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FAKULTA STROJNÍHO INŽENÝRSTVÍ
FACULTY OF MECHANICAL ENGINEERING

ÚSTAV FYZIKÁLNÍHO INŽENÝRSTVÍ
INSTITUTE OF PHYSICAL ENGINEERING

VADY SEŘÍZENÍ HEXAPÓLOVÉHO KOREKTORU SFÉRICKÉ VADY, JEJICH ANALÝZA A KOREKCE

PARASITIC ABERRATIONS OF THE HEXAPOLE CORRECTOR OF SPHERICAL ABERRATION - ANALYSIS AND CORRECTIONS

DIPLOMOVÁ PRÁCE
MASTER'S THESIS

AUTOR PRÁCE Bc. et Bc. Jan Sopoušek
AUTHOR

VEDOUCÍ PRÁCE Mgr. Tomáš Radlička, Ph.D.
SUPERVISOR

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Zadání diplomové práce

Ústav: Ústav fyzikálního inženýrství
Student: **Bc. Jan Sopoušek**
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Vedoucí práce: **Mgr. Tomáš Radlička, Ph.D.**
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Ředitel ústavu Vám v souladu se zákonem č.111/1998 o vysokých školách a se Studijním a zkušebním řádem VUT v Brně určuje následující téma diplomové práce:

Vady seřízení hexapólového korektoru sférické vady, jejich analýza a korekce

Stručná charakteristika problematiky úkolu:

Velikost sférické vady objektivu elektronového mikroskopu významně ovlivňuje jeho rozlišení. V případě systémů s energií primárních elektronů vyšší ne 10 keV se jako jediná realizovatelná cesta korekce jeví využití multipólových korektorů. Standarní systémy používají hexapólové a kvadrupólové-oktupólové korektory. Ačkoli už byl základní princip těchto korektorů publikován a existují komerční realizace takovýchto systémů, relativně málo pozornosti je v publikacích věnováno korekcím vad seřízení, které jsou pro správnou funkčnost korektoru stěžejní.

Cíle diplomové práce:

• Seznámit se se základní funkčností hexapólového korektoru sférické vady
• Seznámit se s vhodnými metodami výpočtu optických vad a jejich aplikace na systém s korektorem
• Analýza vad seřízení a parazitických vad a popis jejich vlivu na výsledné rozlišení systému pomoci difrakčních integrálů.
• Analýza metod korekce parazitických vad v systému s korektorem

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L. S.

prof. RNDr. Tomáš Šikola, CSc. ředitel ústavu	doc. Ing. Jaroslav Katolický, Ph.D. děkan fakulty

Abstrakt
Jednou z možností korekce sférické vady v elektronové mikroskopii je hexapólový korektor. Ačkoliv samotný princip korekce je poměrně dobře v literatuře popsán, jen relativně málo je věnováno samotnému seřízení hexapólového korektoru, jež je stěžejní pro správnou funkčnost. Práce je věnována analytickému rozboru vad seřízení a jejich vlivu na rozlišení obrazu za použití metody eikonálu a aberačních integrálů. Je ukázáno, že nejdůležitější roli v parazitických aberací hrají výchylky a náklon hexapólů. V závěru je pak popsáno, jakým způsobem je třeba hexapólový korektor seřídit pro odstranění parazitických vad.

Klíčová slova
Elektronová mikroskopie, Aberace, Hexapólový korektor

Summary
One of the option of spherical aberration correction in electron microscopy is the hexapole corrector. Although the principle of the corrector is described in literature quite elaborately the adjustment of the corrector, which is crucial for its functionality, is studied just briefly. The thesis is dedicated to the analytic analysis of parasitic aberrations and its influence on resolution of an image by the Eikonal method and aberration integrals. It is shown that off-axial shifts and tilts play the major role in parasitic aberrations. In the end the procedure of adjustment of the hexapole corrector for elimination of parasitic aberrations is described.

Keywords
Electron Microscopy, Aberrations, Hexapole Corrector,

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Prohlašuji, že jsem diplomovou práci *Vady seřízení hexapólového korektoru sférické vady, jejich analýza a korekce* vypracoval samostatně pod vedením Mgr. Tomáše Radličky, Ph.D., s použitím materiálů uvedených v seznamu literatury.

Bc. et Bc. Jan Sopoušek

Děkuji mému vedoucímu Mgr. Tomášovi Radličkovi, Ph.D., za věnovaný čas, cenné rady a připomínky k diplomové práci.

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Introduction

This year, 2017, Samsung started a 10 nm technology of a semiconductor manufacturing process. This is about 100 times an atom. The requirement to have atomic resolution is therefore highly needed and not just in semiconductor industry. With high resolution techniques we can understand nature more deeply. Thanks to our ability to observe more precisely the matter, we can design new materials with higher strength, durability, lighter, more flexible. We can create new promising drugs, we have more efficient way of producing energy.

There are several techniques to measure atoms but not as versatile as electron microscopy. To achieve atomic resolution in the electron microscope one way is to increase the energy of the accelerated electrons to shorten their wavelength. This approach was often used in the past and 1 MV microscopes were built. That, however, is quite impractical because such a microscope needs a special room and is very expensive, but, above all, it creates radiation damage thus a broad spectrum of materials, such as organic materials, cannot be analysed. The current tendency is quite opposite – to use a low voltage microscope to increase interactions with electronic structure. To achieve atomic resolution at 100 keV and even lower it is necessary to use correctors.

