{\partial \boldsymbol{Q}_a}-\frac{\partial g_4}{\partial \boldsymbol{Q}_a}-[g_3,\frac{\partial g_3}{\partial \boldsymbol{Q}_a}]\\ \boldsymbol{Q}_a+\frac{\partial g_3}{\partial \boldsymbol{Q}_o}+\frac{\partial g_4}{\partial \boldsymbol{Q}_o}+[g_3,\frac{\partial g_3}{\partial \boldsymbol{Q}_o}]\end{pmatrix} \tag{5.121}$$

Applying this procedure to higher order terms it is possible to find the canonical transformation which compensates the Hamiltonian up to given order, let us say the k^{th}

$$\tilde{\mathcal{M}}_{k-1}=e^{:g_k(\tilde{\boldsymbol{w}},z):}e^{:g_{k-1}(\tilde{\boldsymbol{w}},z):}\cdots e^{:g_3(\tilde{\boldsymbol{w}},z):}. \tag{5.122}$$

The evolution in original coordinates can be then evaluated as

$$\boldsymbol{w}_{(k-1)}=\mathcal{M}_1\tilde{\mathcal{M}}_{k-1}\boldsymbol{w}_o\,. \tag{5.123}$$

5.5 Dispersion and Chromatic Aberration

So far we were describing the perturbation methods for the system in which the electrons have the same energy. Let us – abandoning this assumption – focus to the cases when the energy of electrons differs. In this subsection the changes and modifications of the perturbation methods invoked by this extension will be presented.

The Trajectory Method

From (2.7) and (4.34a) it is clear that the additional dimension changes the trajectory equations to

$$\hat{P}_1(\boldsymbol{Q})+\frac{F_1}{4e\phi^{*7/4}}\begin{pmatrix}-\cos\Theta\\ \sin\Theta\end{pmatrix}\delta=\boldsymbol{f}_2(\delta,\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',z)+\boldsymbol{f}_3(\delta,\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',z)+\cdots \tag{5.124a}$$

$$\delta=\text{const.} \tag{5.124b}$$

where terms $\boldsymbol{f}_k(\delta,\boldsymbol{Q},\boldsymbol{Q}',\boldsymbol{Q}'',z)$ on the right hand side represent the k-th order homogeneous polynomial in variables δ, $\boldsymbol{Q}$, $\boldsymbol{Q}'$ and $\boldsymbol{Q}''$ with z dependent coefficients.

According to procedure used in monochromatic case using the perturbation parameter λ one can find

$$\begin{aligned}\hat{P}_1(\boldsymbol{Q}_1+\lambda\boldsymbol{Q}_2+\lambda^2\boldsymbol{Q}_3+\cdots)+\frac{F_1}{4e\phi^{*7/4}}\begin{pmatrix}-\cos\Theta\\ \sin\Theta\end{pmatrix}\delta=\\ =\lambda\boldsymbol{f}_2\big(\delta,\boldsymbol{Q}_1+\lambda\boldsymbol{Q}_2+\cdots,\boldsymbol{Q}_1'+\lambda\boldsymbol{Q}_2'+\cdots,\boldsymbol{Q}_1''+\lambda\boldsymbol{Q}_2''+\cdots,z\big)+\lambda^2\boldsymbol{f}_3\big(\delta,\boldsymbol{Q}_1+\cdots,\boldsymbol{Q}_1'+\cdots,\boldsymbol{Q}_1''+\cdots,z\big)\end{aligned}$$

from which comparing of each order in λ it is possible to find equations that determine all $\boldsymbol{Q}^{(i)}$, e.q.

$$\hat{P}_1(\boldsymbol{Q}_1)=-\frac{F_1}{4e\phi^{*\frac{7}{4}}}\begin{pmatrix}-\cos(\Theta)\\ \sin(\Theta)\end{pmatrix}\delta \tag{5.125a}$$

$$\hat{P}_1(\boldsymbol{Q}_2)=\boldsymbol{f}_2\big(\delta,\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z\big) \tag{5.125b}$$

$$\begin{aligned}\hat{P}_1(\boldsymbol{Q}_3)=&\frac{\partial\boldsymbol{f}_2\big(\delta,\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z\big)}{\partial Q_i}Q_{2i}+\frac{\partial\boldsymbol{f}_2\big(\delta,\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z\big)}{\partial Q_i'}Q_{2i}'+\frac{\partial\boldsymbol{f}_2\big(\delta,\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z\big)}{\partial Q_i''}Q_{2i}''+\\ &+\boldsymbol{f}_3\big(\delta,\boldsymbol{Q}_1,\boldsymbol{Q}_1',\boldsymbol{Q}_1'',z\big)\end{aligned} \tag{5.125c}$$

$$\vdots$$

The following procedure will be analogical to procedure mentioned in subsection (4.1).

The Lie Algebra Method

For description of the dispersion case the phase space must include two more canonical conjugate variables τ and p_τ, therefore the Poisson brackets read

$$[f,g] == \frac{\partial f}{\partial \boldsymbol{q}}\frac{\partial g}{\partial \boldsymbol{p}} - \frac{\partial f}{\partial \boldsymbol{p}}\frac{\partial g}{\partial \boldsymbol{q}} + \frac{\partial f}{\partial \tau}\frac{\partial g}{\partial p_\tau} - \frac{\partial f}{\partial p_\tau}\frac{\partial g}{\partial \tau} \tag{5.126}$$

The definition and properties of Lie operator and Lie transform remain unchanged except that Poisson brackets and the phase space change themselves.

Hence, the Hamiltonian must include variable p_τ and its expansion will take form

$$H(\boldsymbol{q},\boldsymbol{p},p_\tau,z) = H_2(\boldsymbol{q},\boldsymbol{p},p_\tau,z) + H_3(\boldsymbol{q},\boldsymbol{p},p_\tau,z) + H_4(\boldsymbol{q},\boldsymbol{p},p_\tau,z) + \cdots . \tag{5.127}$$

Moreover, if the dipole fields represented by coefficient F_1 are presented the paraxial approximation takes form

$$\mathcal{M}_1 = \begin{pmatrix} \hat{R}^{-1} & \hat{0} & \underline{0} \\ \hat{0} & \frac{e}{\eta}\hat{R}^{-1} & \underline{0} \\ \underline{0} & \underline{0} & 1 \end{pmatrix} \begin{pmatrix} g\hat{1} & \phi_0^{*-\frac{1}{2}}\hat{1} & \underline{0} \\ \phi^{*\frac{1}{2}}g'\hat{1} & \sqrt{\frac{\phi^*}{\phi_0^*}}h'\hat{1} & \underline{0} \\ \underline{0} & \underline{0} & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 2mc\eta\hat{\mu}(h) \\ 0 & 1 & 0 & 0 & 2mc\eta\hat{\nu}(h) \\ 0 & 0 & 1 & 0 & -2mc\eta\hat{\mu}(g) \\ 0 & 0 & 0 & 1 & -2mc\eta\hat{\nu}(g) \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

which causes the change of the interaction coordinates

$$\begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \\ p_\tau \end{pmatrix} = \mathcal{M}_1 \begin{pmatrix} \tilde{\boldsymbol{q}} \\ \tilde{\boldsymbol{p}} \\ \tilde{p}_\tau \end{pmatrix} \tag{5.128}$$

and the interaction Hamiltonian as well. The rest of the procedure remains unchanged.

The Differential Algebra Method

Besides the image position and directives the particles trajectories are determined by their energy deviation δ, if one supposes the dispersion case. For this method it causes the differential algebraic basis to include other elements. The general basis elements then read

$$|l_1,l_2,l_3,l_4,d\rangle = X^{l_1}Y^{l_2}P_x^{l_3}P_y^{l_4}P_\tau^d \tag{5.129}$$

and as P_τ remains constant along each ray i.e. $P'_\tau = 0$, the derivative of general differential algebraic element takes form

$$\frac{\mathrm{d}}{\mathrm{d}z}|l_1,l_2,l_3,l_4,d\rangle = -[H_2+H_3+H_4+\cdots,|l_1,l_2,l_3,l_4,d\rangle]\,. \tag{5.130}$$

In this case one can find $\binom{5+k}{k}-1$ linear differential equations of the first order which determine the solution up to the k^{th} order. The procedure that follows is analogous to the monochromatic case.

5.6 Example: Round Magnetic Lens

The round magnetic lens is the base element of the most of electron microscopes. Our intention is to show the application of perturbation methods described above rather than to describe the physical properties of the lens. First we show the calculation using the eikonal method and the Lie algebra method. The trajectory method will be applied at the end. We skip the differential algebra method, because it is not appropriate for analytic calculation of aberrations. We will compare the results of all these methods.

The magnetic axial symmetric field is determined by one function - the axial flux density $B(z)$. We will use the following expansion of the vector potential

$$A_x = -\frac{1}{2}yB(z)+\frac{1}{16}y(x^2+y^2)B''(z) \tag{5.131a}$$

$$A_y = \frac{1}{2}xB(z)-\frac{1}{16}x(x^2+y^2)B''(z) \tag{5.131b}$$

$$A_z = 0 \tag{5.131c}$$

The paraxial equation of the system has been studied, so we start to calculate the aberration.

The eikonal method

The Lagrangian of the system up to the fourth order reads

$$M = M_2 + M_4$$

where

$$M_2 = \frac{1}{2}\phi^{*\frac{1}{2}}\boldsymbol{q}'^2 - \frac{1}{2}\eta B(z)(xy'-x'y) \tag{5.132}$$

$$M_4 = -\frac{1}{8}\phi^{*\frac{1}{2}}(\boldsymbol{q}'^2)^2 + \frac{1}{16}\eta B''(xy'-x'y)\boldsymbol{q}^2 \tag{5.133}$$

hence, the third order Lagrangian is not present in the system. We will solve the problem in rotation coordinates, where the Lagrangian reads

$$M_2 = \frac{1}{2}\phi^{*\frac{1}{2}}\boldsymbol{Q}'^2 - \frac{\eta^2 B^2(z)}{8\phi^{*\frac{1}{2}}}\boldsymbol{Q}^2 \tag{5.134}$$

$$\begin{aligned} M_4 = &-\frac{1}{4}L_1(\boldsymbol{Q}^2)^2 - \frac{1}{2}L_2\boldsymbol{Q}^2\boldsymbol{Q}'^2 - \frac{1}{4}L_3(\boldsymbol{Q}'^2)^2 - R(XY' - X'Y)^2 \\ &- C_P\boldsymbol{Q}^2(XY' - X'Y) - C_Q\boldsymbol{Q}'^2(XY' - X'Y) \end{aligned} \tag{5.135}$$

with the coefficients defined:

$$L_1 = \frac{\eta^4 B^4}{32\phi^{*\frac{3}{2}}} - \frac{\eta^2}{8\phi^{*\frac{1}{2}}}BB'' \tag{5.136a}$$

$$L_2 = \frac{\eta^2 B^2}{8\phi^{*\frac{1}{2}}} \tag{5.136b}$$

$$L_3 = \frac{1}{2}\phi^{*\frac{1}{2}} \tag{5.136c}$$

$$R = \frac{\eta^2 B^2}{8\phi^{*\frac{1}{2}}} \tag{5.136d}$$

$$C_Q = \frac{1}{4}\eta B \tag{5.136e}$$

$$C_P = \frac{\eta^3 B^3}{16\phi^*} - \frac{\eta B''}{16} \tag{5.136f}$$

When we use the paraxial approximation in parameterization with coordinate and momentum in the object plane after substitution (4.27) for $\boldsymbol{Q}$ and $\boldsymbol{Q}'$ and using $L_z^2 = \boldsymbol{Q}^2\boldsymbol{P}^2 - (\boldsymbol{Q}\boldsymbol{P})^2$ we get

$$\begin{aligned}\tilde{M}_4 = &-\frac{1}{4}\phi^{*-2}(L_1h^4+2L_2h^2h'^2+L_3h'^4)(\boldsymbol{P}_o^2)^2- \\ &-\phi^{*-\frac{3}{2}}(L_1gh^3+L_2hh'(gh)'+L_3g'h'^3)\boldsymbol{P}_o^2(\boldsymbol{Q}_o\boldsymbol{P}_o)- \\ &-\phi^{*-1}(L_1g^2h^2+2L_2ghg'h'+L_3g'^2h'^2-R)(\boldsymbol{Q}_o\boldsymbol{P}_o)^2- \\ &-\frac{1}{2}\phi^{*-1}(L_1g^2h^2+L_2(g'^2h^2+g^2h'^2)+L_3g'^2h'^2+2R)\boldsymbol{Q}_o^2\boldsymbol{P}_o^2- \\ &-\phi^{*-\frac{1}{2}}(L_1hg^3+L_2gg'(hg)'+L_3h'g'^3)\boldsymbol{Q}_o^2(\boldsymbol{Q}_o\boldsymbol{P}_o)- \\ &-\frac{1}{4}(L_1g^4+2L_2g^2g'^2+L_3g'^4)(\boldsymbol{Q}_o^2)^2- \\ &-\phi^{*-\frac{3}{2}}(C_Qh'^2+C_Ph^2)\boldsymbol{P}_o^2L_z-2\phi^{*-1}(C_Qg'h'+C_Pgh)\boldsymbol{Q}_o\boldsymbol{P}_oL_z- \\ &-\phi^{*\frac{1}{2}}(C_Qg'^2+C_Pg^2)\boldsymbol{Q}_o^2L_z\end{aligned} \tag{5.137}$$

Let us mention that because there is no electric field in the system, ie. $\phi^* = \phi_o^*$, the Wronskian remains constant

$$gh'-g'h = g(z_o)h'(z_o)-g'(z_o)h(z_o) = 1 \tag{5.138a}$$

$$st'-s't = s(z_o)t'(z_o)-s'(z_o)t(z_o) = W_{so} \tag{5.138b}$$

When we introduce notation

$$C = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1h^4+2L_2h^2h'^2+L_3h'^4)\mathrm{d}z \tag{5.139a}$$

$$K = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1gh^3+L_2hh'(gh)'+L_3g'h'^3)\mathrm{d}z \tag{5.139b}$$

$$A = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1g^2h^2+2L_2ghg'h'+L_3g'^2h'^2-R)\mathrm{d}z \tag{5.139c}$$

$$F = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1g^2h^2+L_2(g'^2h^2+g^2h'^2)+L_3g'^2h'^2+2R)\mathrm{d}z \tag{5.139d}$$

$$D = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1hg^3+L_2gg'(hg)'+L_3h'g'^3)\mathrm{d}z \tag{5.139e}$$

$$E = \phi^{*-\frac{1}{2}}\int_{z_o}^{z}(L_1g^4+2L_2g^2g'^2+L_3g'^4)\mathrm{d}z \tag{5.139f}$$

$$k = \phi^{*-\frac{1}{2}} \int_{z_o}^{z} (C_Q h'^2 + C_P h^2) \mathrm{d}z \tag{5.140a}$$

$$a = \phi^{*-\frac{1}{2}} \int_{z_o}^{z} (C_Q g' h' + C_P g h) \mathrm{d}z \tag{5.140b}$$

$$d = \phi^{*-\frac{1}{2}} \int_{z_o}^{z} (C_Q g'^2 + C_P g^2) \mathrm{d}z \tag{5.140c}$$

the action takes form

$$\begin{aligned} S_{oi}^I = &-\frac{1}{4}\phi^{*-\frac{3}{2}} C(\boldsymbol{P}_o^2)^2 - \phi^{*-1} K \boldsymbol{P}_o^2 (\boldsymbol{Q}_o \boldsymbol{P}_o) - \phi^{*-\frac{1}{2}} A (\boldsymbol{Q}_o \boldsymbol{P}_o)^2 - \frac{1}{2}\phi^{*-\frac{1}{2}} F \boldsymbol{Q}_o^2 \boldsymbol{P}_o^2 \\ &- D\boldsymbol{Q}_o^2 (\boldsymbol{Q}_o \boldsymbol{P}_o) - \frac{1}{4}\phi^{*\frac{1}{2}} E (\boldsymbol{Q}_o^2)^2 - \phi^{*-1} k \boldsymbol{P}_o^2 L_z - 2\phi^{*-\frac{1}{2}} a \boldsymbol{Q}_o \boldsymbol{P}_o L_z - d\boldsymbol{Q}_o^2 L_z \end{aligned} \tag{5.141}$$

and using (54) the perturbation in the image plane reads

$$\begin{aligned} \boldsymbol{Q}_i^{(1)} = M \Big(&\phi^{*-\frac{3}{2}} C \boldsymbol{P}_o^2 \boldsymbol{P}_o + \phi^{*-1} K (\boldsymbol{P}_o^2 \boldsymbol{Q}_o + 2(\boldsymbol{Q}_o \boldsymbol{P}_o)\boldsymbol{P}_o) + 2\phi^{*-\frac{1}{2}} A (\boldsymbol{Q}_o \boldsymbol{P}_o)\boldsymbol{Q}_o + \\ &+ \phi^{*-\frac{1}{2}} F \boldsymbol{Q}_o^2 \boldsymbol{P}_o + D\boldsymbol{Q}_o^2 \boldsymbol{Q}_o + k\phi^{*-1}(2L_z \boldsymbol{P}_o - \boldsymbol{P}_o^2 \hat{J}_2 \boldsymbol{Q}_o) + \\ &+ 2a\,\phi^{*-\frac{1}{2}} (L_z \boldsymbol{Q}_o - (\boldsymbol{Q}_o \boldsymbol{P}_o)\hat{J}_2 \boldsymbol{Q}_o) - d\boldsymbol{Q}_o^2 \hat{J}_2 \boldsymbol{Q}_o \Big) \end{aligned} \tag{5.142}$$

where

$$\hat{J}_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{5.143}$$

and when we use $\boldsymbol{P}_o = \phi^{*\frac{1}{2}} \boldsymbol{Q}'_o$,

$$\begin{aligned} \boldsymbol{Q}^{(1)} = M \big(&C\boldsymbol{Q}_o'^2 \boldsymbol{Q}'_o + K(\boldsymbol{Q}_o'^2 \boldsymbol{Q}_o + 2(\boldsymbol{Q}_o \boldsymbol{Q}'_o)\boldsymbol{Q}'_o) + 2A(\boldsymbol{Q}_o \boldsymbol{Q}'_o)\boldsymbol{Q}_o + F\boldsymbol{Q}_o^2 \boldsymbol{Q}'_o + D\boldsymbol{Q}_o^2 \boldsymbol{Q}_o \\ &+ k(2K_z \boldsymbol{Q}'_o - \boldsymbol{Q}_o'^2 \hat{J}_2 \boldsymbol{Q}_o) + 2a(K_z \boldsymbol{Q}_o - (\boldsymbol{Q}_o \boldsymbol{Q}'_o)\hat{J}_2 \boldsymbol{Q}_o) - d\boldsymbol{Q}_o^2 \hat{J}_2 \boldsymbol{Q}_o \Big) \end{aligned} \tag{5.144}$$

where $K_z = X_o Y'_o - Y_o X'_o$.