In light optics we can deal with aberrations and dispersion by using different materials of lenses with an adequate dispersion relation and optical properties. In electron optics it is not the way how to do it. Any electromagnetic rotational symmetric lens is converging thus we cannot eliminate chromatic aberration by just a combination of those. Furthermore, since 1936 it has been known that spherical aberration of a rotational symmetric lens is always positive (derived by O. Scherzer [17]). The way to obtain negative spherical aberration and to correct chromatic aberration is either an electron mirror, which is used in Low-energy electron microscopy [18], or multipoles[8]. To reach atomic resolution we have first to deal with the spherical aberration. The chromatic aberration becomes mainly dominant if the energy of the electron is in the order of tens of electron volts. The common strategy of dealing with a polychromatic beam is to use a monochromator [19] or a corrector of chromatic aberration[22]. The chromatic aberration corrector has the advantage that a higher electron current can be used, which is especially useful, for example in Energy-dispersive X-ray spectroscopy. On the other hand the use of a monochromator is more adequate when we do high resolution spectroscopy measurements. Monochromators are presently used more often because they are cheaper and easier to construct.

The first attempt on an electrostatic multipole corrector of spherical aberration was made by R. Seeliger in 1951 based on the proposition of O. Scherzer. The design consisted of a combination of octupoles, stigmators and electrostatic cylinders. It was experimentally proved that negative spherical aberration can be achieved but at that time the corrector did not improve resolution. It was mainly because of instabilities of the mechanical parts. Later it was found that resolution of a microscope is determined by two factors – coherent aberrations caused by misalignments together with mechanical imperfections of lenses and incoherent effects of electromagnetic noise with vibrations (and nowadays a thermal noise of the used magnetic materials[20]). Throughout the next forty years multiple attempts of building correctors were made but all were destined to a failure because of technological difficulties. In 1988 a group of experts declared at a meeting in the United States that the successful realization of aberration correction was unthinkable[13].

It must be said that all of the previous designs of correctors were based on some combination of quadrupole and octupole fields. A hexapole field produces in the first approximation three-fold astigmatism thus at the beginning it was not considered for correction of spherical aberration. In the second approximation the hexapole field has the same aberration coefficients as the radial symmetric field. If we manage to cancel the three-fold astigmatism we can use it as a corrector of spherical aberration. Such a concept was first studied by H. Rose in 1981 [14]. It is the same design as is studied in this thesis – consists of two hexapoles with a lens doublet in-between. After 1990 M. Haider noticed that a hexapole corrector requires less stability tolerances than previous quadrupole/octupole correctors and together with H. Rose they built one. In 1995 it was demonstrated that the corrector works satisfactorily but the problem was with residual aberrations due to misalignments[3]. It was later solved by using a computer aid to automatically calculate these aberration coefficients and to minimize them. In 1998 the reduction of the point resolution from 0.24 nm to 0.14 nm was finally reached by the hexapole corrector of spherical aberration[5].

In 1996 an idea of the quadrupole/octupole corrector was revived by Ondrej L. Krivanek[10]. Nowadays there are two main manufacturers of the correctors – CEOS founded by J. Zach and M. Haider with its hexapole corrector and the Nion company of O.L Krivanek with its quadrupole/octupole corrector. The CEOS-like corrector was also adopted by JEOL and FEI.

The topic of this thesis is on the residual aberrations. It brings an analytical study of aberration coefficients which gives a deep insight to the origin of parasitic aberrations and what is the best solution how to eliminate them.

1. Multipole Expansion of Field

We start with a theoretical background. At first we derive the multipole expansion of an electrostatic and magnetostatic field in vacuum. The multipole expansion is derived along an optical axis in the tangential plane and provide an useful form of the field which can be used for simplified calculation.

1.1 Maxwell's Equations

We start with the Maxwell's equations in vacuum:

$$\begin{array}{rclcrcl} \nabla \cdot \boldsymbol{B} & = & 0 & & \nabla \times \boldsymbol{E} + \frac{\partial \boldsymbol{B}}{\partial t} & = & 0 \\ \nabla \cdot \boldsymbol{E} & = & \frac{\rho}{\epsilon_0} & & \nabla \times \boldsymbol{B} - \mu_0 \epsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} & = & \mu_0 \boldsymbol{j} \end{array}$$

Now we assume that any charge and current is not present in the investigated area.* We also assume that the fields are static thus they are not functions of time. Using these assumptions we get:

$$\begin{array}{ll} \nabla \cdot \boldsymbol{B} = 0 & \nabla \times \boldsymbol{E} = 0 \\ \nabla \cdot \boldsymbol{E} = 0 & \nabla \times \boldsymbol{B} = 0 \end{array}$$

We can solve the second pair of equations by introducing an electric potential Φ and a magnetic potential W such that:

$$\begin{aligned} \boldsymbol{E} &= -\nabla \Phi \\ \boldsymbol{B} &= -\nabla W \end{aligned} \tag{1.1}$$

We can find the solutions of the potentials by solving Laplace equations:

$$\begin{aligned} \Delta \Phi &= 0 \\ \Delta W &= 0 \end{aligned} \tag{1.2}$$

1.2 Vector Potential

We also need a magnetic vector potential which is defined as:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{1.3}$$

Let us derive its link to the magnetostatic potential W. We compare 1.3 with 1.1:

$$\nabla \times \boldsymbol{A} = -\nabla W \tag{1.4}$$

The vector potential is not fully determined by this equation. In fact we can choose one of its component freely. We chose it in a way such as the A_z component (it does not

*That assumption is not correct because we are dealing with an electron beam which consists of more than one electron. But if the beam current is low than we can use the assumption.

matter which one due to the symmetry) is equal to the function $f(x, y, z)$. Then we can evaluate x and y component of $\boldsymbol{A}$ from the first two equations 1.4:

$$\begin{aligned} A_x &= \int \left(-\frac{\partial W}{\partial y} + \frac{\partial f}{\partial x} \right) \mathrm{d}z + g(x, y) \\ A_y &= \int \left(\frac{\partial W}{\partial x} + \frac{\partial f}{\partial y} \right) \mathrm{d}z + h(x, y) \end{aligned} \tag{1.5}$$

Where g, h are any functions of x and y. Now we put these components to the last equation:

$$\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = -\frac{\partial W}{\partial z} \tag{1.6}$$

We obtain:

$$\int \left(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} + \frac{\partial^2 f}{\partial y \partial x} - \frac{\partial^2 f}{\partial x \partial y} \right) \mathrm{d}z + \frac{\partial h}{\partial x} - \frac{\partial g}{\partial y} = -\frac{\partial W}{\partial z} \tag{1.7}$$

If f is a smooth function and $\frac{\partial h}{\partial x} - \frac{\partial g}{\partial y} = 0$ (it is natural to choose $g = 0$, $h = 0$) we get:

$$\int \left(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} \right) \mathrm{d}z = -\frac{\partial W}{\partial z} \tag{1.8}$$

And differentiating with respect to z:

$$\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} + \frac{\partial^2 W}{\partial z^2} = 0 \tag{1.9}$$

Which is the required Laplace equation of W. In this text I will choose $A_z = 0$ †. Then x, y-components are calculated from W by:

$$\begin{aligned} A_x &= \int \left(-\frac{\partial W}{\partial y} \right) \mathrm{d}z \\ A_y &= \int \left(\frac{\partial W}{\partial x} \right) \mathrm{d}z \end{aligned} \tag{1.10}$$

1.3 Solution of Laplace Equation

We now derive the solution of the Laplace equation:

$$\Delta \Phi = 0 \tag{1.11}$$

in the form of power series. In cylindrical coordinates it looks like:

$$\frac{\partial^2 \Phi}{\partial r^2} + \frac{1}{r} \frac{\partial \Phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \Phi}{\partial \theta^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0 \tag{1.12}$$

We find the solution in the form:

$$\Phi = R(r, z) S(\theta) \tag{1.13}$$

† P. W. Hawkes[9] uses $A_z = W$ instead

Putting it into 1.12, dividing by R, S and multiplying by r^2 we get:

$$\frac{r^2}{R}\frac{\partial^2 R}{\partial r^2} + \frac{r}{R}\frac{\partial R}{\partial r} + \frac{r^2}{R}\frac{\partial^2 R}{\partial z^2} = -\frac{S''}{S} \tag{1.14}$$

Because R is only a function of r, z and S is only a function of θ the both sides of the equation have to be equal to a constant. At first we solve the equation:

$$-\frac{S''}{S} = \lambda \tag{1.15}$$

S has to be 2π-periodic thus λ is equal to a positive number. Further more the solution looks like:

$$S = e^{\mathrm{i}k\theta} \tag{1.16}$$

where k is an integer (due to 2π-periodicity). λ is thus equal to k^2.

Let us find the solution of the function $R(r, z)$. We are looking for the solution in the form of power series:

$$R(r, z) = \sum_{n=0}^{\infty} a_{n,k}(z) r^{n+s} \tag{1.17}$$

Where s is an integer. The sum starts from zero because we require finiteness of the solution on the optical axis. By putting the power of series into the equation 1.14:

$$r^2\frac{\partial^2 R}{\partial r^2} + r\frac{\partial R}{\partial r} + r^2\frac{\partial^2 R}{\partial z^2} - k^2 R = 0 \tag{1.18}$$

We get:

$$\sum_{n=0}^{\infty} a_{n,k}(z)(n+s)(n+s-1)r^{n+s} + \sum_{n=0}^{\infty} a_{n,k}(z)(n+s)r^{n+s} + \\ + \sum_{n=0}^{\infty} a_{n,k}(z)'' r^{n+s+2} - \sum_{n=0}^{\infty} a_{n,k}(z)k^2 r^{n+s} = 0 \tag{1.19}$$

We shift the index of the third sum and simplify it:

$$a_{0,k}(s^2 - k^2)r^s + a_{1,k}\left((1+s^2) - k^2\right) r^{s+1} + \\ + \sum_{n=2}^{\infty} \left[a_{n,k}\left((n+s)^2 - k^2\right) + a''_{n-2,k}\right] r^{n+s} = 0 \tag{1.20}$$

To fulfil the equation for all r each coefficient of different power of r has to be equal to zero:

$$\begin{aligned} a_{0,k}(s^2 - k^2) &= 0 \\ a_{1,k}\left((1+s^2) - k^2\right) &= 0 \\ a_{n,k}\left((n+s)^2 - k^2\right) + a''_{n-2,k} &= 0 \quad \text{for} \quad n > 2 \end{aligned} \tag{1.21}$$

From the first equation we get $s = |k|$ [‡]. Thus $a_{1,k}$ is zero and also all coefficients with odd n because we can get the recursive formula for $n > 2$:

$$a_{n,k} = -\frac{a''_{n-2,k}}{n(n+2|k|)} \tag{1.22}$$

The recursive formula can be also rewritten to the explicit form (n is replaced by $2n$):

$$a_{2n,k} = \frac{(-1)^n a_{0,k}^{(2n)} |k|!}{2^{2n} n!(n+|k|)!} \tag{1.23}$$

Bringing it all together we get the final multipole expansion of the electrostatics potential Φ:

$$\Phi = \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \frac{(-1)^n |k|!}{2^{2n} n!(n+|k|)!} \phi_k^{(2n)}(z) r^{2n+|k|} e^{\mathrm{i}k\theta} \tag{1.24}$$

Where $a_{0,k}$ was replaced by ϕ_k. Similarly, the multipole expansion of the magnetic potential W is:

$$W = \sum_{n=0}^{\infty} \sum_{k=-\infty}^{\infty} \frac{(-1)^n |k|!}{2^{2n} n!(n+|k|)!} \psi_k^{(2n)}(z) r^{2n+|k|} e^{\mathrm{i}k\theta} \tag{1.25}$$