In case of parameterization with position in the object and aperture plane we will proceed similarly

$$\begin{aligned}\tilde{M}_4 = &-\frac{1}{4}(L_1t^4+2L_2t^2t'^2+L_3t'^4)(\boldsymbol{Q}_a^2)^2-(L_1st^3+L_2tt'(st)'+L_3s't'^3)\boldsymbol{Q}_a^2(\boldsymbol{Q}_o\boldsymbol{Q}_a)\\ &-(L_1s^2t^2+2L_2sts't'+L_3s'^2t'^2-RW_s^2)(\boldsymbol{Q}_o\boldsymbol{Q}_a)^2-\\ &-\frac{1}{2}(L_1s^2t^2+L_2(s'^2t^2+s^2t'^2)+L_3s'^2t'^2+2RW_s^2)\boldsymbol{Q}_o^2\boldsymbol{Q}_a^2-\\ &-(L_1ts^3+L_2ss'(ts)'+L_3t's'^3)\boldsymbol{Q}_o^2(\boldsymbol{Q}_o\boldsymbol{Q}_a)-\frac{1}{4}(L_1s^4+2L_2s^2s'^2+L_3s'^4)(\boldsymbol{Q}_o^2)^2-\\ &-W_s(C_Qt'^2+C_Pt^2)\boldsymbol{Q}_a^2L_z-2W_s(C_Qs't'+C_Pst)\boldsymbol{Q}_o\boldsymbol{Q}_aL_z-\\ &-W_s(C_Qs'^2+C_Ps^2)\boldsymbol{Q}_o^2L_z \end{aligned} \tag{5.145}$$

where now $L_z = X_oY_a - X_aY_o$. Using coefficients

$$C = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1t^4+2L_2t^2t'^2+L_3t'^4)\mathrm{d}z \tag{5.146a}$$

$$K = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1st^3+L_2tt'(st)'+L_3s't'^3)\mathrm{d}z \tag{5.146b}$$

$$A = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1s^2t^2+2L_2sts't'+L_3s'^2t'^2-RW_s^2)\mathrm{d}z \tag{5.146c}$$

$$F = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1s^2t^2+L_2(s'^2t^2+s^2t'^2)+L_3s'^2t'^2+2RW_s^2)\mathrm{d}z \tag{5.146d}$$

$$D = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1ts^3+L_2ss'(ts)'+L_3t's'^3)\mathrm{d}z \tag{5.146e}$$

$$E = \phi^{*-\frac{1}{2}}W_s^{-1}\int_{z_o}^{z}(L_1s^4+2L_2s^2s'^2+L_3s'^4)\mathrm{d}z \tag{5.146f}$$

$$k=\phi^{*-\frac{1}{2}}\int_{z_o}^{z}(C_Qt'^2+C_Pt^2)\mathrm{d}z \tag{5.147a}$$

$$a=\phi^{*-\frac{1}{2}}\int_{z_o}^{z}(C_Qs't'+C_Pst)\mathrm{d}z \tag{5.147b}$$

$$d=\phi^{*-\frac{1}{2}}\int_{z_o}^{z}(C_Qs'^2+C_Ps^2)\mathrm{d}z \tag{5.147c}$$

the action takes form

$$\begin{aligned}S^I_{oi}=&-\frac{C}{4}(\boldsymbol{Q}_a^2)^2-K\boldsymbol{Q}_a^2(\boldsymbol{Q}_o\boldsymbol{Q}_a)-A(\boldsymbol{Q}_o\boldsymbol{Q}_a)^2-\frac{F}{2}\boldsymbol{Q}_o^2\boldsymbol{Q}_a^2-D\boldsymbol{Q}_o^2(\boldsymbol{Q}_o\boldsymbol{Q}_a)-\frac{E}{4}(\boldsymbol{Q}_o^2)^2\\&-k\boldsymbol{Q}_a^2L_z-2a\boldsymbol{Q}_o\boldsymbol{Q}_aL_z-d\boldsymbol{Q}_o^2L_z\end{aligned} \tag{5.148}$$

and using (63) one gets

$$\begin{aligned}\boldsymbol{Q}^{(1)}=M\big(&C\boldsymbol{Q}_a^2\boldsymbol{Q}_a+K\boldsymbol{Q}_a^2\boldsymbol{Q}_o+2(\boldsymbol{Q}_o\boldsymbol{Q}_a)\boldsymbol{Q}_a+2A(\boldsymbol{Q}_o\boldsymbol{Q}_a)\boldsymbol{Q}_o+F\boldsymbol{Q}_o^2\boldsymbol{Q}_a+D\boldsymbol{Q}_o^2\boldsymbol{Q}_o+\\&+k(2L_z\boldsymbol{Q}_a-\boldsymbol{Q}_a^2\hat{J}_2\boldsymbol{Q}_o)+2a(L_z\boldsymbol{Q}_o-(\boldsymbol{Q}_o\boldsymbol{Q}_a)\hat{J}_2\boldsymbol{Q}_o)-d\boldsymbol{Q}_o^2\hat{J}_2\boldsymbol{Q}_o\big)\end{aligned} \tag{5.149}$$

The Lie algebra method

The Hamiltonian up to the fourth order takes form

$$H=H_2+H_4 \tag{5.150}$$

where

$$H_2=\frac{\eta}{2e\phi^{*\frac{1}{2}}}\boldsymbol{p}^2+\frac{\eta B}{2\phi^{*\frac{1}{2}}}L_z+\frac{\eta eB^2}{4\phi^{*\frac{1}{2}}}\boldsymbol{q}^2 \tag{5.151}$$

$$\begin{aligned}H_4=&\frac{\eta^3}{8e^3\phi^{*\frac{3}{2}}}(\boldsymbol{p}^2)^2+\frac{\eta^3B^2}{16e\phi^{*\frac{3}{2}}}\boldsymbol{p}^2\boldsymbol{q}^2+\left(\frac{e\eta^3}{128\phi^{*\frac{3}{2}}}B^4-\frac{e\eta}{32\phi^{*\frac{1}{2}}}BB''\right)(\boldsymbol{q}^2)^2+\frac{\eta^3B^2}{8e\phi^{*\frac{3}{2}}}L_z^2\\&+\left(\frac{\eta^3B^3}{16\phi^{*\frac{3}{2}}}-\frac{\eta B''}{16\phi^{*\frac{1}{2}}}\right)L_z\boldsymbol{q}^2+\frac{\eta^3B}{4e^2\phi^{*\frac{3}{2}}}L_z\boldsymbol{p}^2\end{aligned} \tag{5.152}$$

which in rotation coordinates takes form

$$H_2=\frac{\boldsymbol{P}^2}{2\phi^{*\frac{1}{2}}}+\frac{\eta^2B^2}{8\phi^{*\frac{1}{2}}}\boldsymbol{Q}^2 \tag{5.153}$$

$$\begin{aligned}H_4=&\frac{1}{4}L_1(\boldsymbol{Q}^2)^2+\frac{1}{2}\phi^{*-1}L_2\boldsymbol{Q}^2\boldsymbol{P}^2+\frac{1}{4}\phi^{*-2}L_3(\boldsymbol{P}^2)^2-\phi^{*-1}RL_z^2\\&+\phi^{*-\frac{1}{2}}C_P\boldsymbol{Q}^2L_z+\phi^{*-\frac{3}{2}}C_Q\boldsymbol{P}^2L_z\end{aligned} \tag{5.154}$$

In case of parameterization with coordinates and momentum in the object plane the interaction Hamiltonian can be calculated using

$$H_4^{\mathsf{int}} = H_4(\boldsymbol{Q}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}}),\boldsymbol{P}(\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}})) \tag{5.155}$$

where the transformation $(\boldsymbol{Q},\boldsymbol{P}) \to (\tilde{\boldsymbol{Q}},\tilde{\boldsymbol{P}})$ is paraxial approximation described in (4.27); hence,

$$\begin{aligned} H_4^{\mathsf{int}} =& \frac{1}{4}\phi^{*-2}(L_1h^4+2L_2h^2h'^2+L_3h'^4)(\tilde{\boldsymbol{P}}^2)^2+ \\ &+\phi^{*-\frac{3}{2}}(L_1gh^3+L_2hh'(gh)'+L_3g'h'^3)\tilde{\boldsymbol{P}}^2(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{P}})+ \\ &+\phi^{*-1}(L_1g^2h^2+2L_2ghg'h'+L_3g'^2h'^2-R)(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{P}})^2+ \\ &+\frac{1}{2}\phi^{*-1}(L_1g^2h^2+L_2(g'^2h^2+g^2h'^2)+L_3g'^2h'^2+2R)\tilde{\boldsymbol{Q}}^2\tilde{\boldsymbol{P}}^2+ \\ &+\phi^{*-\frac{1}{2}}(L_1hg^3+L_2gg'(hg)'+L_3h'g'^3)\tilde{\boldsymbol{Q}}^2(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{P}})+ \\ &+\frac{1}{4}(L_1g^4+2L_2g^2g'^2+L_3g'^4)(\tilde{\boldsymbol{Q}}^2)^2+ \\ &+\phi^{*-\frac{3}{2}}(C_Qh'^2+C_Ph^2)\tilde{\boldsymbol{P}}^2L_z+2\phi^{*-1}(C_Qg'h'+C_Pgh)\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{P}}L_z+ \\ &+\phi^{*\frac{1}{2}}(C_Qg'^2+C_Pg^2)\tilde{\boldsymbol{Q}}^2L_z \end{aligned} \tag{5.156}$$

where we used $L_z^2 = \boldsymbol{p}^2\boldsymbol{q}^2-(\boldsymbol{qp})^2$. Using (107, 114 and 118) we can write

$$g_3 = 0 \tag{5.157}$$

$$g_4 = -\int_{z_o}^{z} H_4^{\mathsf{int}}(\boldsymbol{Q}^{[2]},\boldsymbol{P}^{[2]},z)\mathrm{d}z \tag{5.158}$$

ie.

$$\begin{aligned} g_4 =& -\frac{1}{4}\phi^{*-\frac{3}{2}}C(\boldsymbol{P}^{[2]2})^2-\phi^{*-1}K\boldsymbol{P}^{[2]2}(\boldsymbol{Q}^{[2]}\boldsymbol{P}^{[2]})-\phi^{*-\frac{1}{2}}A(\boldsymbol{Q}^{[2]}\boldsymbol{P}^{[2]})^2-\frac{1}{2}\phi^{*-\frac{1}{2}}F\boldsymbol{Q}^{[2]2}\boldsymbol{P}^{[2]2} \\ &-D\boldsymbol{Q}^{[2]2}(\boldsymbol{Q}^{[2]}\boldsymbol{P}^{[2]})-\frac{1}{4}\phi^{*\frac{1}{2}}E(\boldsymbol{Q}^{[2]2})^2-\phi^{*-1}k\boldsymbol{P}^{[2]2}L_z-2\phi^{*-\frac{1}{2}}a\boldsymbol{Q}^{[2]}\boldsymbol{P}^{[2]}L_z-d\boldsymbol{Q}^{[2]2}L_z \end{aligned}$$

The position in the image plane can be calculated using (120)

$$\boldsymbol{Q}_{(3)} = M\left(\boldsymbol{Q}_o - \frac{\partial g_4(\boldsymbol{Q}_o,\boldsymbol{P}_o)}{\partial \boldsymbol{P}_o}\right) \tag{5.159}$$

where the second term $-M\frac{\partial g_4(\boldsymbol{w}_o)}{\partial \boldsymbol{P}_o}$ agrees with $\boldsymbol{Q}^{(1)}$ from (142).

When the parameterization with position in image and aperture plane is used, the interaction Hamiltonian reads

$$\begin{aligned} H_4^{\text{int}} =& \frac{1}{4}(L_1 t^4 + 2L_2 t^2 t'^2 + L_3 t'^4)(\tilde{\boldsymbol{Q}}_a^2)^2 + (L_1 s t^3 + L_2 t t'(st)' + L_3 s' t'^3)\tilde{\boldsymbol{Q}}_a^2(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}_a) \\ &+ (L_1 s^2 t^2 + 2L_2 s t s' t' + L_3 s'^2 t'^2 - R)(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}_a)^2 \\ &+ \frac{1}{2}(L_1 s^2 t^2 + L_2(s'^2 t^2 + s^2 t'^2) + L_3 s'^2 t'^2 + 2R)\tilde{\boldsymbol{Q}}^2\tilde{\boldsymbol{Q}}_a^2 \\ &+ (L_1 t s^3 + L_2 s s'(ts)' + L_3 t' s'^3)\tilde{\boldsymbol{Q}}^2(\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}_a) + \frac{1}{4}(L_1 s^4 + 2L_2 s^2 s'^2 + L_3 s'^4)(\tilde{\boldsymbol{Q}}^2)^2 + \\ &+ (C_Q t'^2 + C_P t^2)\tilde{\boldsymbol{Q}}_a^2 L_z - 2(C_Q s' t' + C_P s t)\tilde{\boldsymbol{Q}}\tilde{\boldsymbol{Q}}_a L_z + (C_Q s'^2 + C_P s^2)\tilde{\boldsymbol{Q}}^2 L_z \end{aligned} \tag{5.160}$$

$$\begin{aligned} g_4 =& -\frac{1}{4}C(\boldsymbol{Q}_a^{[2]2})^2 - K\boldsymbol{Q}_a^{[2]2}(\boldsymbol{Q}^{[2]}\boldsymbol{Q}_a^{[2]}) - A(\boldsymbol{Q}^{[2]}\boldsymbol{Q}_a^{[2]})^2 - \frac{1}{2}F\boldsymbol{Q}^{[2]2}\boldsymbol{Q}_a^{[2]2} - \\ &- D\boldsymbol{Q}^{[2]2}(\boldsymbol{Q}^{[2]}\boldsymbol{Q}_a^{[2]}) - \frac{1}{4}E(\boldsymbol{Q}^{[2]2})^2 - k\boldsymbol{Q}_a^{[2]2}L_z - 2a\boldsymbol{Q}^{[2]}\boldsymbol{Q}_a^{[2]}L_z - d\boldsymbol{Q}^{[2]2}L_z \end{aligned} \tag{5.161}$$

and

$$\boldsymbol{Q}_{(3)} = M\left(\boldsymbol{Q}_o - \frac{\partial g_4(\boldsymbol{Q}_o, \boldsymbol{Q}_a)}{\partial \boldsymbol{Q}_a}\right) \tag{5.162}$$

which corresponds to (149).