1.4 Potential in Different Coordinates

Potentials in formula 1.24 and 1.25 are in cylindrical coordinates. Since θ is not defined on the optical axis it is better to use different coordinate system. The best option, due to the potential term, seems to be the 'circular polarization' coordinates $(z, w, \bar{w})$, where transition between cylindrical and circular polarization coordinates is defined by:

$$\begin{aligned} z &= z \\ w &= re^{\mathrm{i}\theta} \\ \bar{w} &= re^{-\mathrm{i}\theta} \end{aligned} \tag{1.26}$$

We notice that ϕ_k and ϕ_{-k} are complex conjugates (due to the real potential). The potential than looks like:

$$\Phi = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-1)^n k!}{2^{2n} n!(n+k)!} (w\bar{w})^n (\phi_k^{(2n)}(z) w^k + \bar{\phi}_k^{(2n)}(z) \bar{w}^k) \tag{1.27}$$

Where ϕ_k are the same as in the formula 1.24 with only exception of ϕ_0 which is only half of the ϕ_0 from the original 1.24. The formula of the magnetic potential is similar:

$$W = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-1)^n k!}{2^{2n} n!(n+k)!} (w\bar{w})^n (\psi_k^{(2n)}(z) w^k + \bar{\psi}_k^{(2n)}(z) \bar{w}^k) \tag{1.28}$$

[‡]We can also solve that by $s = -|k|$ or $a_{0,k} = 0$ but since k is an integer it does not matter - we would only get the solution corresponding to different k.

2. Trajectory Equation

We will derive the trajectory equation based on the variational formalisms. We start with a Lagrangian of a relativistic charged particle in a static electromagnetic field:

$$L = mc^2\left(1 - \sqrt{1 - \frac{v^2}{c^2}}\right) + q(-\Phi + \boldsymbol{v}\cdot\boldsymbol{A}) \tag{2.1}$$

Where m is the rest mass of the particle, q its charge, c speed of light, $\boldsymbol{v}$ its speed, $\Phi(\boldsymbol{x})$ an electric potential and $A(\boldsymbol{x})$ a magnetic vector potential. The corresponding canonical momentum and the Hamiltonian are:

$$\begin{aligned} \boldsymbol{p} &= \frac{m\boldsymbol{v}}{\sqrt{1-\frac{v^2}{c^2}}} + q\boldsymbol{A} \\ H &= mc^2\left(\frac{1}{\sqrt{1-\frac{v^2}{c^2}}} - 1\right) + q\Phi \end{aligned} \tag{2.2}$$

The field is static thus the Hamiltonian is a constant of motion (E_0). We can evaluate the formula of the absolute value of the velocity and kinetic momentum $g = mv\gamma$:

$$\begin{aligned} v &= c\sqrt{1 - \left(\frac{mc^2}{E_0 + mc^2 - q\Phi}\right)^2} \\ g &= \sqrt{2m(E_0 - q\Phi)\left(1 + \frac{E_0 - q\Phi}{2mc^2}\right)} \end{aligned} \tag{2.3}$$

Now derive the trajectory equation. The action for the realized trajectory has to be extremal:

$$S = \int L\,\mathrm{d}t = \text{extr.} \tag{2.4}$$

We have a static system where the Hamiltonian $H = \boldsymbol{p}\cdot\boldsymbol{v} - L$ is conserved and thus its contribution to the action is a constant*. We can extremalise modified action instead:

$$\tilde{S} = \int \boldsymbol{p}\cdot\boldsymbol{v}\,\mathrm{d}t = \text{extr.} \tag{2.5}$$

This action is invariant with respect to the parametrization (due to $\boldsymbol{v} = \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t}$) Thus we can re-parametrize it by using the optical axis coordinate z:

$$\tilde{S} = \int (\boldsymbol{g} + q\boldsymbol{A})\cdot\boldsymbol{r}'(z)\,\mathrm{d}z \tag{2.6}$$

The absolute value of kinetic momentum is determined by the equation 2.4 and its direction is always tangential to the trajectory. Thus we can write:

$$\tilde{S} = \int \left(g\sqrt{1 + x'^2 + y'^2} + q(A_x x' + A_y y' + A_z)\right)\,\mathrm{d}z \tag{2.7}$$

*If we assume that the strat and end time are fixed then $\int H\mathrm{d}t = E_0(t_{end} - t_{start})$

If the action is extremal, the integrand (M) has to satisfy Lagrange equations of the second kind:

$$\begin{aligned} \left(\frac{\partial M}{\partial x'}\right)' - \frac{\partial M}{\partial x} = 0 \\ \left(\frac{\partial M}{\partial y'}\right)' - \frac{\partial M}{\partial y} = 0 \end{aligned} \tag{2.8}$$

By evaluating it, we would get the exact solution of the trajectory in Cartesian coordinates. But we will do more simplifications. First of all we replace the magnetic vector potential by the scalar potential. We use $A_z = 0$ and the equations 1.11:

$$M = g\sqrt{1 + x'^2 + y'^2} + q\left(\left[-\int \frac{\partial W}{\partial y}\,\mathrm{d}z\right] x' + \left[\int \frac{\partial W}{\partial x}\,\mathrm{d}z\right] y'\right) \tag{2.9}$$

Now we go to circular polarization coordinates $(z, w, \bar{w})$:

$$\begin{aligned} M = g\sqrt{1 + w'\bar{w}'} + q\Bigg(-\left[\mathrm{i}\int \frac{\partial W}{\partial w} - \frac{\partial W}{\partial \bar{w}}\,\mathrm{d}z\right]\left(\frac{w' + \bar{w}'}{2}\right) + \\ + \left[\mathrm{i}\int \frac{\partial W}{\partial w} + \frac{\partial W}{\partial \bar{w}}\,\mathrm{d}z\right]\left(\frac{w' - \bar{w}'}{2i}\right)\Bigg) \end{aligned} \tag{2.10}$$

Where we used:

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial}{\partial w} + \frac{\partial}{\partial \bar{w}} \\ \frac{\partial}{\partial y} &= \mathrm{i}\frac{\partial}{\partial w} - \mathrm{i}\frac{\partial}{\partial \bar{w}} \\ x' &= \frac{w' + \bar{w}'}{2} \\ y' &= \frac{w' - \bar{w}'}{2\mathrm{i}} \end{aligned} \tag{2.11}$$

The magnetic term can be further simplified into the formula:

$$M = g\sqrt{1 + w'\bar{w}'} + \mathrm{i}q\left(\bar{w}'\left[\int \frac{\partial W}{\partial \bar{w}}\,\mathrm{d}z\right] - w'\left[\int \frac{\partial W}{\partial w}\,\mathrm{d}z\right]\right) \tag{2.12}$$

The trajectory can be found by applying the Lagrange equations with respect to the circular polarization coordinates.

$$\begin{aligned} \left(\frac{\partial M}{\partial w'}\right)' - \frac{\partial M}{\partial w} = 0 \\ \left(\frac{\partial M}{\partial \bar{w}'}\right)' - \frac{\partial M}{\partial \bar{w}} = 0 \end{aligned} \tag{2.13}$$

2.1 Paraxial Approximation

The paraxial approximation of the trajectory equation is an useful tool for deriving the behaviour of the electron/ion optical system. The main assumption is that the beam trajectory is close to the optical axis. Thus the coordinates x, y (or $w, \bar{w}$) are small. We can linearize the trajectory equations. In the Lagrangian it means to find the terms up to the quadratic.

We will start with expansion of the electric term of the Lagrangian. The square root term can be simplified to:

$$\sqrt{1 + w'\bar{w}'} \approx 1 + \frac{1}{2} w'\bar{w}' \tag{2.14}$$

and the kinetic momentum:

$$g = \sqrt{-2mq\Phi \left(1 - \frac{q\Phi}{2mc^2}\right)} \tag{2.15}$$

Where we already involve initial energy into the scalar potential†. It can be quadratised by splitting the potential into the constant part and the part dependent on w and $\bar{w}$:

$$\Phi = \phi_0 + \phi_n \tag{2.16}$$

Then the kinetic momentum is:

$$g = \sqrt{-2mq\phi_r} \sqrt{1 + \frac{\phi_n}{\phi_r} \left(1 - \frac{q(2\phi_0 + \phi_n)}{2mc^2}\right)} \tag{2.17}$$

Where ϕ_r is a relativistically corrected potential on the optical axis:

$$\phi_r = \phi_0 \left(1 - \frac{q\phi_0}{2mc^2}\right) \tag{2.18}$$

The Taylor series of kinetic momentum up to the second order of ϕ_n is then:

$$g \approx \sqrt{-2mq\phi_r} \left(1 + \frac{1}{2}\frac{\gamma_0\phi_n}{\phi_r} - \frac{1}{8}\frac{\phi_n^2}{\phi_r^2}\right) \tag{2.19}$$

Where γ_0 is γ-factor on the optical axis:

$$\gamma_0 = 1 - \frac{q\phi_0}{mc^2} \tag{2.20}$$

Bringing it all together we get the following estimation of the Lagrangian:

$$\begin{aligned} \tilde{M} = \sqrt{\phi_r} \left(1 + \frac{1}{2}\frac{\gamma_0\phi_n}{\phi_r} - \frac{1}{8}\frac{\phi_n^2}{\phi_r^2}\right) \left(1 + \frac{1}{2} w'\bar{w}'\right) + \\ + \mathrm{i}\eta \left(\bar{w}' \left[\int \frac{\partial W}{\partial \bar{w}}\, \mathrm{d}z\right] - w' \left[\int \frac{\partial W}{\partial w}\, \mathrm{d}z\right]\right) \end{aligned} \tag{2.21}$$

†If the potential change by constant, the electric field remain the same.

Where we divided the original the Lagrangian by a constant $\sqrt{-2mq}$. The parameter η equals to:

$$\eta = \sqrt{-\frac{q}{2m}} \tag{2.22}$$

The next thing to do is to insert the electric and magnetic potential in the form of power series of w and $\bar{w}$ up to the second term. From equations 1.27 and 1.28 we have:

$$\begin{aligned} \Phi &\approx \phi_0 - \frac{1}{4}\phi_0'' w\bar{w} + \phi_1 w + \bar{\phi}_1\bar{w} + \phi_2 w^2 + \bar{\phi}_2\bar{w}^2 \\ W &\approx \psi_0 - \frac{1}{4}\psi_0'' w\bar{w} + \psi_1 w + \bar{\psi}_1\bar{w} + \psi_2 w^2 + \bar{\psi}_2\bar{w}^2 \end{aligned} \tag{2.23}$$