Trajectory method

The trajectory equation can be derived from the Lagrangian equations

$$\frac{\mathrm{d}}{\mathrm{d}z}\frac{\partial M}{\partial \boldsymbol{Q}'} - \frac{\partial M}{\partial \boldsymbol{Q}} = 0 \tag{5.163}$$

which leads to

$$\phi^{*\frac{1}{2}}\boldsymbol{Q}'' + \frac{\eta^2 B^2}{4\phi^{*\frac{1}{2}}}\boldsymbol{Q} = \left(L_3\boldsymbol{Q}'' - L_2\boldsymbol{Q} - C_Q'\hat{J}_2\boldsymbol{Q} - 2C_Q\hat{J}_2\boldsymbol{Q}'\right)\boldsymbol{Q}'^2 + 2(L_2\boldsymbol{Q}' - C_P\hat{J}_2\boldsymbol{Q})\boldsymbol{Q}\boldsymbol{Q}' \tag{5.164}$$

$$\begin{aligned} &+ \left(L_2\boldsymbol{Q}'' + L_2'\boldsymbol{Q}' - L_1\boldsymbol{Q} - C_P'\hat{J}_2\boldsymbol{Q} - 2C_p\hat{J}_2\boldsymbol{Q}'\right)\boldsymbol{Q}^2 + 2\left(L_3\boldsymbol{Q}' - C_Q\hat{J}_2\boldsymbol{Q}\right)\boldsymbol{Q}'\boldsymbol{Q}'' + \\ &+ 2\left(C_Q\boldsymbol{Q}' - R\hat{J}_2\boldsymbol{Q}\right)K_z' + 2\left(C_Q\boldsymbol{Q}'' + C_Q'\boldsymbol{Q}' - C_P\boldsymbol{Q} - 2R\hat{J}_2\boldsymbol{Q}' - R'\hat{J}_2\boldsymbol{Q}\right)K_z \end{aligned}$$

where

$$K_z = XY' - YX'$$

was defined. Hence, the trajectory equation takes form

$$\boldsymbol{Q}'' + \frac{\eta^2 B^2}{4\phi}\boldsymbol{Q} = \boldsymbol{f}_3(\boldsymbol{Q}, \boldsymbol{Q}', \boldsymbol{Q}'', z) \tag{5.165}$$

ie. there is no polynomial of the second order on the right hand side. It causes that the $\boldsymbol{Q}_2 = 0$ (26) and the equation (28) is reduced to

$$\boldsymbol{Q}_3'' + \frac{\eta^2 B^2}{4\phi}\boldsymbol{Q}_3 = \boldsymbol{f}_3(\boldsymbol{Q}_1, \boldsymbol{Q}_1', \boldsymbol{Q}_1'', z) \tag{5.166}$$

and using parameter variation method one can find

$$\boldsymbol{Q}_3 = -M\phi_o^{*-\frac{1}{2}} \int_{z_o}^{z_i} \phi^{*\frac{1}{2}} h(t) \boldsymbol{f}_3(\boldsymbol{Q}_1, \boldsymbol{Q}_1', \boldsymbol{Q}_1'', t)\,\mathrm{d}t = -M \int_{z_o}^{z_i} h(t) \boldsymbol{f}_3(\boldsymbol{Q}_1, \boldsymbol{Q}_1', \boldsymbol{Q}_1'', t)\,\mathrm{d}t \tag{5.167}$$

or

$$\boldsymbol{Q}_3 = -\frac{M}{W_{so}\phi_o^{*\frac{1}{2}}} \int_{z_o}^{z_i} \phi^{*\frac{1}{2}} t(\alpha) \boldsymbol{f}_3(\boldsymbol{Q}_1, \boldsymbol{Q}_1', \boldsymbol{Q}_1''\alpha)\,\mathrm{d}\alpha = -\frac{M}{W_{so}} \int_{z_o}^{z_i} t(\alpha) \boldsymbol{f}_3(\boldsymbol{Q}_1, \boldsymbol{Q}_1', \boldsymbol{Q}_1''\alpha)\,\mathrm{d}\alpha \tag{5.168}$$

depending on the parameterization used.

Because the practical calculation is lengthy we will show it only for case of parameterization by position and directives in the object plane. In such a case the $\boldsymbol{Q}_1 = g\boldsymbol{Q}_o + h\boldsymbol{Q}_o'$, $W_g = gh' - hg' = 1$ and $\boldsymbol{Q}_1'' = -\frac{L_2}{L_3}\boldsymbol{Q}_1$; hence, the equation (166) reads

$$\begin{aligned}
&\boldsymbol{Q}_3'' + \frac{\eta^2 B^2}{4\phi^*}\boldsymbol{Q}_3 = \qquad\qquad (5.169)\\
&= \phi^{*-\frac{1}{2}} \big[I_1 \boldsymbol{Q}_o'^2 \boldsymbol{Q}_o' + I_2 \boldsymbol{Q}_o'^2 \boldsymbol{Q}_o + I_3 (\boldsymbol{Q}_o \boldsymbol{Q}_o') \boldsymbol{Q}_o' + I_4 (\boldsymbol{Q}_o \boldsymbol{Q}_o') \boldsymbol{Q}_o + I_5 \boldsymbol{Q}_o^2 \boldsymbol{Q}_o' + I_6 \boldsymbol{Q}_o^2 \boldsymbol{Q}_o \\
&\quad + A_1 K_z \boldsymbol{Q}_o' + A_2 \boldsymbol{Q}_o'^2 \hat{J}_2 \boldsymbol{Q}_o + A_3 K_z \boldsymbol{Q}_o + A_4 (\boldsymbol{Q}_o \boldsymbol{Q}_o') \hat{J}_2 \boldsymbol{Q}_o + A_5 \boldsymbol{Q}_o^2 \hat{J}_2 \boldsymbol{Q}_o + \\
&\quad + N_1 (\boldsymbol{Q}_o \boldsymbol{Q}_o') \hat{J}_2 \boldsymbol{Q}' + N_2 \boldsymbol{Q}_o'^2 \hat{J}_2 \boldsymbol{Q}_o' + N_3 \boldsymbol{Q}_o^2 \hat{J}_2 \boldsymbol{Q}_o' \big]
\end{aligned}$$

where the coefficients read

$$I_1 = -(L_1 + \frac{L_2^2}{L_3})h^3 - 2L_2 h'^2 h + L_2' h^2 h' \tag{5.170a}$$

$$I_2 = -(L_1 + \frac{L_2^2}{L_3})gh^2 - 2L_2 h'^2 g + L_2' g' h^2 - 2R' h - 4Rh' \tag{5.170b}$$

$$I_3 = -2(L_1 + \frac{L_2^2}{L_3})gh^2 - 4L_2 hg' h' + 2L_2' ghh' + 2R' h + 4Rh' \tag{5.170c}$$

$$I_4 = -2(L_1 + \frac{L_2^2}{L_3})hg^2 - 4L_2 gg' h' - 4Rg' - 2R' g + 2L_2' ghg' \tag{5.170d}$$

$$I_5 = -(L_1 + \frac{L_2^2}{L_3})g^2 h - 2L_2 hg'^2 + L_2' g^2 h' + 4Rg' + 2R' g \tag{5.170e}$$

$$I_6 = -(L_1 + \frac{L_2^2}{L_3})g^3 - 2L_2 g'^2 g + L_2' g^2 g' \tag{5.170f}$$

$$A_1 = 2C'_Q h' - 2(C_P + C_Q \frac{L_2}{L_3})h \tag{5.171a}$$

$$A_2 = -C'_Q h'^2 g - C'_P h^2 g - 2C_Q h'^2 g' - 2C_P h^2 g' - 2(C_P - C_Q \frac{L_2}{L_3})ghh' \tag{5.171b}$$

$$A_3 = -2(C_P + C_Q \frac{L_2}{L_3})g + 2C'_Q g' \tag{5.171c}$$

$$A_4 = -2C'_Q gg'h' - 2C'_P g^2 h - 4C_Q g'^2 h' - (6C_P - 2C_Q \frac{L_2}{L_3})ghg' - 2(C_P - C_Q \frac{L_2}{L_3})g^2 h' \tag{5.171d}$$

$$A_5 = -2C_Q g'^3 - C'_P g^3 - C'_Q gg'^2 - 2(2C_P - C_Q \frac{L_2}{L_3})g^2 g' \tag{5.171e}$$

$$N_1 = -(6C_P - 2C_Q \frac{L_2}{L_3})ghh' - 2(C_P - C_Q \frac{L_2}{L_3})h^2 g' - 4C_Q g' h'^2 - 2C'_Q hg' h' - 2C'_P gh^2 \tag{5.172a}$$

$$N_2 = -2(2C_P - C_Q \frac{L_2}{L_3})h^2 h' - 2C_Q h'^3 - C'_P h^3 - C'_Q hh'^2 \tag{5.172b}$$

$$N_3 = -2(C_P - C_Q \frac{L_2}{L_3})ghg' - 2C_P g^2 h' - 2C_Q g'^2 h' - C'_P g^2 h - C'_Q hg'^2 \tag{5.172c}$$

$$\tag{5.172d}$$

where we used

$$K_z \hat{J}_2 \boldsymbol{Q}' = \boldsymbol{Q}'^2 \boldsymbol{Q} - (\boldsymbol{Q}\boldsymbol{Q}')\boldsymbol{Q}' \tag{5.173a}$$

$$K_z \hat{J}_2 \boldsymbol{Q} = (\boldsymbol{Q}\boldsymbol{Q}')\boldsymbol{Q} - \boldsymbol{Q}^2 \boldsymbol{Q}' \tag{5.173b}$$

Using (167) one can write

$$\begin{aligned} \boldsymbol{Q}_3 = & M(\tilde{I}_1 \boldsymbol{Q}'^2_o \boldsymbol{Q}'_o + \tilde{I}_2 \boldsymbol{Q}'^2_o \boldsymbol{Q}_o + \tilde{I}_3 (\boldsymbol{Q}_o \boldsymbol{Q}'_o)\boldsymbol{Q}'_o + \tilde{I}_4 (\boldsymbol{Q}_o \boldsymbol{Q}'_o)\boldsymbol{Q}_o + \tilde{I}_5 \boldsymbol{Q}^2_o \boldsymbol{Q}'_o + \tilde{I}_6 \boldsymbol{Q}^2_o \boldsymbol{Q}_o + \\ & + \tilde{A}_1 K_z \boldsymbol{Q}'_o + \tilde{A}_2 \boldsymbol{Q}'^2_o \hat{J}_2 \boldsymbol{Q}_o + \tilde{A}_3 K_z \boldsymbol{Q}_o + \tilde{A}_4 (\boldsymbol{Q}_o \boldsymbol{Q}'_o)\hat{J}_2 \boldsymbol{Q}_o + \tilde{A}_5 \boldsymbol{Q}^2_o \hat{J}_2 \boldsymbol{Q}_o + \\ & + \tilde{N}_1 (\boldsymbol{Q}_o \boldsymbol{Q}'_o)\hat{J}_2 \boldsymbol{Q} + \tilde{N}_2 \boldsymbol{Q}'^2_o \hat{J}_2 \boldsymbol{Q}_o + \tilde{N}_3 \boldsymbol{Q}^2_o \hat{J}_2 \boldsymbol{Q}'_o) \end{aligned} \tag{5.174}$$

where coefficients with tilde are calculated like

$$\tilde{I}_1 = -\phi_o^{*-\frac{1}{2}} \int_{z_o}^{z_i} h(t) I_1(t) \mathrm{d}t, \ldots \tag{5.175}$$

It is clear that (174) must correspond to (144); hence, we express the coefficients from (174)

$$\tilde{I}_1 = \phi_o^{*-\frac{1}{2}} \int_{z_o}^{z_i} \left((L_1 + \frac{L_2^2}{L_3}) h^4 - L_2' h' h'^3 + 2 L_2 h'^2 h^2 \right) \mathrm{d}z = \tag{5.176}$$

$$= \phi_o^{*-\frac{1}{2}} \int_{z_o}^{z_i} \left(L_1 h^4 + 2 L_2 h'^2 h^2 + L_3 h'^4 - \frac{\mathrm{d}}{\mathrm{d}z} (L_3 h'^3 h + L_2 h^3 h') \right) \mathrm{d}z =$$

$$= C - \phi_o^{*-\frac{1}{2}} [L_3 h'^3 h + L_2 h^3 h']_{z_o}^{z_i} = C$$

where we used $h'' = -\frac{L_2}{L_3} h$ and $h(z_o) = h(z_i) = 0$. At evaluation of the other coefficients we will proceed similarly

$$\tilde{I}_2 = K - \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z} (L_3 h h'^2 g' + L_2 h^3 g' - 2 R h^2) \mathrm{d}z = K \tag{5.177a}$$

$$\tilde{I}_3 = 2(K - \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z} (L_3 h h'^2 g' + L_2 g h^2 h' + R h^2) \mathrm{d}z) = 2K \tag{5.177b}$$

$$\tilde{I}_4 = 2(A - \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z} (-R g h + L_2 g g' h^2 + L_3 g'^2 h h') \mathrm{d}z) = 2A \tag{5.177c}$$

$$\tilde{I}_5 = F - \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z} (2 R g h + L_2 h g^2 h' + L_3 h h' g'^2) \mathrm{d}z = F \tag{5.177d}$$

$$\tilde{I}_6 = D - \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z} (L_3 h g'^3 + L_2 h g^2 g') \mathrm{d}z = D \tag{5.177e}$$

$$\tilde{A}_1 = 2k - 2\phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_Q h' h)\mathrm{d}z = 2k \tag{5.178a}$$

$$\tilde{A}_2 = -k + \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_Q h'^2 hg + C_P h^3 g)\mathrm{d}z = -k \tag{5.178b}$$

$$\tilde{A}_3 = 2a - 2\phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_Q g' h)\mathrm{d}z = 2a \tag{5.178c}$$

$$\tilde{A}_4 = -2a + 2\phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_P g^2 h^2 + C_Q ghg' h')\mathrm{d}z = -2a \tag{5.178d}$$

$$\tilde{A}_5 = -d + \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_P g^3 h + C_Q ghg'^2)\mathrm{d}z = -d \tag{5.178e}$$

$$\tilde{N}_1 = 2\phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_P gh^3 + C_Q h^2 g' h')\mathrm{d}z = 0 \tag{5.179a}$$

$$\tilde{N}_2 = \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_P h^4 + C_Q h^2 h'^2)\mathrm{d}z = 0 \tag{5.179b}$$

$$\tilde{N}_3 = \phi^{*-\frac{1}{2}} \int_{z_o}^{z_i} \frac{\mathrm{d}}{\mathrm{d}z}(C_P g^2 h^2 + C_Q h^2 g'^2)\mathrm{d}z = 0 \tag{5.179c}$$

The third order aberration polynomial then takes form

$$\begin{aligned}\boldsymbol{Q}_3 = M\big(&C\boldsymbol{Q}_o'^2\boldsymbol{Q}_o' + K(\boldsymbol{Q}_o'^2\boldsymbol{Q}_o + 2(\boldsymbol{Q}_o\boldsymbol{Q}_o')\boldsymbol{Q}_o') + 2A(\boldsymbol{Q}_o\boldsymbol{Q}_o')\boldsymbol{Q}_o + F\boldsymbol{Q}_o^2\boldsymbol{Q}_o' + D\boldsymbol{Q}_o^2\boldsymbol{Q}_o \\ &+ k(2K_z\boldsymbol{Q}_o' - \boldsymbol{Q}_o'^2\hat{J}_2\boldsymbol{Q}_o) + 2a(K_z\boldsymbol{Q}_o - (\boldsymbol{Q}_o\boldsymbol{Q}_o')\hat{J}_2\boldsymbol{Q}_o) - d\boldsymbol{Q}_o^2\hat{J}_2\boldsymbol{Q}_o\big)\end{aligned} \tag{5.180}$$

which is coincident to (144).

6 The Symplectic Classification of Geometric Aberrations

The theory of aberrations describes a manner of the optic imperfections of various devices. The aberrations describe the deviation of an electron trajectory from the ideal paraxial ray, determined as linear function of positions and directives in the object plane. From mathematical point of view the ray is function

$$\boldsymbol{r} = \boldsymbol{r}(z; \boldsymbol{r}_0, \boldsymbol{r}_0') \tag{6.1}$$

which can be for each z expanded to Taylor series in initial conditions $\boldsymbol{r}_0$ and $\boldsymbol{r}_0'$. Hence, aberration part denotes the nonlinear part of the expansion.

Unfortunately, as the ray is function of four initial variables the Taylor polynomial contains high number of members even in relatively low order,

$$P_n = \frac{1}{6}(n+3)(n+2)(n+1). \tag{6.2}$$

P_n denotes number of members in Taylor polynomial of n-th order. It gives 20 members of the third order, 56 members of the fifth order, 220 members of the 9^{th} order etc. There are raising two questions. The first one is the meaning of each member in the aberration polynomial including its influence on the optical properties of the system. The second is whether there exists any structure in the aberration coefficients which might be useful for understanding of the system properties. Both are partly explained with symplectic classification of aberrations.

The symplectic classification of the aberration polynomial of the axial symmetric system was presented in [4], the general systems were classified in series of works [21, 22, 23]. We will present the classification of aberration polynomials of the stigmatic system according to representation of group adjoint to the algebra of quadratic polynomials that are determined by the quadratic part of Hamiltonian. We also show the essential influence of the form of paraxial approximation on the relationship among the aberration polynomials. The classification will be also described for the real aberration polynomials.

6.1 Aberrations and Lie transformations

In the last chapter we showed the consequence between aberrations and Lie transformations. We found the transfer map in form of Lie transformation

$$\mathcal{M} = \mathcal{M}_1 \cdots e^{:g_k(\boldsymbol{w}_o, z):} \cdots e^{:g_3(\boldsymbol{w}_o, z):} \tag{6.3}$$

Now we can find the aberrations as the expansion of

$$\boldsymbol{w}(\boldsymbol{w}_o,z)=\mathcal{M}(\boldsymbol{w}_o) \tag{6.4}$$

into Taylor series in power of $\boldsymbol{w}_o$, ie.

$$\boldsymbol{w}=f_1(\boldsymbol{w}_o,z)+f_2(\boldsymbol{w}_o,z)+\cdots f_{k-1}(\boldsymbol{w}_o,z)+\cdots \tag{6.5}$$

Hence, we can describe aberrations using Lie transformation, particulary using of homogeneous polynomials g_k.

One from the most significant properties of aberrations is the invariance according to a canonical transformation $e^{:f:}$ that can represent eq. the rotation around the optical axis. The invariance of the aberrations according to a canonical transformation $e^{:f:}$ is defined:
When the phase space in the object plane is transformed by $e^{:f(\boldsymbol{w}_o):}$ and then is applied the transfer map, the result is the same as in case when the transfer map is applied first and the Lie transformation $e^{:f(\boldsymbol{w}_i):}$ is applied in image plane.
Hence, the diagram

$$\begin{array}{ccc} \boldsymbol{w} & \xrightarrow{e^{:g(\boldsymbol{w}):}} & \tilde{\boldsymbol{w}} \\ {\scriptstyle e^{:f(\boldsymbol{w}):}}\downarrow & & \downarrow{\scriptstyle e^{:f(\tilde{\boldsymbol{w}}):}} \\ \boldsymbol{w}^I & \xrightarrow[e^{:g(\tilde{\boldsymbol{w}}):}]{} & \tilde{\boldsymbol{w}}^I \end{array} \tag{6.6}$$

must commute. Such a property of aberration must influent the form of Lie transformation, namely $g(\boldsymbol{w}_o)$

$$\begin{aligned} e^{:g(\boldsymbol{w}_o):} &= e^{-:f(\tilde{\boldsymbol{w}}^I):}e^{:g(\boldsymbol{w}^I):}e^{:f(\boldsymbol{w}):} = e^{:g:(\boldsymbol{w}^I)}e^{-f(\boldsymbol{w}^I)}e^{-:g(\boldsymbol{w}^I):}e^{:g(\boldsymbol{w}^I):}e^{f(\boldsymbol{w}^I)} = \\ &= \exp(:e^{:f(\boldsymbol{w}):}g(\boldsymbol{w}):) \end{aligned} \tag{6.7}$$

hence, $g(\boldsymbol{w})$ must fulfill

$$g(\boldsymbol{w})=e^{:f(\boldsymbol{w}):}g(\boldsymbol{w}) \tag{6.8}$$

hence, the canonical transformation does not change the form of g. The invariance of aberrations with respect to a canonical transformation determines easy condition on the Lie transformation. We will explore the properties of Lie transformation in the following text.

6.2 Aberrations and Paraxial approximation

However, the paraxial approximation describes the optimal electron paths, we have formerly seen that it plays an important role in the aberration theory as well. It was signified in all perturbation methods. We will focus our attention on the Lie algebra method, where the paraxial approximation is described by the linear operator $\mathcal{M}_1$ that fulfills the equation

$$\frac{\mathrm{d}}{\mathrm{d}z}\mathcal{M}_1 = -\mathcal{M}_1 : H_2 : . \tag{6.9}$$

Generally this equation cannot be analytically solved; however, using Magnus formula [16] we can find the operator in form of exponential map,

$$\mathcal{M}_1 = \exp(: g_2(\boldsymbol{w},z) :) \tag{6.10}$$

where

$$g_2(\boldsymbol{w},z) = -\int_{z_o}^{z} \mathrm{d}z_1 H_2(\boldsymbol{w},z_1) + \frac{1}{2}\int_{z_o}^{z}\mathrm{d}z_2 \int_{z_o}^{z_2}\mathrm{d}z_1 [H_2(z_1),H_2(z_2)] + \cdots . \tag{6.11}$$

It is a member of subalgebra $\mathfrak{h}_2$ of the Lie algebra of the quadratic polynomials in phase space variables with z-dependent coefficients, where the Poisson bracket plays role of Lie brackets. Mathematically, $\mathfrak{h}_2$ is the smallest subalgebra of the algebra that contains the quadratic part of Hamiltonian. In case when $[H_2(z_1),H_2(z_2)] = 0$ for each z_1 and z_2 $\mathfrak{h}_2$ is reduced into one dimensional subspace; hence, (11) is reduced to

$$g_2(\boldsymbol{w},z) = \int_{z_o}^{z} \mathrm{d}z_1 H_2(\boldsymbol{w},z_1), \qquad \text{if } [H_2(z_1),H_2(z_2)] = 0 \quad \forall z_1,z_2$$

Unfortunately, this condition is not generally fulfilled and previous equation is not longer valid. However, if one knows the structure of $\mathfrak{h}_2$, he can also describe the general structure of action of $\mathcal{M}_1$ on the polynomial subspace.

The map that assigns for each element $g \in \mathfrak{h}_2$ the adjoint Lie operator $: g : \in \mathfrak{gl}(P)$ is representation of the algebra $\mathfrak{h}_2$ into the space P. P is the vector space of polynomial in the phase space variables. Using standard procedure we can decompose P into the irreducible subspaces according to the representation of $\mathfrak{h}_2$. Let us consider any polynomial f_0 that is the element of invariant subspace $U \subset P$ and the series

$$f_0, \quad f_1 =: g_2 : f_0, \quad f_2 =: g_2 : f_1, \quad \ldots$$

As the first member of the series $f_0 \in U$ and U is invariant according to the representation of $\mathfrak{h}_2$, if $f_{i-1} \in U$ then $f_i \in U$. Hence, all members of the series are elements of U. Moreover, U is a vector space; thus, any linear combination of members of U is member of U as well. Hence,

$$\mathcal{M}_1 f = \exp(:g_2:) f = \sum_{n=0}^{\infty} \frac{:g_2:^n}{n!} f \in U \tag{6.12}$$

ie. if the space is invariant under the representation of $\mathfrak{h}_2$ then it is invarian under the action $\mathcal{M}_1 = \exp(:g_2:)$ where $g_2 \in \mathfrak{h}_2$.

Hereby we showed that if we find the decomposition of the polynomial subspace on the irreducible subspaces under the representation of $\mathfrak{h}_2$, these subspaces are invariant also under the action of $\mathcal{M}_1$. But why should we do that? We can find three reasons.

The n-th order part of the Hamiltonian takes form

$$H_n = \sum_{i+j+k+l=n} a_{ijkl} x^i y^j p_x^k p_y^l$$

The transition to the interaction Hamiltonian(5.101)

$$H^{\mathsf{int}}(\tilde{\boldsymbol{w}}, z) = H_n(\boldsymbol{w}(\tilde{\boldsymbol{w}}, z), z) = \mathcal{M}_1 H_n(\tilde{\boldsymbol{w}}, z) \tag{6.13}$$

is of complicated form in these coordinates; however, when we decompose the n-th order polynomials on irreducible subspaces $V_n = V_{n1} \oplus \cdots \oplus V_{nk}$, the parts of Hamiltonian belonging to different invariant subspaces do not mix. It simplifies the transition.

The action of $\mathcal{M}_1$ also arises in two other situations. The first one is at recalculation the aberration coefficients expressed in object coordinates to those expressed in paraxial coordinates in the image. Generally, the coordinates in the image can be expressed

$$\begin{aligned} \boldsymbol{w}_i =& \mathcal{M}_1 \boldsymbol{w}_o + \boldsymbol{f}_2(\boldsymbol{w}_o) + \boldsymbol{f}_3(\boldsymbol{w}_o) + \cdots = \\ =& \boldsymbol{w}_i^p + \boldsymbol{f}_2(\mathcal{M}_1^{-1} \boldsymbol{w}_i^p) + \boldsymbol{f}_3(\mathcal{M}_1^{-1} \boldsymbol{w}_i^p) + \cdots \end{aligned} \tag{6.14}$$

where $\boldsymbol{w}_i^p = \mathcal{M}_1 \boldsymbol{w}_o$ denotes paraxial coordinates in the image. By using the feature of the Lie transformation [3] the previous equation takes

$$\boldsymbol{w}_i = \boldsymbol{w}_i^p + \mathcal{M}_1^{-1} \boldsymbol{f}_2(\boldsymbol{w}_i^p) + \mathcal{M}_1^{-1} \boldsymbol{f}_3(\boldsymbol{w}_i^p) + \cdots \tag{6.15}$$

which is in the form of the previous case. Similarly we can say that the parts of the aberration polynomials belonging to different irreducible subspaces do not mix at the transformation.

The last motivation example is the combining of the systems. Let us have two systems where the first one is described by transition map $\mathcal{M}^I$ and the second one by transition map $\mathcal{M}^{II}$. The result map of system which is formed by their combination these two ones is described by transfer map [3] $\mathcal{M}=\mathcal{M}^I\mathcal{M}^{II}$. By using decomposition of transfer maps into paraxial and nonlinear part we can find

$$\begin{aligned}\mathcal{M}=\mathcal{M}_1\exp(:g_3(\boldsymbol{w}_o)+g_4(\boldsymbol{w}_o)+\cdots:)=\mathcal{M}_1^I\exp(:g_3^I(\boldsymbol{w}_o)+g_4^I(\boldsymbol{w}_o)+\cdots:)\cdot\\ \cdot\mathcal{M}_1^{II}\exp(:g_3^{II}(\boldsymbol{w}_o)+g_4^{II}(\boldsymbol{w}_o)+\cdots:)\end{aligned}\tag{6.16}$$

which can be written by using manipulations described in previous section in form

$$\mathcal{M}=\mathcal{M}_1^I\mathcal{M}_1^{II}e^{:(\mathcal{M}_1^{II})^{-1}(g_3(\boldsymbol{w}_o)+g_4(\boldsymbol{w}_o)+\cdots):}e^{:g_3^{II}(\boldsymbol{w}_o)+g_4^{II}(\boldsymbol{w}_o)+\cdots:}.\tag{6.17}$$

using famous Baker–Campbell–Hausdorff formula one can find

$$g_3(\boldsymbol{w}_o)=(\mathcal{M}_1^{II})^{-1}g_3^I(\boldsymbol{w}_o)+g_3^{II}(\boldsymbol{w}_o)\tag{6.18a}$$

$$g_4(\boldsymbol{w}_o)=(\mathcal{M}_1^{II})^{-1}g_4^I(\boldsymbol{w}_o)+g_4^{II}(\boldsymbol{w}_o)+\frac{1}{2}[(\mathcal{M}_1^{II})^{-1}g_3^I(\boldsymbol{w}_o),g_3^{II}(\boldsymbol{w}_o)]\tag{6.18b}$$

...

From the last equation it is clear that just aberrations belonging to corresponding irreducible subspaces are mixing at combining the transfer map.

These entire examples show the important role of the paraxial approximation, which can be described by action of $\mathcal{M}_1$. The decomposition of aberration polynomial into irreducible subspaces shows the structure of the aberration and might be helpful for understanding of the optical properties of the system. In particular we will proceed by:

- We find general form of the algebra $\mathfrak{h}_2$ for stigmatic systems
- We find the decomposition of the polynomial space in irreducible subspaces according the representation of $\mathfrak{h}_2$
- We describe the structure of invariant subspaces of the polynomial space under the action $\mathcal{M}_1$

6.3 Lie algebra $\mathfrak{h}_2$

In general case the quadratic part of the Hamiltonian is described by (4.22), consequently the subalgebra $\mathfrak{h}_2$ is generated by four polynomials $\boldsymbol{q}^2$, $\boldsymbol{p}^2$, L_z and x^2-y^2. Hence, the

algebra $\mathfrak{h}_2$ is equal to algebra of all quadratic polynomials, which is via (2) the 10–dimensional vector space. The structure of such a space is too complicated. Fortunately, the general form of the quadratic part of Hamiltonian is not necessary, as the most of optical devices is constructed to be stigmatic.

When one applies the stigmatic condition (4.6) the quadratic part of the Hamiltonian reduces into

$$H_2 = \frac{\eta}{2e\phi^{*\frac{1}{2}}}\boldsymbol{p}^2 + \frac{\eta B}{2\phi^{*\frac{1}{2}}}L_z + \frac{1}{2}\left(\frac{e\gamma_0\phi''}{4\eta\phi^{*\frac{1}{2}}} + \frac{e\eta B^2}{4\phi^{*\frac{1}{2}}} + \frac{eF_1^2}{8\eta\phi^{*\frac{3}{2}}}\right)\boldsymbol{q}^2 \tag{6.19}$$

The subalgebra $\mathfrak{h}_2$ is then formed by four polynomials $\boldsymbol{p}^2$, $\boldsymbol{q}^2$, $\boldsymbol{qp}$ and L_z. It is common to introduce notation [4]

$$a^+ = -\frac{1}{2}\boldsymbol{p}^2 \tag{6.20a}$$

$$a^- = \frac{1}{2}\boldsymbol{q}^2 \tag{6.20b}$$

$$a_0 = \frac{1}{2}[a^+, a^-] = \frac{1}{2}\boldsymbol{qp} \tag{6.20c}$$

$$L_z = xp_y - yp_x \tag{6.20d}$$

One can then find the commutation relations

$$[L_z, a^+] = 0 \qquad [L_z, a^-] = 0 \qquad [L_z, a_0] = 0$$
$$[a^+, a^-] = 2a_0 \qquad [a_0, a^+] = a^+ \qquad [a_0, a^-] = -a^-.$$

The polynomials a^+, a^- and a_0 form the Lie subalgebra of the quadratic polynomial algebra which is isomorphic to $\mathfrak{sp}(2,\mathbb{R})$; moreover, as the polynomial L_z commutes with the others the structure of $\mathfrak{h}_2$ can be written

$$\mathfrak{h}_2 \cong \mathfrak{sp}(2,\mathbb{R}) \oplus \mathbb{R} \tag{6.21}$$

This is the structure we will consider in the following text.

Let us denote the adjoint operator to a^+, a^-, a_0 and L_z

$$\hat{a}^+ =: a^+ : = -\frac{1}{2} : \boldsymbol{p}^2 : \tag{6.22a}$$

$$\hat{a}^- =: a^- : = \frac{1}{2} : \boldsymbol{q}^2 : \tag{6.22b}$$

$$\hat{a}_0 =: a_0 : = \frac{1}{2} : [a^+, a^-] := \frac{1}{2} : \boldsymbol{qp} : \tag{6.22c}$$

$$\hat{L}_z =: L_z : =: xp_y - yp_x : \tag{6.22d}$$

which form basis of adjoint algebra $:\mathfrak{h}_2:$, which has the same algebraic structure as algebra $\mathfrak{h}_2$.

6.4 Representation of $\mathfrak{h}_2$ on the space of complex polynomials

When we know the structure of $\mathfrak{h}_2$ we can describe the adjoint representation on the polynomial space. The first important property of the action is that the polynomial order remains unchanged under the action of $\mathfrak{h}_2$, the homogeneous polynomials of different order do not mix and they can be investigated independently. Hence, the polynomial space can be decomposed to

$$V = \bigoplus_{n=1}^{\infty} V_n \tag{6.23}$$

where each V_n is reducible representation of $\mathfrak{h}_2$.