Where the terms with index zero are half of the original (they are the same as in the equation 1.24 and 1.25) We put it into 2.21 and take only terms up to the second order of $w, \bar{w}, w'$ and $\bar{w}'$:

$$\begin{aligned} \tilde{M} = \sqrt{\phi_r} &+ \frac{1}{2}\frac{\phi_1}{\sqrt{\phi_r}}w + \frac{1}{2}\frac{\bar{\phi}_1}{\sqrt{\phi_r}}\bar{w} + \mathrm{i}\eta\left[\int\psi_1\right]w' - \mathrm{i}\eta\left[\int\bar{\psi}_1\right]\bar{w}' \\ &+ \left(\frac{1}{2}\frac{\gamma_0\phi_2}{\phi_r^{\frac{1}{2}}} - \frac{1}{8}\frac{\phi_1^2}{\phi_r^{\frac{3}{2}}}\right)w^2 + \left(\frac{1}{2}\frac{\gamma_0\bar{\phi}_2}{\phi_r^{\frac{1}{2}}} - \frac{1}{8}\frac{\bar{\phi}_1^2}{\phi_r^{\frac{3}{2}}}\right)\bar{w}^2 + \left(-\frac{1}{8}\frac{\gamma_0\phi_0''}{\phi_r^{\frac{1}{2}}} - \frac{1}{4}\frac{\phi_1\bar{\phi}_1}{\phi_r^{\frac{3}{2}}}\right)w\bar{w} \\ &+ 2\mathrm{i}\eta\left[\int\psi_2\right]ww' - 2\mathrm{i}\eta\left[\int\bar{\psi}_2\right]\bar{w}\bar{w}' + \frac{1}{4}\mathrm{i}\eta\psi_0'(w\bar{w}' - \bar{w}w') + \frac{1}{2}\sqrt{\phi_r}w'\bar{w}' \end{aligned} \tag{2.24}$$

Since the trajectory equations does not change if we add the total derivative of z to the Lagrangian we can simplify it to:

$$\begin{aligned} \tilde{M} = \sqrt{\phi_r} &+ \left(\frac{1}{2}\frac{\phi_1}{\sqrt{\phi_r}} + \mathrm{i}\eta\psi_1\right)w + \left(\frac{1}{2}\frac{\bar{\phi}_1}{\sqrt{\phi_r}} - \mathrm{i}\eta\bar{\psi}_1\right)\bar{w} \\ &+ \left(\frac{1}{2}\frac{\gamma_0\phi_2}{\phi_r^{\frac{1}{2}}} - \frac{1}{8}\frac{\phi_1^2}{\phi_r^{\frac{3}{2}}} + \mathrm{i}\eta\psi_2\right)w^2 + \left(\frac{1}{2}\frac{\gamma_0\bar{\phi}_2}{\phi_r^{\frac{1}{2}}} - \frac{1}{8}\frac{\bar{\phi}_1^2}{\phi_r^{\frac{3}{2}}} - \mathrm{i}\eta\bar{\psi}_2\right)\bar{w}^2 \\ &+ \left(-\frac{1}{8}\frac{\gamma_0\phi_0''}{\phi_r^{\frac{1}{2}}} - \frac{1}{4}\frac{\phi_1\bar{\phi}_1}{\phi_r^{\frac{3}{2}}}\right)w\bar{w} + \frac{1}{4}\mathrm{i}\eta\psi_0'(w\bar{w}' - \bar{w}w') + \frac{1}{2}\sqrt{\phi_r}w'\bar{w}' \end{aligned} \tag{2.25}$$

We now assume two sets of condition. The first are Wien's condition:

$$\left(\frac{1}{2}\frac{\phi_1}{\sqrt{\phi_r}} + \mathrm{i}\eta\psi_1\right) = 0 \tag{2.26}$$

which link the electric dipole to the magnetic dipole. And the second the stigmatic conditions:

$$\left(\frac{1}{2}\frac{\gamma_0\phi_2}{\phi_r^{\frac{1}{2}}} - \frac{1}{8}\frac{\phi_1^2}{\phi_r^{\frac{3}{2}}} + \mathrm{i}\eta\psi_2\right) = 0 \tag{2.27}$$

which link quadrupole terms of potentials. Thus the Lagrangian reduces to:

$$\tilde{M} = \sqrt{\phi_r} + \left(-\frac{1}{8}\frac{\gamma_0\phi_0''}{\phi_r^{\frac{1}{2}}} - \frac{1}{4}\frac{\phi_1\bar{\phi}_1}{\phi_r^{\frac{3}{2}}}\right)w\bar{w} + \frac{1}{4}\mathrm{i}\eta\psi_0'(w\bar{w}' - \bar{w}w') + \frac{1}{2}\sqrt{\phi_r}w'\bar{w}' \tag{2.28}$$

We can now introduce the co-rotating coordinates $(\omega, \bar{\omega})$:

$$w = \omega e^{\mathrm{i}\theta} \quad , \quad \bar{w} = \bar{\omega} e^{-\mathrm{i}\theta} \tag{2.29}$$

where θ is dependent on z according to the equation:

$$\theta' = \frac{\eta \psi_0'}{2\sqrt{\phi_r}} \tag{2.30}$$

Then the Lagrangian looks like:

$$\tilde{M} = \sqrt{\phi_r} - \frac{1}{8}\left(\frac{\eta^2 \psi'^2}{\phi_r^{\frac{1}{2}}} + \frac{\gamma_0 \phi_0''}{\phi_r^{\frac{1}{2}}} + \frac{2\phi_1 \bar{\phi}_1}{\phi_r^{\frac{3}{2}}}\right) \omega \bar{\omega} + \frac{1}{2}\sqrt{\phi_r} \omega' \bar{\omega}' \tag{2.31}$$

And the trajectory equations are:

$$\left(\frac{1}{2}\sqrt{\phi_r} \bar{\omega}'\right)' + \frac{1}{8}\left(\frac{\eta^2 \psi'^2}{\phi_r^{\frac{1}{2}}} + \frac{\gamma_0 \phi_0''}{\phi_r^{\frac{1}{2}}} + \frac{2\phi_1 \bar{\phi}_1}{\phi_r^{\frac{3}{2}}}\right) \bar{\omega} = 0 \tag{2.32}$$