The order of a polynomial can be calculated as an eigenvalue of number operator

$$\hat{\mathcal{N}} = x\frac{\mathrm{d}}{\mathrm{d}x} + y\frac{\mathrm{d}}{\mathrm{d}y} + p_x\frac{\mathrm{d}}{\mathrm{d}p_x} + p_y\frac{\mathrm{d}}{\mathrm{d}p_y} \tag{6.24}$$

hence, as the action $\mathfrak{h}_2$ conserves the order of homogeneous polynomial, there must be fulfil

$$[\hat{\mathcal{N}}, \hat{a}_0] = [\hat{\mathcal{N}}, \hat{a}^+] = [\hat{\mathcal{N}}, \hat{a}^-] = [\hat{\mathcal{N}}, \hat{L}_z] = 0. \tag{6.25}$$

Now we must find decomposition of each V_n to irreducible subspaces. As the first step we describe the eigen subspaces of $\hat{L}_z$. This operator is the generator of rotation around the axis z [10]. The transformation has no eigen direction in the real plane perpendicular to the axis z. The standard way how to describe the decomposition on the irreducible subspaces is to extend the real space to complex. In the complex extension it is possible to find the basis of eingen vectors of any linear operator. Let us introduce the coordinates

$$z = (x + \mathrm{i}y)/\sqrt{2} \tag{6.26a}$$

$$\bar{z} = (x - \mathrm{i}y)/\sqrt{2} \tag{6.26b}$$

and canonically adjoint impulses found by a standard way [10] read

$$p_z = (p_x - \mathrm{i}p_y)/\sqrt{2} \tag{6.26c}$$

$$p_{\bar{z}} = (p_x + \mathrm{i}p_y)/\sqrt{2}. \tag{6.26d}$$

z - coordinate of angular momentum takes form

$$L_z = \mathrm{i}(zp_z - \bar{z}p_{\bar{z}}) \tag{6.27}$$

the action of which is described by

$$\hat{L}_z z^{i_1}\bar{z}^{i_2}p_z^{i_3}\bar{p}_z^{i_4} = \mathrm{i}(i_3 - i_4 - i_1 + i_2) z^{i_1}\bar{z}^{i_2}p_z^{i_3}\bar{p}_z^{i_4}, \tag{6.28}$$

ie. the polynomials of form $z^{i_1}\bar{z}^{i_2}p_z^{i_3}\bar{p}_z^{i_4}$ are eigenvectors of $\hat{L}_z$. Let us denote

$$l = (i_3 - i_4 - i_1 + i_2),$$

Using $n = i_1 + i_2 + i_3 + i_4$ one can find that $l = n - 2(i_1 + i_4)$. Because $i_1 + i_4$ can take value from 0 to n; hence, for given polynomial order n

$$l \in \{-n, -n+2, \ldots, n-2, n\}. \tag{6.29}$$

The eigenvectors with the same value of l form subspace of V_n. As $[\mathfrak{sp}(2,\mathbb{R}), L_z] = 0$ these subspaces are invariant under the action of $\mathfrak{h}_2$ and one can write

$$V_n = \bigoplus_{k=0}^{n} V_{n,n-2k} \tag{6.30}$$

Let us consider the polynomial $u = z^{i_1}\bar{z}^{i_2}p_z^{i_3}p_{\bar{z}}^{i_4} \in V_{n,l}$, then in subspace V_n there must exist polynomial $\bar{u} = z^{i_2}\bar{z}^{i_1}p_z^{i_4}p_{\bar{z}}^{i_3} \in V_{n,l}$. As $\hat{L}_z u = \mathrm{i}lu$ the action of $\hat{L}_z$ on $\bar{u}$ takes form

$$\hat{L}_z \bar{u} = -\mathrm{i}(i_3 - i_4 - i_1 + i_2)\bar{u} = -\mathrm{i}l\bar{u}$$

hence, $\bar{u} \in V_{n,-l}$. Using the linearity of $\hat{L}_z$ one can find for each $u \in V_{n,l}$ complex conjugate polynomial $\bar{u} \in V_{n,-l}$. Thus, it was shown that subspaces $V_{n,l}$ and $V_{n,-l}$ are complex conjugate, ie.

$$V_{n,l} = \bar{V}_{n,-l} \tag{6.31}$$

The next step is to describe the action of $\mathfrak{sp}(2,\mathbb{R})$ on the polynomial subspace V_{nl}. The polynomials a^+, a^- and a_0 are transformed like

$$a^+ = -p_z p_{\bar{z}} \tag{6.32a}$$

$$a^- = z\bar{z} \tag{6.32b}$$

$$a_0 = \frac{1}{2}(zp_z + \bar{z}p_{\bar{z}}) \tag{6.32c}$$

Let us note that all of the polynomials L_z, a^+, a^- and a_0 are actually real polynomials expressed in complex coordinates.

First we describe general properties of a finite dimensional complex representations of $\mathfrak{sp}(2,\mathbb{R})$, which is for our case represented by operators $\hat{a}^+$, $\hat{a}^-$ and $\hat{a}_0$. Here it is usual to introduce the Casimir operator [17],

$$\hat{a}^2 = \hat{a}^-\hat{a}^+ + \hat{a}_0^2 + \hat{a}_0 = \hat{a}^+\hat{a}^- + \hat{a}_0^2 - \hat{a}_0. \tag{6.33}$$

It commutes with all elements of $\mathfrak{sp}(2,\mathbb{R})$

$$[\hat{a}^2,\hat{a}^-] = [\hat{a}^2,\hat{a}^+] = [\hat{a}^2,\hat{a}_0] = 0,$$

hence, in the irreducible subspace there exists base formed by common eigenvectors of $\hat{a}^2$ and $\hat{a}_0$. Let us denote them $|\,j,m\rangle$,

$$\hat{a}^2\,|\,j,m\rangle = j(j+1)\,|\,j,m\rangle \tag{6.34}$$

$$\hat{a}_0\,|\,j,m\rangle = m\,|\,j,m\rangle \tag{6.35}$$

From the commutation relations one can find the meaning of $\hat{a}^+$ and $\hat{a}^-$ as raising or descending operator respectively,

$$\hat{a}_0\hat{a}^\pm\,|\,j,m\rangle = \hat{a}^\pm\hat{a}_0 \pm a^\pm\,|\,j,m\rangle = (m\pm 1)a^\pm\,|\,j,m\rangle \tag{6.36}$$

$$a^\pm\,|\,j,m\rangle \sim |\,j,m\pm 1\rangle \tag{6.37}$$

ie. the action of $\hat{a}^+$ transforms vector with an eigenvalue m relative to $\hat{a}_0$ to vector with the eigenvalue $m+1$, similarly the action of $\hat{a}^-$ transforms vector with the eigenvalue m to vector with the eigenvalue $m-1$.

The representation is finite, the consequence of which there must exist vector $|\,j,m_1\rangle \neq 0$ that vanishes under the action of $\hat{a}^+$, ie. $a^+\,|\,j,m_1\rangle = 0$. Using the definition (33) one can find

$$\hat{a}^2\,|\,j,m_1\rangle = (m_1^2 + m_1)\,|\,j,m_1\rangle$$

and comparing with (34) $m_1 = j$. Hence, in the irreducible subspace there exists vector $|\,j,j\rangle \neq 0$ which vanish under the action of $\hat{a}^+$.

Applying operator $\hat{a}^-$ we can generate chain of vectors,

$$|\,j,j-k\rangle \sim (\hat{a}^-)^k\,|\,j,j\rangle, \tag{6.38}$$

which is invariant under the action of $\mathfrak{sp}(2,\mathbb{R})$ and forms an irreducible subspace. As we suppose for the representation to be finite, the chain must be finite as well; hence, there must exist k_m such that $|\,j,j-k_m\rangle \neq 0$ that vanishes under the action of $\hat{a}^-$, ie.

$$\hat{a}^- \,|\, j,j-k_m\rangle = |\, j,j-k_m-1\rangle = 0 \tag{6.39}$$

and when one calculates the action of $\hat{a}^2$

$$\begin{aligned}\hat{a}^2 \,|\, j,j-k_m\rangle &= (\hat{a}^+\hat{a}^- + \hat{a}_0^2 - \hat{a}_0)\,|\, j,j-k_m\rangle = ((j-k_m)^2 - j + k_m)\,|\, j,j-k_m\rangle \\ &= (j^2+j)\,|\, j,j-k_m\rangle \end{aligned} \tag{6.40}$$

and compares the coefficients in last equation he can find $k_m = 2j$. Hence, we can write the possible eigenvalue of $\hat{a}_0$

$$m \in \{j, j-1, \cdots -j+1, -j\} \tag{6.41}$$

moreover, as k_m is integer the possible values of j are constrained to

$$j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \ldots\} \tag{6.42}$$

Thus, the irreducible representation of $\mathfrak{sp}(2,\mathbb{R})$ can be characterised by eigenvalues of $\hat{a}^2$. We will denote them D_j,

$$D_j = <|\, j,j\rangle, |\, j,j-1, \ldots, |\, j,-j+1\rangle, |\, j,-j\rangle> \tag{6.43}$$

We did not completely defined the polynomial $|\, j,m\rangle$ yet, we only note that it is proportional to $(a^-)^{j-m}\,|\, j,m\rangle$, now we will determine the multiplicative factor. We will use different normalisation than is used in quantum mechanics, where the representation of $\mathfrak{sl}(2,\mathbb{R}) \cong \mathfrak{sp}(2,\mathbb{R})$ is used at description of angular momentum operator. We will use the normalisation introduced in [4]

$$|\, j,m-1\rangle = \frac{1}{m+j}\hat{a}^- \,|\, j,m\rangle \tag{6.44a}$$

$$|\, j,m+1\rangle = \frac{1}{m-j}\hat{a}^+ \,|\, j,m\rangle \tag{6.44b}$$

It is well known [17] that representation of the $\mathfrak{sp}(2,\mathbb{R})$ is completely reducible, which for our case means that the space $V_{n,l}$ can be written as a direct sum

$$V_{n,l} = \bigoplus_{j\in\mathcal{K}} V_{n,l,j} = \bigoplus_{j\in\mathcal{K}} D_j\,, \tag{6.45}$$

where $\mathcal{K}$ is an index set. Now two questions are raising, what is the form of elements in D_j and what can be said about the index set $\mathcal{K}$.

It was shown that each irreducible space D_j is determined by the appropriate vector $|\,j,j\rangle$; hence, if one wants to describe all $D_j \in V_{nl}$ he must find all polynomial $u \in V_{nl}$ that vanishes after the action of $\hat{a}_+$ and are eigenvectors of $\hat{a}_0$ and $\hat{a}^2$. The polynomials

$$u = p_z^a p_{\bar{z}}^b (\mathrm{i}(z p_z - \bar{z} p_{\bar{z}}))^c = p_z^a p_{\bar{z}}^b L_z^c, \qquad a+b+2c = n$$

fulfil such conditions. Really $\hat{a}_+ u = 0$, $\hat{a}_0 u = \frac{1}{2}(a+b)u$ and $\hat{a}^2 u = (\frac{1}{4}(a+b)^2 + \frac{1}{2}(a+b))u$. Moreover, we require for the polynomial to be element of V_{nl}. Let us find the connection between a, b, c and n, l, j.

$$\hat{\mathcal{N}} u = (a+b+2c)u = nu \tag{6.46a}$$

$$\hat{L}_z u = \mathrm{i}(a-b)u = \mathrm{i}l u \tag{6.46b}$$

$$\hat{a}^2 u = \frac{1}{2}(a+b)(\frac{1}{2}(a+b)+1)u = j(j+1)u \tag{6.46c}$$

Comparing the results and solving the algebraic equation one can find u in form

$$u = p_z^{j+\frac{1}{2}l} p_{\bar{z}}^{j-\frac{1}{2}l} L_z^{\frac{1}{2}n-j} =: {}^n\mathcal{P}_j^{j;l}, \tag{6.47}$$

where the notation for the polynomial using its eigenvalues relative to operators $\mathcal{N}$, $\hat{L}_z$, $\hat{a}^2$ and $\hat{a}_0$ were introduce, ie.

$$\hat{\mathcal{N}}\ {}^n\mathcal{P}_m^{j;l} = n\ {}^n\mathcal{P}_m^{j;l} \tag{6.48a}$$

$$\hat{L}_z\ {}^n\mathcal{P}_m^{j;l} = \mathrm{i}l\ {}^n\mathcal{P}_m^{j;l} \tag{6.48b}$$

$$\hat{a}^2\ {}^n\mathcal{P}_m^{j;l} = j(j+1)\ {}^n\mathcal{P}_m^{j;l} \tag{6.48c}$$

$$\hat{a}_0\ {}^n\mathcal{P}_m^{j;l} = m\ {}^n\mathcal{P}_m^{j;l} \tag{6.48d}$$

more over one can easily show that

$${}^n\mathcal{P}_j^{j;l} = L_z^{\frac{n}{2}-j}\ {}^{2j}\mathcal{P}_j^{j;l} \tag{6.49}$$

Because the exponent cannot be negative, the value of j is constrained with the others, ie.

$$j \le \frac{1}{2}n, \qquad j \ge \frac{1}{2}l, \qquad j \ge -\frac{1}{2}l \tag{6.50}$$

hence,

$$j \in \{\frac{|\,l\,|}{2}, \frac{|\,l\,|}{2}+1, \ldots, \frac{n}{2}\} \tag{6.51}$$

and subspace

$$V_{n,l} \cong D_{\frac{|l|}{2}} \oplus D_{\frac{|l|}{2}+1} \oplus \cdots \oplus D_{\frac{n}{2}} \oplus U_{n,l} \tag{6.52}$$

where each D_j is generated by the action of $\hat{a}^-$ on the polynomial ${}^n\mathcal{P}_j^{j;l}$,

$${}^n\mathcal{P}_m^{j;l} = \alpha(j,m) L_z^{\frac{1}{2}n-j} (\hat{a}^-)^{j-m} p_z^{j+\frac{1}{2}l} p_{\bar{z}}^{j-\frac{1}{2}l} = L_z^{\frac{1}{2}n-j}\ {}^{2j}\mathcal{P}_m^{j;l} \tag{6.53}$$

the multiplicative factor $\alpha(j,m) = \prod_{i=m+1}^{j} 1/(i+j)$ and U_{nl} is some rest subspace. Using (53) it is easy to see that

$$V_{nlj} = L_z^{\frac{n}{2}-j} \cdot V_{2j,l,j} \tag{6.54}$$

Now we will show that $U_{nl} = 0$. It is possible by comparing of the subspace dimensions. The dimension of n^{th} order polynomials subspace can be evaluated

$$\dim V_n = \frac{(n+3)!}{n!3!} = \frac{1}{6}(n+3)(n+2)(n+1). \tag{6.55}$$

On the other hand one can find the dimension

$$\dim V_n = \sum_{k=0}^{n} V_{n,n-2k} = \sum_{k=0}^{n} \Big(\sum_{j=|n-2k|/2}^{n/2} \dim D_j + \dim U_{n,n-2k} \Big)$$

and as the dimension of D_j is $2j+1$,

$$\begin{aligned} \dim V_n &= \sum_{k=0}^{n} \Big(\sum_{j=|n-2k|/2}^{n/2} (2j+1) + \dim U_{n,n-2k} \Big) = \\ &= \sum_{k=0}^{n} \frac{1}{2}(n+1+|\,n-2k\,|+1)\Big(\frac{n}{2} - \frac{|\,n-2k\,|}{2} + 1\Big) + \dim U_{n,n-2k} \\ &\sum_{k=0}^{n} \Big(\frac{n}{2}+1\Big)^2 - \frac{(n-2k)^2}{4} + \sum_{k=0}^{n} \dim(U_{n,n-2k}) = \\ &= \frac{1}{6}(n+3)(n+2)(n+1) + \sum_{k=0}^{n} \dim(U_{n,n-2k}) \end{aligned} \tag{6.56}$$

comparing (55) and (56) it is showed that $\dim U_{nl} = 0$ and

$$V_{n,l} \cong V_{n,l,\frac{|l|}{2}} \oplus V_{n,l,\frac{|l|}{2}+1} \oplus \cdots \oplus V_{n,l,\frac{n}{2}} \tag{6.57}$$

where each $V_{n,l,j} \cong D_j$.

We have shown that $V_{n,l} = \bar{V}_{n,-l}$, when we use the decomposition (57) it is easy to see that each of the subspaces $V_{n,l,j}$ is complex conjugate to the subspace $V_{n,-l,j}$, or more particularly

$$ {}^{n}\mathcal{P}_{m}^{j;l} = {}^{n}\bar{\mathcal{P}}_{m}^{j;-l}. \tag{6.58}$$

The description of the decomposition of polynomial space to irreducible subspaces is done by combining (23), (30) and (57). The particular form of the polynomials is described by (53).