3. Aberrations

Design of an optical system require also calculation of aberrations. The method which is used in this thesis to calculate them is called the Eikonal method[9]. We assume that Lagrangian can be written in perturbation series:

$$M = \sum_{j=0}^{N} \lambda^j M^{(j)} \tag{3.1}$$

Where $|\lambda| < 1^*$. We are looking for the solution also in perturbation series:

$$\boldsymbol{q}(z) = \sum_{j=0}^{N} \lambda^j \boldsymbol{q}^{(j)} \tag{3.2}$$

We are looking for the trajectory which minimize the action S. The variation of the action S can be evaluated by two different ways. At first we can vary the total Lagrangian:

$$\delta S = \int_{z_o}^{z_i} \left(\frac{\partial M}{\partial q_i} \delta q_i + \frac{\partial M}{\partial q_i'} \delta q_i' \right) \mathrm{d}z \tag{3.3}$$

Where it is integrated from the object position z_o to the image position z_i. We use summing nomenclature – $\frac{\partial M}{\partial q_i} \delta q_i$ means summing over all coordinates (either x, y or $w, \bar{w}$). By integrating by parts we get:

$$\delta S = \int_{z_o}^{z_i} \left(\left(\frac{\partial M}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}z} \frac{\partial M}{\partial q_i'} \right) \delta q_i \right) \mathrm{d}z + \Big[p_i \delta q_i \Big]_{z_o}^{z_i} \tag{3.4}$$

Where p_i is canonical momentum defined:

$$p_i = \frac{\partial M}{\partial q_i'} \tag{3.5}$$

The first part of the variation of the action is zero due to the Lagrange equation. Thus we get the formula for the variation:

$$\delta S = \Big[p_i \delta q_i \Big]_{z_o}^{z_i} \tag{3.6}$$

Now the p_i and q_i can be expressed in form of the perturbation series:

$$q_i(z) = \sum_{j=0}^{N} \lambda^j q_i^{(j)}(z) \tag{3.7}$$

$$q_i'(z) = \sum_{j=0}^{N} \lambda^j q_i'^{(j)}(z)$$

$$p_i(z) = \sum_{j=0}^{N} \lambda^j p_i^{(j)}(z)$$

*In our case it will not be true ($\lambda = 1$) but the M_{j+1} will be already much smaller than M_j though we can use the model.

The variation of the action is then:

$$\begin{aligned} \delta S &= \sum_{k=0}^{2N}\sum_{j=0}^{k}\lambda^k\left[p_i^{(k-j)}\delta q_i^{(j)}\right]_{z_o}^{z_i} \\ &\approx \left[p_i^{(0)}\delta q_i^{(0)}\right]_{z_o}^{z_i} \\ &+ \lambda\left[p_i^{(1)}\delta q_i^{(0)} + p_i^{(0)}\delta q_i^{(1)}\right]_{z_o}^{z_i} \\ &+ \lambda^2\left[p_i^{(2)}\delta q_i^{(0)} + p_i^{(1)}\delta q_i^{(1)} + p_i^{(0)}\delta q_i^{(2)}\right] \\ &+ \lambda^3\left[p_i^{(3)}\delta q_i^{(0)} + p_i^{(2)}\delta q_i^{(1)} + p_i^{(1)}\delta q_i^{(2)} + p_i^{(0)}\delta q_i^{(3)}\right]_{z_o}^{z_i} \end{aligned} \tag{3.8}$$

On the other hand we can first decompose Lagrangian in the power of series of λ. We do it only to the third order:

$$\begin{aligned} M &= \sum \lambda^j M^{(j)}\left(\sum \lambda^j q_i^{(j)}, \sum \lambda^j q_i'^{(j)}\right) \\ &\approx M^{(0)} + \lambda\left(M^{(1)} + D^{(1)}M^{(0)}\right) \\ &+ \lambda^2\left(M^{(2)} + D^{(1)}M^{(1)} + D^{(2)}M^{(0)} + \frac{1}{2}\left(D^{(1)}\right)^2 M^{(0)}\right) \\ &+ \lambda^3\left(M^{(3)} + D^{(1)}M^{(2)} + D^{(2)}M^{(1)} + D^{(3)}M^{(0)} + \frac{1}{2}\left(D^{(1)}\right)^2 M^{(1)} + \right. \\ &\left. + D^{(1)}D^{(2)}M^{(0)} + \frac{1}{6}\left(D^{(1)}\right)^3 M^{(0)}\right) \end{aligned} \tag{3.9}$$

The Lagrangian $M^{(0)}, M^{(1)}, M^{(2)}$ are express by zeroth order of the trajectory:

$$\begin{aligned} M^{(0)} &= M^{(0)}(w_i^{(0)}, p_i^{(0)}) \\ M^{(1)} &= M^{(1)}(w_i^{(0)}, p_i^{(0)}) \\ M^{(2)} &= M^{(2)}(w_i^{(0)}, p_i^{(0)}) \\ M^{(3)} &= M^{(3)}(w_i^{(0)}, p_i^{(0)}) \end{aligned} \tag{3.10}$$

And the differential operators $D^{(1)}, D^{(2)}$ are defined as:

$$\begin{aligned} D^{(1)} &= q_i^{(1)}\frac{\partial}{\partial q_i} + q_i'^{(1)}\frac{\partial}{\partial q_i'} \\ D^{(2)} &= q_i^{(2)}\frac{\partial}{\partial q_i} + q_i'^{(2)}\frac{\partial}{\partial q_i'} \\ D^{(3)} &= q_i^{(3)}\frac{\partial}{\partial q_i} + q_i'^{(3)}\frac{\partial}{\partial q_i'} \end{aligned} \tag{3.11}$$