6.5 Example: Decomposition of polynomial space up to 4^{th} order

We use the method mentioned in the previous subsection. As the irreducible subspaces of different orders do not mix we can describe the decomposition of each order independently.

Polynomials of the third order

For the subspace V_3 $n=3$ and using (29) $l \in \{-3,-1,1,3\}$. Hence,

$$ V_3 = V_{3,-3} \oplus V_{3,-1} \oplus V_{3,1} \oplus V_{3,3} \tag{6.59}$$

For $V_{3,-3}$, $n=3$ and $l=-3$ using (51) $j \in \{\frac{3}{2}\}$; hence,

$$ V_{3,-3} = V_{3,-3,\frac{3}{2}} \cong D_{3/2} \tag{6.60}$$

The irreducible subspace $D_{3/2}$ is generated from polynomial (47), ie.

$$ {}^{3}\mathcal{P}_{\frac{3}{2}}^{\frac{3}{2};-3} = p_{\bar{z}}^{3} \tag{6.61a}$$

applying the operator $\hat{a}^{-}$

$$ {}^{3}\mathcal{P}_{\frac{1}{2}}^{\frac{3}{2};-3} = \frac{1}{3}\hat{a}^{-}\ {}^{3}\mathcal{P}_{\frac{3}{2}}^{\frac{3}{2};-3} = \frac{1}{3}\hat{a}^{-}p_{\bar{z}}^{3} = z p_{\bar{z}}^{2} \tag{6.61b}$$

$$ {}^{3}\mathcal{P}_{-\frac{1}{2}}^{\frac{3}{2};-3} = \frac{1}{2}\hat{a}^{-}\ {}^{3}\mathcal{P}_{\frac{3}{2}}^{\frac{1}{2};-3} = \frac{1}{2}\hat{a}^{-}z p_{\bar{z}}^{2} = z^{2} p_{\bar{z}} \tag{6.61c}$$

$$ {}^{3}\mathcal{P}_{-\frac{3}{2}}^{\frac{3}{2};-3} = \hat{a}^{-}\ {}^{3}\mathcal{P}_{\frac{3}{2}}^{-\frac{1}{2};-3} = \hat{a}^{-}z^{2} p_{\bar{z}} = z^{3} \tag{6.61d}$$

hence,

$$ V_{3,-3} = < p_{\bar{z}}^{3}, z p_{\bar{z}}^{2}, z^{2} p_{\bar{z}}, z^{3} > \tag{6.62}$$

Using the same procedure one can find for $l=-1$, $j\in\{\frac{1}{2},\frac{3}{2}\}$ and $V_{3,-1}\cong D_{1/2}\oplus D_{3/2}$, with $D_{1/2}$ formed by polynomials

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{\frac{1}{2}} = \mathrm{i}p_{\bar{z}}(zp_z-\bar{z}p_{\bar{z}}) = p_{\bar{z}}L_z \tag{6.63a} $$

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{-\frac{1}{2}} = \mathrm{i}z(zp_z-\bar{z}p_{\bar{z}}) = zL_z \tag{6.63b} $$

and $D_{3/2}$ by

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{\frac{3}{2}} = p_z p_{\bar{z}}^2 \tag{6.64a} $$

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{\frac{1}{2}} = \frac{1}{3}\bar{z}p_{\bar{z}}^2+\frac{2}{3}zp_{\bar{z}}p_z \tag{6.64b} $$

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{-\frac{1}{2}} = \frac{2}{3}\bar{z}zp_{\bar{z}}+\frac{1}{3}z^2p_z \tag{6.64c} $$

$$ {}^3\mathcal{P}^{\frac{1}{2};-1}_{-\frac{3}{2}} = \bar{z}z^2 \tag{6.64d} $$

The subspace $V_{3,1}\cong D_{1/2}\oplus D_{3/2}$ with

$$ D_{1/2} = <p_zL_z, \bar{z}L_z> \tag{6.65a} $$

$$ D_{3/2} = <p_z^2p_{\bar{z}}, \frac{2}{3}\bar{z}p_zp_{\bar{z}}+\frac{1}{3}zp_z^2, \frac{1}{3}\bar{z}^2p_{\bar{z}}+\frac{2}{3}z\bar{z}p_z, z\bar{z}^2> \tag{6.65b} $$

and subspace $V_{3,3}\cong D_{3/2}$, ie.

$$ V_{3,3} = <p_z^3, \bar{z}p_z^2, \bar{z}^2p_z, \bar{z}^3> \tag{6.66} $$

Polynomials of the forth order

For $n=4$ the values of l are elements of the set $\{-4,-2,0,2,4\}$. We will show the procedure only for the case $l=0$, for the other we will present only the results.

When $l=0$, j goes through the set $\{0,1,2\}$; thus, $V_{4,0}\cong V_{4,0,0}\oplus V_{4,0,1}\oplus V_{4,0,2}$. The irreducible space $V_{4,0,0}\cong D_0$ is a one dimensional vector space generated by vector

$$ {}^4\mathcal{P}_0^{0;0} = L_z^2 = -(zp_z-\bar{z}p_{\bar{z}})^2 \tag{6.67} $$

The irreducible subspace $V_{4,0,1}\cong D_1$ is generated by the polynomial

$$ {}^4\mathcal{P}_1^{1;0} = p_zp_{\bar{z}}L_z \tag{6.68a} $$

and applaying apperator $\hat{a}^-$ we generate the basis

$$ {}^4\mathcal{P}_0^{1;0} = \frac{1}{2}\hat{a}^- \ {}^4\mathcal{P}_1^{1;0} = \frac{1}{2}(zp_z + \bar{z}p_{\bar{z}})L_z \tag{6.68b} $$

$$ {}^4\mathcal{P}_{-1}^{1;0} = \hat{a}^- \ {}^4\mathcal{P}_0^{1;0} = z\bar{z}L_z \tag{6.68c} $$

and the subspace $V_{4,0,2} \cong D_2$ is generated by the polynomial

$$ {}^4\mathcal{P}_2^{2;0} = (p_z p_{\bar{z}})^2 \tag{6.69a} $$

and the other basis elements take form

$$ {}^4\mathcal{P}_1^{2;0} = \frac{1}{2}p_z p_{\bar{z}}(zp_z + \bar{z}p_{\bar{z}}) \tag{6.69b} $$

$$ {}^4\mathcal{P}_0^{2;0} = \frac{1}{6}(zp_z + \bar{z}p_{\bar{z}})^2 + \frac{1}{3}z\bar{z}p_z p_{\bar{z}} \tag{6.69c} $$

$$ {}^4\mathcal{P}_{-1}^{2;0} = \frac{1}{2}z\bar{z}(zp_z + \bar{z}p_{\bar{z}}) \tag{6.69d} $$

$$ {}^4\mathcal{P}_{-2}^{2;0} = \bar{z}^2 z^2 \tag{6.69e} $$

For $l = -4$, j must be equal 2; hence, $V_{4,-4} = V_{4,-4,2} \cong D_2$, which is generated by

$$ V_{4,-4,2} = < p_{\bar{z}}^4, zp_{\bar{z}}^3, z^2 p_{\bar{z}}^2, z^3 p_{\bar{z}}, z^4 > \tag{6.70} $$

For $l = -2$, j goes through the set $\{1,2\}$; hence, $V_{4,-2} = V_{4,-2,1} \oplus V_{4,-2,2} \cong D_1 \oplus D_2$ where

$$ V_{4,-2,1} = < p_{\bar{z}}^2 L_z, zp_{\bar{z}} L_z, z^2 L_z > \tag{6.71} $$

and

$$ V_{4,-2,2} = < p_z p_{\bar{z}}^3, \frac{1}{4}p_{\bar{z}}^2(\bar{z}p_{\bar{z}} + 3zp_z), \frac{1}{2}zp_{\bar{z}}(zp_z + \bar{z}p_{\bar{z}}), \frac{1}{4}z^2(zp_z + 3\bar{z}p_{\bar{z}}), \bar{z}z^3 > \tag{6.72} $$

The subspace $V_{4,2}$ is complex conjugate to $V_{4,-2}$ and $V_{4,4}$ is complex conjugate to $V_{4,-4}$.

6.6 Representation of $\mathfrak{h}_2$ on the real space of polynomials

We have described the representation of $\mathfrak{h}_2$ on the space of complex polynomials, but the real representation is more complicated. We have noted that except of the axial symmetric polynomials there exists no eigen vectors of L_z in the real polynomial space.

Fortunately, using the decomposition of the space of complex polynomials we can find the irreducible subspaces of real polynomials.

Let us consider the irreducible subspaces $V_{n,l,j}$ and $V_{n,-l,j}$. We showed that these subspaces are complex conjugate and each element ${}^{n}\mathcal{P}_m^{j;l} \in V_{n,l,j}$, ${}^{n}\mathcal{P}_m^{j;l}$ is complex conjugate to ${}^{n}\mathcal{P}_m^{j;-l} \in V_{n,-l,j}$. Let us define two real polynomials

$$\xi = \frac{1}{2}({}^{n}\mathcal{P}_m^{j;l} + {}^{n}\mathcal{P}_m^{j;-l}) \tag{6.73a}$$

$$\eta = -\frac{\mathrm{i}}{2}({}^{n}\mathcal{P}_m^{j;l} - {}^{n}\mathcal{P}_m^{j;-l}) \tag{6.73b}$$

Even though these two polynomials are not eigen vectors of $\hat{L}_z$, the subspace $<\xi,\eta>$ is invariant under the action, ie.

$$\hat{L}_z\xi = \frac{1}{2}(\mathrm{i}l\ {}^{n}\mathcal{P}_m^{j;l} - \mathrm{i}l\ {}^{n}\mathcal{P}_m^{j;-l}) = -l\eta \tag{6.74a}$$

$$\hat{L}_z\eta = \frac{1}{2\mathrm{i}}(\mathrm{i}l\ {}^{n}\mathcal{P}_m^{j;l} + \mathrm{i}l\ {}^{n}\mathcal{P}_m^{j;-l}) = l\xi \tag{6.74b}$$

Now we will apply this approach to the whole space V. Let us define the real vectors

$${}^{n}\mathcal{C}_m^{j;l} = 2^{j-1}({}^{n}\mathcal{P}_m^{j;l} + {}^{n}\mathcal{P}_m^{j;-l}) \tag{6.75a}$$

$${}^{n}\mathcal{S}_m^{j;l} = -\mathrm{i}2^{j-1}({}^{n}\mathcal{P}_m^{j;l} - {}^{n}\mathcal{P}_m^{j;-l}) \tag{6.75b}$$

and for each n, $l>0$, and j the real subspaces

$$U_{n,l,j}^{+} = <{}^{n}\mathcal{C}_j^{j;l}, \cdots, {}^{n}\mathcal{C}_{-j}^{j;l}> \tag{6.76a}$$

$$U_{n,l,j}^{-} = <{}^{n}\mathcal{S}_j^{j;l}, \cdots, {}^{n}\mathcal{S}_{-j}^{j;l}> \tag{6.76b}$$

Using the properties of representation $\mathfrak{h}_2$ on the space of complex polynomials we find

$$\begin{aligned}\frac{\hat{a}^{-}}{j+m}\ {}^{n}\mathcal{C}_m^{j;l} &= 2^{j-1}(\frac{a^{-}}{j+m}\ {}^{n}\mathcal{P}_m^{j;l} + \frac{a^{-}}{j+m}\ {}^{n}\mathcal{P}_m^{j;-l}) = \\ &= 2^{j-1}({}^{n}\mathcal{P}_{m-1}^{j;l} + {}^{n}\mathcal{P}_m^{j;-l}) = {}^{n}\mathcal{C}_{m-1}^{j;l}\end{aligned} \tag{6.77}$$

and similarly

$$\frac{\hat{a}^{-}}{j+m}\ {}^{n}\mathcal{S}_m^{j;l} = {}^{n}\mathcal{S}_{m-1}^{j;l} \tag{6.78}$$

The subspace $U^{+}_{n,l,j}$ can also be generated from ${}^{n}\mathcal{C}^{j;l}_{j}$ by lowering with $\hat{a}^{-}$ and similarly the subspace $U^{-}_{n,l,j}$ from the polynomial ${}^{n}\mathcal{S}^{j;l}_{m}$. Hence, these subspaces are irreducible under the action of $\mathfrak{sp}(2,\mathbb{R})$ isomorphic to D_j. Unfortunately, they are not invariant under the action of $\hat{L}_z$,

$$\hat{L}_z\ {}^{n}\mathcal{C}^{j;l}_{m} = -l\ {}^{n}\mathcal{S}^{j;l}_{m} \tag{6.79a}$$

$$\hat{L}_z\ {}^{n}\mathcal{S}^{j;l}_{m} = \ \ l\ {}^{n}\mathcal{C}^{j;l}_{m} \tag{6.79b}$$

which causes mixing these two subspaces. The irreducible subspace under the action of $\mathfrak{h}_2$ is then

$$U_{n,l,j} = U^{+}_{n,l,j} \oplus U^{-}_{n,l,j} \tag{6.80}$$

where $\oplus$ for this once means just vector space addition.

When $l=0$ the situation is much easier because all of polynomials ${}^{n}\mathcal{P}^{j;0}_{m}$ are real polynomials expressed in complex coordinates. Thus, we must only express the polynomials in real coordinates and normalize, ie.

$${}^{n}\mathcal{C}^{j;0}_{m} = 2^{j}\ {}^{n}\mathcal{P}^{j;0}_{m} \tag{6.81}$$

Hence, the decomposition of the real polynomial space

$$U = \sum_{n} \sum_{k=0}^{\frac{n}{2}} \sum_{j=k}^{\frac{1}{2}} U_{n,2k,j} \tag{6.82}$$

is the decomposition on the irreducible subspaces according to the action oh $\mathfrak{h}_2$.

6.7 Example: Real polynomials up to the fourth order

We have calculated the decomposition of space of complex polynomials to irreducible subspaces according to the action of $\mathfrak{h}_2$. Now we will use that result and applying the procedure described in last section we will show the decomposition of the real polynomial space up to fourth order.

The third order polynomials

We will show the procedure on construction of the space $U_{3,3,3/2}$. Using (62), (66) and (75b) one can find the basis of $U^{+}_{3,3,3/2}$

$$
\begin{aligned}
{}^3\mathcal{C}^{\frac{3}{2};3}_{\frac{3}{2}} &= 2^{\frac{1}{2}}\left({}^3\mathcal{P}^{\frac{3}{2};3}_{\frac{3}{2}} + {}^3\mathcal{P}^{\frac{3}{2};-3}_{\frac{3}{2}}\right) && \text{(6.83a)}\\
&= \sqrt{2}(p_z^3 + p_{\bar z}^3) = px^3 - 3p_x p_y^2 &&\\
{}^3\mathcal{C}^{\frac{3}{2};3}_{\frac{1}{2}} &= 2^{\frac{1}{2}}(\bar z p_z + z p_{\bar z}) = x(p_x^2 - p_y^2) - 2yp_x p_y && \text{(6.83b)}\\
{}^3\mathcal{C}^{\frac{3}{2};3}_{-\frac{1}{2}} &= 2^{\frac{1}{2}}(p_z \bar z^2 + p_{\bar z} z^2) = px(x^2 - y^2) - 2xyp_y && \text{(6.83c)}\\
{}^3\mathcal{C}^{\frac{3}{2};3}_{-\frac{3}{2}} &= 2^{\frac{1}{2}}(z^3 + \bar z^3) = x^3 - 3xy^2 && \text{(6.83d)}
\end{aligned}
$$

alternatively one can find the basis by descending polynomial ${}^3\mathcal{C}^{3/2;3}_{3/2}$. The basis of $U^{-}_{3,3,3/2}$ takes

$$
\begin{aligned}
{}^3\mathcal{S}^{\frac{3}{2};3}_{\frac{3}{2}} &= -\mathrm{i}2^{\frac{1}{2}}\left({}^3\mathcal{P}^{\frac{3}{2};3}_{\frac{3}{2}} - {}^3\mathcal{P}^{\frac{3}{2};-3}_{\frac{3}{2}}\right) && \text{(6.84a)}\\
&= -\mathrm{i}\sqrt{2}(p_z^3 - p_{\bar z}^3) = 3p_x^2 p_y - p_y^3 &&\\
{}^3\mathcal{S}^{\frac{3}{2};3}_{\frac{1}{2}} &= -\mathrm{i}2^{\frac{1}{2}}(\bar z p_z - z p_{\bar z}) = y(p_x^2 - p_y^2) + 2xp_x p_y && \text{(6.84b)}\\
{}^3\mathcal{S}^{\frac{3}{2};3}_{-\frac{1}{2}} &= -\mathrm{i}2^{\frac{1}{2}}(p_z \bar z^2 - p_{\bar z} z^2) = p_y(x^2 - y^2) + 2xyp_x && \text{(6.84c)}\\
{}^3\mathcal{S}^{\frac{3}{2};3}_{-\frac{3}{2}} &= -\mathrm{i}2^{\frac{1}{2}}(z^3 - \bar z^3) = 3x^2 y - y^3 && \text{(6.84d)}
\end{aligned}
$$

Hence,

$$
\begin{aligned}
U^{+}_{3,3,\frac{3}{2}} &= < px^3 - 3p_x p_y^2, x(p_x^2 - p_y^2) - 2yp_x p_y, px(x^2 - y^2) - 2xyp_y, x^3 - 3xy^2 > && \text{(6.85a)}\\
U^{-}_{3,3,\frac{3}{2}} &= < 3p_x^2 p_y - p_y^3, y(p_x^2 - p_y^2) + 2xp_x p_y, p_y(x^2 - y^2) + 2xyp_x, 3x^2 y - y^3 > && \text{(6.85b)}
\end{aligned}
$$

Now we present the results for the other subspaces.

$$
U^{+}_{3,1,\frac{1}{2}} = < p_x L_z, x L_z > \qquad U^{-}_{3,1,\frac{1}{2}} = < p_y L_z, y L_z > \tag{6.86}
$$

$$
\begin{aligned}
U^{+}_{3,1,\frac{3}{2}} &= < p_x \boldsymbol{p}^2, \frac{1}{3} x \boldsymbol{p}^2 + \frac{2}{3} p_x \boldsymbol{qp}, \frac{1}{3} p_x \boldsymbol{q}^2 + \frac{2}{3} x \boldsymbol{qp}, x \boldsymbol{q}^2 > && \text{(6.87a)}\\
U^{-}_{3,1,\frac{3}{2}} &= < p_y \boldsymbol{p}^2, \frac{1}{3} y \boldsymbol{p}^2 + \frac{2}{3} p_y \boldsymbol{qp}, \frac{1}{3} p_y \boldsymbol{q}^2 + \frac{2}{3} y \boldsymbol{qp}, y \boldsymbol{q}^2 > && \text{(6.87b)}
\end{aligned}
$$

Polynomials of the forth order

The procedure is except case $l=0$ similar as in case of the polynomials of third order. We will present only the results

$U_{4,4,2}=U^{+}_{4,4,2}\oplus U^{-}_{4,4,2}$, where

$$
\begin{aligned}
{}^{4}\mathcal{C}^{2;4}_{2} &= (p_x^2-p_y^2)^2-4p_x^2p_y^2 && \text{(6.88a)}\\
{}^{4}\mathcal{C}^{2;4}_{1} &= (xp_x-yp_y)(px^2-p_y^2)-2p_xp_y(xp_y+yp_x) && \text{(6.88b)}\\
{}^{4}\mathcal{C}^{2;4}_{0} &= (x^2-y^2)(p_x^2-p_y^2)-4xyp_xp_y && \text{(6.88c)}\\
{}^{4}\mathcal{C}^{2;4}_{-1} &= (xp_x-yp_y)(x^2-y^2)-2xy(xp_y+yp_x) && \text{(6.88d)}\\
{}^{4}\mathcal{C}^{2;4}_{-2} &= (x^2-y^2)^2-4x^2y^2 && \text{(6.88e)}
\end{aligned}
$$

is bases of $U^{+}_{4,4,2}$ and polynomials

$$
\begin{aligned}
{}^{4}\mathcal{S}^{2;4}_{2} &= 4p_xp_y(p_x^2-p_y^2) && \text{(6.89a)}\\
{}^{4}\mathcal{S}^{2;4}_{1} &= (xp_y+yp_x)(p_x^2-p_y^2)+2p_xp_y(xp_x-yp_y) && \text{(6.89b)}\\
{}^{4}\mathcal{S}^{2;4}_{0} &= 2(xp_x-yp_y)(xp_y+yp_x) && \text{(6.89c)}\\
{}^{4}\mathcal{S}^{2;4}_{-1} &= (xp_y+yp_x)(x^2-y^2)+2xy(xp_x-yp_y) && \text{(6.89d)}\\
{}^{4}\mathcal{S}^{2;4}_{-2} &= 4xy(x^2-y^2) && \text{(6.89e)}
\end{aligned}
$$

form bases of $U^{-}_{4,4,2}$.

The subspace $U_{4,2}$ is formed from subspaces

$$
\begin{aligned}
U^{+}_{4,2,2} &= <(p_x^2-p_y^2)\boldsymbol{p}^2, xp_x^3-yp_y^3, (xp_x-yp_y)\boldsymbol{qp}, x^3p_x-y^3p_y, (x^2-y^2)\boldsymbol{q}^2> && \text{(6.90a)}\\
U^{-}_{4,2,2} &= <2p_xp_y\boldsymbol{p}^2, \frac{1}{2}\boldsymbol{p}^2(xp_y+yp_x)+p_xp_y\boldsymbol{qp}, (xp_y+yp_x)\boldsymbol{qp}, && \text{(6.90b)}\\
&\quad \frac{1}{2}(xp_y+yp_x)\boldsymbol{q}^2+xy\boldsymbol{qp}, 2xy\boldsymbol{q}^2>
\end{aligned}
$$

$$
\begin{aligned}
U^{+}_{4,2,1} &= <(p_x^2-p_y^2)L_z, (xp_x-yp_y)L_z, (x^2-y^2)L_z> && \text{(6.91a)}\\
U^{-}_{4,2,1} &= <2p_xp_yL_z, (xp_y+yp_x)L_z, 2xyL_z> && \text{(6.91b)}
\end{aligned}
$$

The subspace belonging to $l=0$ is formed from irreducible subspaces

$$
U_{4,0,2} = <(\boldsymbol{p}^2)^2, \boldsymbol{p}^2\boldsymbol{qp}, \frac{1}{3}(\boldsymbol{p}^2\boldsymbol{q}^2+2(\boldsymbol{qp})^2), \boldsymbol{q}^2\boldsymbol{qp}, (\boldsymbol{q}^2)^2> \qquad \text{(6.92a)}
$$

$$U_{4,0,1} = < \boldsymbol{p}^2 L_z, \boldsymbol{qp} L_z, \boldsymbol{q}^2 L_z > \tag{6.92b}$$

$$U_{4,0,0} = < L_z^2 > \tag{6.92c}$$

6.8 Decomposition of polynomial with respect to $\mathcal{M}_1$

As we showed before the irreducible subspaces in real polynomial subspace according to action of $\mathfrak{h}_2$ are also invariant with respect to

$$\mathcal{M}_1 = e^{:g_2:}, \qquad g_2 \in \mathfrak{h}_2. \tag{6.93}$$

Moreover, if $B(z) \neq 0$ using (11) and (19)

$$g_2 = a(z)\boldsymbol{p}^2 + b(z)\boldsymbol{qp} + c(z)\boldsymbol{q}^2 + d(z)L_z \tag{6.94}$$

where each coefficient is nonzero, these invariant subspaces are irreducible. The decomposition into irreducible subspaces is then described by (82). Now we can easily find the physical meaning of numbers that characterize the bases vector of irreducible subspaces.

First we will show the meaning of number l. In complex polynomial space it determines the eigenvalue of L_z, ie.

$$\hat{L}_z \ {}^n\mathcal{P}_m^{j;l} = \mathrm{i}l \ {}^n\mathcal{P}_m^{j;l} \tag{6.95}$$

the meaning of l cannot be found in the real polynomial because except the axial symmetric polynomials there are no eigenvectors of L_z. Let us consider polynomial

$${}^n\mathcal{C}_m^{j;l} = 2^{j-1}(\ {}^n\mathcal{P}_m^{j;l} + \ {}^n\mathcal{P}_m^{j;-l}) \tag{6.96}$$

which according to the action of $\exp(\varphi : L_z :)$ takes form

$$\begin{aligned} \exp(\varphi : L_z :) \ {}^n\mathcal{C}_m^{j;l} &= 2^{j-1}(e^{\varphi : L_z : \ {}^n\mathcal{P}_m^{j;l}} + e^{\varphi : L_z : \ {}^n\mathcal{P}_m^{j;-l}}) = \\ &= 2^{j-1}(e^{\mathrm{i}\varphi l \ {}^n\mathcal{P}_m^{j;l}} + e^{-\mathrm{i}\varphi l \ {}^n\mathcal{P}_m^{j;-l}}) \end{aligned} \tag{6.97}$$

In case of $\varphi l = 2\pi k$, the polynomial ${}^n\mathcal{C}_m^{j;l}$ is invariant according to Lie transformation $\exp(\varphi : L_z :)$. This transformation represents the rotation in phase space around the optical axis about angle $\varphi = 2\pi k/l$. The polynomials ${}^n\mathcal{C}_m^{j;l}$ and ${}^n\mathcal{S}_m^{j;l}$ remained unchanged when the phase space is rotated around the origin obout angle $2\pi k/l$.

The next interesting characteristic of homogeneous polynomials is eigenvalue m of Lie operator $\hat{a}_0$. The operator a_0 generates Lie transformation $\exp(\tau : a_0 :)$ which acts as pure magnification in four dimensional phase space,

$$\exp(\tau : a_0 :) \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} = \exp(\tau : \boldsymbol{qp} :) \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} e^{-\tau}\boldsymbol{q} \\ e^{\tau}\boldsymbol{p} \end{pmatrix} \tag{6.98}$$

Thus, the value m describes how the influence of aberrations changes with magnification, or more trivial it expresses excess of $\boldsymbol{p}$'s over $\boldsymbol{q}$'s, m is known as Seidel weight [21]. In practical calculations the most important are aberrations with the highest weight because they contain just p_x or p_y and their influence does not change with distance from the axis.

The eigenvalue j of operator $\hat{a}^2$ has the worst explained meaning. It expresses the order of skewness variable $L_z = xp_y - yp_x$ in the homogeneous polynomial ${}^n\mathcal{C}_m^{j;l}$ which takes $n/2 - j$. In the axial symmetric case, when the order of L_z is odd the polynomial is not invariant under the discrete space reflection $x \to -x$, $p_x \to -p_x$, $y \to y$, $p_y \to p_y$ or $y \to -y$, $p_y \to -p_y$, $x \to x$, $p_x \to p_x$ respectively and the aberrations that it describes are anisotropic.

6.9 The third order axial symmetric aberrations

The third order axial symmetric aberrations are described by the Lie transformation $\exp(: g_4 :)$, where $g_4 \in V_{4,0}$, ie.

$$\begin{aligned} g_4 = &-\frac{C}{4}\ {}^4\mathcal{C}_2^{2;0} - K\ {}^4\mathcal{C}_1^{2;0} - \frac{\alpha}{2}\ {}^4\mathcal{C}_0^{2;0} - \frac{\beta}{2}\ {}^4\mathcal{C}_0^{0;0} - D\ {}^4\mathcal{C}_{-1}^{2;0} - \frac{E}{4}\ {}^4\mathcal{C}_{-2}^{2;0} \\ &- k\ {}^4\mathcal{C}_1^{1;0} - 2a\ {}^4\mathcal{C}_0^{1;0} - d\ {}^4\mathcal{C}_{-1}^{1;0} \end{aligned} \tag{6.99}$$

This type of aberration is well described and classified, we will mention the standard meaning of each member in (99). The first term $-\frac{C}{4}\ {}^4\mathcal{C}_2^{2;0}$ describes the spherical aberration

$$\exp(-\frac{C}{4} :\ {}^4\mathcal{C}_2^{2;0} :)\boldsymbol{q} = \exp(-\frac{C}{4} : (\boldsymbol{p}^2)^2 :)\boldsymbol{q} = \boldsymbol{q} + C\boldsymbol{p}^2\boldsymbol{p} + o(5) \tag{6.100}$$

the second one describes the coma

$$\exp(-K :\ {}^4\mathcal{C}_1^{2;0} :)\boldsymbol{q} = \exp(-K : \boldsymbol{p}^2\boldsymbol{qp} :)\boldsymbol{q} = \boldsymbol{q} + K(\boldsymbol{p}^2\boldsymbol{q} + 2(\boldsymbol{qp})\boldsymbol{p}) + o(5). \tag{6.101}$$

The polynomial $D\ {}^4\mathcal{C}_{-1}^{2;0}$ generates the distorsion

$$\exp(-D :\ {}^4\mathcal{C}_{-1}^{2;0} :)\boldsymbol{q} = \exp(-D : \boldsymbol{q}^2\boldsymbol{qp} :)\boldsymbol{q} = \boldsymbol{q} + D\boldsymbol{q}^2\boldsymbol{q} + o(5). \tag{6.102}$$

and the polynomial ${}^4\mathcal{C}_{-2}^{2;0}$ has no effect on the change of coordinates, it affects the final directives.

The effect of ${}^4\mathcal{C}_0^{2;0}$ and ${}^4\mathcal{C}_0^{0;0}$ is necessary to describe together, they generate the astigmatism and the field curvature. One can find two definitions of the astigmatism, the first one [3] is defined as

$$\exp(-A:\ {}^4\mathcal{C}_0^{2;0} - \frac{1}{3}\ {}^4\mathcal{C}_0^{0;0}:)\boldsymbol{q} = \exp(-A:(\boldsymbol{qp})^2:)\boldsymbol{q} = \boldsymbol{q} + 2A(\boldsymbol{qp})\boldsymbol{q} + o(5) \tag{6.103}$$

the second one used eq. in [1] reads

$$\exp(-A:\frac{1}{2}\ {}^4\mathcal{C}_0^{2;0} - \frac{2}{3}\ {}^4\mathcal{C}_0^{0;0}:)\boldsymbol{q} = \exp(-A:(\boldsymbol{qp})^2 - \frac{1}{2}\boldsymbol{q}^2\boldsymbol{p}:^2)\boldsymbol{q} = \tag{6.104}$$
$$= \boldsymbol{q} + A(2(\boldsymbol{qp})\boldsymbol{q} - \boldsymbol{q}^2\boldsymbol{p}) + o(5)$$

The field curvature is defined

$$\exp(-F:\frac{1}{2}\ {}^4\mathcal{C}_0^{2;0} + \frac{1}{3}\ {}^4\mathcal{C}_0^{0;0}:)\boldsymbol{q} = \exp(-\frac{1}{2}F:\boldsymbol{q}^2\boldsymbol{p}^2:)\boldsymbol{q} = \boldsymbol{q} + F\boldsymbol{p}^2\boldsymbol{q} + o(5) \tag{6.105}$$

Both these aberrations mix effect of action of polynomials ${}^4\mathcal{C}_0^{2;0}$ and ${}^4\mathcal{C}_0^{0;0}$. In fact these polynomials differ only in value of spin, other characteristics are identical.

The polynomials from the space $V_{4,0,1}$ are not invariant according to reflection with respect to any plane, that contains the optical axis. Thus, the aberrations that are described by these polynomials are anisotropic. The first is anisotropic koma

$$\exp(-k:\ {}^4\mathcal{C}_1^{1;0}:)\boldsymbol{q} = \exp(-k:L_z\boldsymbol{p}^2:)\boldsymbol{q} = \boldsymbol{q} + k(2L_z\boldsymbol{p} - \boldsymbol{p}^2\hat{J}_2\boldsymbol{q}) + o(5) \tag{6.106}$$

the second one is the anisotropic astigmatism

$$\exp(-2a:\ {}^4\mathcal{C}_0^{1;0}:)\boldsymbol{q} = \exp(-2a:L_z\boldsymbol{pq}:)\boldsymbol{q} = \boldsymbol{q} + 2a(L_z\boldsymbol{q} - \boldsymbol{qp}\hat{J}_2\boldsymbol{q}) + o(5) \tag{6.107}$$

and the last is the anisotropic distorsion

$$\exp(-d:\ {}^4\mathcal{C}_{-1}^{1;0}:)\boldsymbol{q} = \exp(-d:L_z\boldsymbol{q}^2:)\boldsymbol{q} = \boldsymbol{q} - d\boldsymbol{q}^2\hat{J}_2\boldsymbol{q} + o(5). \tag{6.108}$$

These coefficients have no analogue in light optics; their existence is caused by presence of magnetic field [1]

Let us say more about the structure of aberration polynomials. They are represent by the third order homogeneous polynomials as the results of poisson bracket $[V_{4,0}, \boldsymbol{q}]$ and because each $g \in V_{4,0}$ fulfills

$$\hat{L}_z[g,\boldsymbol{q}] = [\hat{L}_z g,\boldsymbol{q}] + [g,\hat{L}_z\boldsymbol{q}] = [g,\boldsymbol{q}] \tag{6.109}$$

$[V_{4,0}, \boldsymbol{q}] \in V_{3,1}$. The polynomial space $V_{3,1}$ is formed by 12 polynomials and considering the phase space dimension it takes 12^4 possible combinations. However, we showed that there are just nine independent aberration coefficients. This is caused by the fact that the transformation is canonical and can be described by $g_4 \in V_{4,0}$ like Lie transformation $\exp(:g_4:)$. Hence, general axial symmetric aberration polynomial reads

$$\begin{aligned}\begin{pmatrix}\tilde{\boldsymbol{q}}\\ \tilde{\boldsymbol{p}}\end{pmatrix} = \exp(:g_4:)\begin{pmatrix}\boldsymbol{q}_o\\ \boldsymbol{p}_o\end{pmatrix} = \begin{pmatrix}\boldsymbol{q}_o\\ \boldsymbol{p}_o\end{pmatrix} + C\begin{pmatrix}\boldsymbol{p}_o^2\boldsymbol{p}_o\\ 0\end{pmatrix} + K\begin{pmatrix}2(\boldsymbol{q}_o\boldsymbol{p}_o)\boldsymbol{p}_o + \boldsymbol{p}_o^2\boldsymbol{q}_o\\ -\boldsymbol{p}_o^2\boldsymbol{p}_o\end{pmatrix} + \\ 2A\begin{pmatrix}(\boldsymbol{q}_o\boldsymbol{p}_o)\boldsymbol{q}_o\\ -(\boldsymbol{q}_o\boldsymbol{p}_o)\boldsymbol{p}_o\end{pmatrix} + F\begin{pmatrix}\boldsymbol{q}_o^2\boldsymbol{p}_o\\ -\boldsymbol{p}_o^2\boldsymbol{q}_o\end{pmatrix} + D\begin{pmatrix}\boldsymbol{q}_o^2\boldsymbol{q}_o\\ -2(\boldsymbol{q}_o\boldsymbol{p}_o)\boldsymbol{q}_o - \boldsymbol{q}_o^2\boldsymbol{p}_o\end{pmatrix} + E\begin{pmatrix}0\\ -\boldsymbol{q}_o^2\boldsymbol{q}_o\end{pmatrix} + \\ + k\begin{pmatrix}L_z\boldsymbol{p}_o - p_o^2\hat{J}_2\boldsymbol{q}_o\\ -p_o^2\hat{J}_2\boldsymbol{p}_o\end{pmatrix} + 2a\begin{pmatrix}L_z\boldsymbol{q}_o - (\boldsymbol{q}_o\boldsymbol{p}_o)\hat{J}_2\boldsymbol{q}_o\\ -L_z\boldsymbol{q}_o - \boldsymbol{q}_o\boldsymbol{p}_o\hat{J}_2\boldsymbol{p}_o\end{pmatrix} - d\begin{pmatrix}\boldsymbol{q}_o^2\hat{J}_2\boldsymbol{q}_o\\ 2L_z\boldsymbol{q}_o + \boldsymbol{q}_o^2\hat{J}_2\boldsymbol{q}_o\end{pmatrix}\end{aligned} \tag{6.110}$$

6.10 Reflection symmetry

We have seen that the reflection symmetry has interesting consequences in properties of aberration in axial symmetric case. Hence, we will describe the reflection symmetry of the aberrations polynomials in general case.

Let us denote $\hat{\Omega}_\alpha$ the reflection with respect to the plane $-x\sin\alpha + y\cos\alpha = 0$, the plane that arises from the plane xz by the rotation around the z-axis about the angle α. Such a transformation can be described by composition of transformations

$$\Omega_\alpha = \hat{R}_{-\alpha}\hat{\Omega}_0\hat{R}_\alpha \tag{6.111}$$

Now we find the transformation property for the complex polynomial ${}^{n}\mathcal{P}_m^{j;l}$.

It is easy to see that $\hat{\Omega}_0 L_z = -L_z$; hence,

$$\hat{\Omega}_0\ {}^{n}\mathcal{P}_m^{j;l} = \hat{\Omega}_0(L_z^{\frac{n}{2}-j}\ {}^{2j}\mathcal{P}_m^{j;l}) = (-1)^{\frac{n}{2}-j}L_z^{\frac{n}{2}-j}\hat{\Omega}_0\ {}^{2j}\mathcal{P}_m^{j;l} \tag{6.112}$$

The transformation $\hat{\Omega}_0$, which in fact changes the sign at y and p_y, is equivalent to complex conjugation for the complex polynomials ${}^{2j}\mathcal{P}_m^{l;j}$. Hence, using (58)

$$\hat{\Omega}_0\ {}^{2j}\mathcal{P}_m^{j;l} = {}^{2j}\mathcal{P}_m^{j;-l} \tag{6.113}$$

and combining previous results we find

$$\hat{\Omega}_0\ {}^{n}\mathcal{P}_m^{j;l} = (-1)^{\frac{n}{2}-j}L_z^{\frac{n}{2}-j}\ {}^{2j}\mathcal{P}_m^{j;-l} = (-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{P}_m^{j;-l}. \tag{6.114}$$

The transformation property of ${}^{n}\mathcal{P}_m^{j;l}$ according to $\hat{\Omega}_\alpha$ can be found

$$\hat{\Omega}_\alpha\ {}^{n}\mathcal{P}_m^{j;l} = \hat{R}_{-\alpha}\hat{\Omega}_0\hat{R}_\alpha\ {}^{n}\mathcal{P}_m^{j;l} = \hat{R}_{-\alpha}\hat{\Omega}_0 e^{\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;l} = (-1)^{\frac{n}{2}-j}e^{\mathrm{i}l\alpha}\hat{R}_{-\alpha}\ {}^{n}\mathcal{P}_m^{j;-l} = \\ = (-1)^{\frac{n}{2}-j}e^{2\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;-l} \tag{6.115}$$

There are two interesting cases, the first one $\alpha = k\pi/l$ then

$$\hat{\Omega}_{k\frac{\pi}{l}}\ {}^{n}\mathcal{P}_m^{j;l} = (-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{P}_m^{j;-l} \tag{6.116}$$

and the second $\alpha = \pi/2l + k\pi/l$ then

$$\hat{\Omega}_{\frac{\pi}{2l}+k\frac{\pi}{l}}\ {}^{n}\mathcal{P}_m^{j;l} = -(-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{P}_m^{j;-l}. \tag{6.117}$$

These properties can be used for description of transformation properties of real polynomials. First we will focus our attention to polynomial ${}^{n}\mathcal{C}_m^{j;l}$

$$\hat{\Omega}_\alpha\ {}^{n}\mathcal{C}_m^{j;l} = \hat{\Omega}_\alpha 2^{j-1}(\ {}^{n}\mathcal{P}_m^{j;l} + \ {}^{n}\mathcal{P}_m^{j;-l}) = (-1)^{\frac{n}{2}-l}(e^{2\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;-l} + e^{-2\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;l}) \tag{6.118}$$

hence,

$$\hat{\Omega}_{k\frac{\pi}{l}}\ {}^{n}\mathcal{C}_m^{j;l} = \ \ (-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{C}_m^{j;l} \tag{6.119a}$$

$$\hat{\Omega}_{\frac{\pi}{2l}+k\frac{\pi}{l}}\ {}^{n}\mathcal{C}_m^{j;l} = -(-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{C}_m^{j;l} \tag{6.119b}$$

and similarly for the polynomial ${}^{n}\mathcal{S}_m^{j;l}$

$$\hat{\Omega}_\alpha\ {}^{n}\mathcal{S}_m^{j;l} = \hat{\Omega}_\alpha \mathrm{i}2^{j-1}(\ {}^{n}\mathcal{P}_m^{j;l} - \ {}^{n}\mathcal{P}_m^{j;-l}) = \mathrm{i}(-1)^{\frac{n}{2}-l}(e^{2\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;-l} - e^{-2\mathrm{i}l\alpha}\ {}^{n}\mathcal{P}_m^{j;l}) \tag{6.120}$$

hence,

$$\hat{\Omega}_{k\frac{\pi}{l}}\ {}^{n}\mathcal{S}_m^{j;l} = -(-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{S}_m^{j;l} \tag{6.121a}$$

$$\hat{\Omega}_{\frac{\pi}{2l}+k\frac{\pi}{l}}\ {}^{n}\mathcal{S}_m^{j;l} = \ \ (-1)^{\frac{n}{2}-j}\ {}^{n}\mathcal{S}_m^{j;l} \tag{6.121b}$$

The previous equation completely describes the reflection symmetry of polynomials. Unfortunately, from the reflection symmetry of the optical system it is not possible to find the refraction symmetry of the aberration coefficients. It is caused by the anisotropic effect magnetic field, which mixes the polynomials ${}^{n}\mathcal{C}_m^{j;l}$ with ${}^{n}\mathcal{S}_m^{j;l}$. Similarly we can proceed only in electrostatic case or in the light optics.

7 Conclusion

The mathematical background of the Lie algebra method is the canonical perturbation theory. There exists a significant relationship between the factorization theorem and the canonical perturbation theory which is shown in the part 5.4, where we extended the Lie algebra method to the parameterization by the position in the object and aperture plane which is often used in the electron microscopy.

In part 5.6. all described analytical perturbation methods were applied to a simple example of a round magnetic lens. The calculation is not new but the reason for it is to compare the different approaches of the perturbation method. The comparison shows that even though the formulation of the trajectory method is very straightforward, the practical application is very demanding. On the other hand, there are no significant differences in complexity between the eikonal and the Lie algebra method.

During the next study I solved an issue of advisable classification of the aberration polynomials and their relationship (chapter 6). It was shown that the way of classification is connected to the form of the paraxial approximation – it affects the relationship among the aberration coefficients. Because of the complexity of general system classification, we aimed the effort to the classification of stigmatic systems. The classification of the aberration polynomials is described as a representation of the Lie group adjoint to the algebra of the quadratic polynomials that were determined by the quadratic part of Hamiltonian. This representation is explicitly presented. The symmetry of aberration coefficients according to the reflection is also discussed.

Periodical systems were the subject of the next study. A typical system is an accelerator. We investigated a method for determination of the normal form of Hamiltonian which is used for description of the global stability of the system. These results were published in Nuclear Instruments and Method in Physical Research [34]. Unfortunately, this subject is not mentioned in the thesis as the length of the work would grow too much. Furthermore, the article that is connected to the thesis provides the basic orientation.

The properties of the analytical perturbation methods were tested on the case of a round magnetic lens. We could not find any more simple system. For example, trivial systems such as top-hat field is very simple in paraxial approximation but far from trivial for calculations of aberrations. The methods for systems with the straight line optical axis and periodical systems were compared separately.

In general, in case of systems with the straight optical axis, it can be said that the trajectory method is applicable for the first perturbation. It means that either calculation of the second order of aberration for systems that contain dipole or sextupole field or the calculation of the third order of aberrations for systems that do not contain such fields. In case of the second and higher perturbation, the method is rather lengthy. Moreover, the method provides no view into the structure of aberration coefficients like mutual dependency or independency of the aberration coefficients. The aberration integrals of the vanishing coefficients have a form that does not seem to lead to zero from the first point of view. We must use integration by parts to show that such coefficients really vanish.

On the other hand, the eikonal method and the Lie algebra method are much more advisable for the calculations of higher order aberrations. As both methods are formed by using symplectic structure of the phase space, the relationship among the aberration coefficients is much more visible. However, whereas the procedure of derivation of the second order perturbation relations (5.72) is not transparent, the calculation of higher order perturbation in the Lie algebra method is a straightforward procedure.

Even though the numerical values of the aberration coefficients do not have to be dependent on the method used, it does not mean that the form of derived aberration integrals is also identical. However, they can be transformed into the identical form by using integration by parts. Moreover, the Lie algebra method provides insight into the structure of the aberration polynomials — by using symplectic classification we can describe the relationship among aberrations and find out which fields influence a given aberration coefficient.

While the Lie algebra method is not often used for description of systems with the straight optical axis, the situation is completely different in description of the periodical systems. The Lie algebra method is the most commonly used method in accelerator physics. This is caused by the different form of the problems solved. The global stability of the system is the most important property that is studied. This problem is connected with the theory of dynamic systems in which the Hamiltonian formalism is very common and powerful tool. The stability of the phase space according to the transfer map is investigated and the normal form method is the standard tool used for the description of the stability of the system [19, 35]. Nevertheless, it cannot be said that the use of the Lie algebra method is really necessary.

Finally, we can say that the trajectory method is not advisable for calculation of higher order of aberration coefficients. However, I was not able to show any great differences between the eikonal method and the Lie algebra method. I showed that introduction of the Lie algebra structure into the polynomial space brings some advantages, mostly used in the aberrations classification or in the study of periodical systems, but the calculation of the aberration coefficients is still a lengthy work that cannot be done without the use of computer programs for symbolic computation like MAPLE or MAXIMA.

8 Appendix: The Hamiltonian transformation

Although the transformation rule for the Hamiltonian at a z-dependent canonical transformation has been derived by Cary [12], for completeness it will be summarized here. We will start from the rule valid in z-independent case and the extension to z-dependent case will be derived using the extended phase space formalism.

Let us consider two canonical coordinate systems $\boldsymbol{w}$, $\tilde{\boldsymbol{w}}$ with 2 degrees of freedom and an s-dependent Lie transformation $\boldsymbol{w} = e^{:g(\tilde{\boldsymbol{w}},z):}\tilde{\boldsymbol{w}}$ describing their relationship $\boldsymbol{w} = e^{:g(\tilde{\boldsymbol{w}},z):}\tilde{\boldsymbol{w}}$. Although the transformation rule for Hamiltonian in z-independent case does not differ from the functions' one, in this case it might not be obvious. Fortunately, each canonical z-dependent system with two degrees of freedom is equivalent to the canonical z-independent system with three degrees of freedom known as the extended phase space [10], in which z is one of canonical variables with canonical conjugate momentum p_z. A vector in the extended phase space then reads $\boldsymbol{W} = (\boldsymbol{w}, z, p_z)$ and the Hamiltonian takes form $\bar{H} = H + p_z$. The canonical transformation $e^{:g(\tilde{\boldsymbol{w}},z):}$ is represented by a canonical transformation $e^{:g(\tilde{\boldsymbol{W}}):_E}$ which does not depend on independent variable t in the extended phase space. Notation for the Lie operator in the extended phase space $:f:_E$ – with the Poisson bracket defined according to $[g,h]_E = [g,h] + \frac{\partial g}{\partial z}\frac{\partial h}{\partial p_z} - \frac{\partial g}{\partial p_z}\frac{\partial h}{\partial z}$ were used.

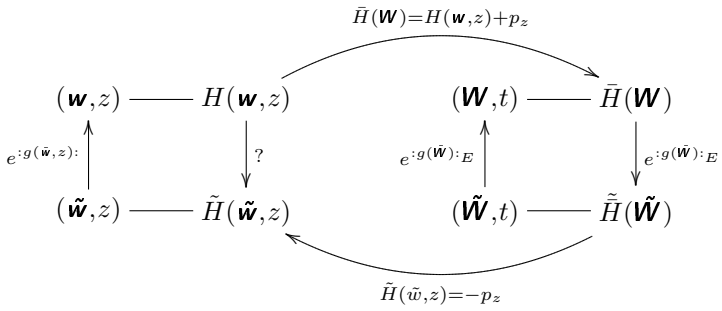
The transformed Hamiltonian then reads

$$\tilde{\bar{H}}(\tilde{\boldsymbol{W}}) = e^{:g(\tilde{\boldsymbol{W}}):_E}\bar{H}(\tilde{\boldsymbol{W}}) \tag{8.1}$$

and using the coordinates in the original phase space one can write

$$\begin{aligned}
\tilde{H}(\tilde{\boldsymbol{w}},s) + \tilde{p}_z &= e^{:g(\tilde{\boldsymbol{w}},s):_E}(H(\tilde{\boldsymbol{w}},s) + p_z) = \\
&= e^{:g(\tilde{\boldsymbol{w}},z):}H(\tilde{\boldsymbol{w}},z) + \frac{\partial g}{\partial z} + \frac{1}{2}[g,\frac{\partial g}{\partial z}] + \frac{1}{6}[g,[g,\frac{\partial g}{\partial z}]] + \cdots \tilde{p}_z \\
\tilde{H}(\tilde{\boldsymbol{w}},z) &= e^{:g(\tilde{\boldsymbol{w}},z):}H(\tilde{\boldsymbol{w}},z) + \int_0^1 \mathrm{d}\theta e^{\theta:g:(\tilde{\boldsymbol{w}},z)}\frac{\partial g(\tilde{\boldsymbol{w}},z)}{\partial z},
\end{aligned} \tag{8.2}$$

what is the sought for expression. The situation is described by the diagram



(8.3)

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