We can now compute first terms of the action $S = S^{(0)} + \lambda S^{(1)} + \lambda^2 S^{(2)} + \lambda^3 S^{(3)}$:

$$\begin{aligned} S^{(0)} &= \int_{z_o}^{z_i} M^{(0)} \mathrm{d}z \\ S^{(1)} &= \int_{z_o}^{z_i} \left(M^{(1)} + D^{(1)} M^{(0)}\right) \mathrm{d}z \\ S^{(2)} &= \int_{z_o}^{z_i} \left(M^{(2)} + D^{(1)} M^{(1)} + D^{(2)} M^{(0)} + \frac{1}{2}\left(D^{(1)}\right)^2 M^{(0)}\right) \mathrm{d}z \\ S^{(2)} &= \int_{z_o}^{z_i} \left(M^{(3)} + D^{(1)} M^{(2)} + D^{(2)} M^{(1)} + D^{(3)} M^{(0)} + \frac{1}{2}\left(D^{(1)}\right)^2 M^{(1)} + \right. \\ & \left. + D^{(1)} D^{(2)} M^{(0)} + \frac{1}{6}\left(D^{(1)}\right)^3 M^{(0)}\right) \mathrm{d}z \end{aligned} \tag{3.12}$$

Which can be further simplified. We notice than for any set of parameters ζ_i and realized trajectories q_i the equation:

$$\int_{z_o}^{z_i} \left(\frac{\partial M}{\partial q_i}\zeta_i + \frac{\partial M}{\partial q_i'}\zeta_i'\right) \mathrm{d}z = \left[p_i \zeta_i\right]_{z_o}^{z_i} \tag{3.13}$$

is satisfied. We substitute $\zeta_i = q_i^{(1)}$ and expand it into power series of λ. Comparing zero, first and second order terms of λ we get:

$$\begin{aligned} &\int_{z_o}^{z_i} D^{(1)} M^{(0)} \, \mathrm{d}z = \left[p_i^{(0)} q_i^{(1)}\right]_{z_o}^{z_i} \\ &\int_{z_o}^{z_i} D^{(1)} M^{(1)} + \left(D^{(1)}\right)^2 M^{(0)} \mathrm{d}z = \left[p_i^{(1)} q_i^{(1)}\right]_{z_o}^{z_i} \\ &\int_{z_o}^{z_i} D^{(1)} M^{(2)} + \left(D^{(1)}\right)^2 M^{(1)} + D^{(1)} D^{(2)} M^{(0)} + \frac{1}{2}\left(D^{(1)}\right)^3 M^{(0)} \mathrm{d}z = \left[p_i^{(2)} q_i^{(1)}\right]_{z_o}^{z_i} \end{aligned} \tag{3.14}$$

Similarly, substituting $\zeta_i = q_i^{(2)}$ we get equation:

$$\begin{aligned} &\int_{z_o}^{z_i} D^{(2)} M^{(0)} \, \mathrm{d}z = \left[p_i^{(0)} q_i^{(2)}\right]_{z_o}^{z_i} \\ &\int_{z_o}^{z_i} D^{(2)} M^{(1)} + D^{(2)} D^{(1)} M^{(0)} \mathrm{d}z = \left[p_i^{(1)} q_i^{(2)}\right]_{z_o}^{z_i} \end{aligned} \tag{3.15}$$

And $\zeta_i = q_i^{(3)}$:

$$\int_{z_o}^{z_i} D^{(3)} M^{(0)} \, \mathrm{d}z = \left[p_i^{(0)} q_i^{(3)}\right]_{z_o}^{z_i} \tag{3.16}$$

Thus we can rewrite 3.12 as:

$$
\begin{aligned}
S^{(0)} &= \int_{z_o}^{z_i} M^{(0)} \mathrm{d}z \\
S^{(1)} &= \int_{z_o}^{z_i} \left(M^{(1)}\right) \mathrm{d}z + \left[p_i^{(0)} q_i^{(1)}\right]_{z_o}^{z_i} \\
S^{(2)} &= \int_{z_o}^{z_i} \left(M^{(2)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(0)}\right) \mathrm{d}z + \left[p_i^{(0)} q_i^{(2)} + p_i^{(1)} q_i^{(1)}\right]_{z_o}^{z_i} \\
S^{(3)} &= \int_{z_o}^{z_i} \left(M^{(3)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(1)} + \frac{1}{3}\left(D^{(1)}\right)^3 M^{(0)} - D^{(1)} D^{(2)} M^{(0)}\right) \mathrm{d}z \\
&\quad + \left[p_i^{(0)} q_i^{(3)} + p_i^{(1)} q_i^{(2)} + p_i^{(2)} q_i^{(1)}\right]_{z_o}^{z_i}
\end{aligned}
\tag{3.17}
$$

For further calculation we name integrals as S^I, S^{II}, S^{III}:

$$
\begin{aligned}
S^{I} &= \int_{z_o}^{z_i} \left(M^{(1)}\right) \mathrm{d}z \\
S^{II} &= \int_{z_o}^{z_i} \left(M^{(2)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(0)}\right) \mathrm{d}z \\
S^{III} &= \int_{z_o}^{z_i} \left(M^{(3)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(1)} - D^{(1)} D^{(2)} M^{(0)}\right) \mathrm{d}z
\end{aligned}
\tag{3.18}
$$

Which are now only function of initial coordinates and momentums. Furthermore, the term $\left(D^{(1)}\right)^3 M^{(0)}$ is zero since there are only quadratic terms of q_i, q_i' in $M^{(0)}$. For further calculation of aberrations we define vectors:

$$
\boldsymbol{Q}^{(j)} = \begin{pmatrix} q_1^{(j)} \\ q_2^{(j)} \\ q_1'^{(j)} \\ q_2'^{(j)} \end{pmatrix}
\tag{3.19}
$$

Operator:

$$
\nabla_0 = \begin{pmatrix} \frac{\partial}{\partial q_{1,o}} \\ \frac{\partial}{\partial q_{2,o}} \\ \frac{\partial}{\partial p_{1,o}} \\ \frac{\partial}{\partial p_{2,o}} \end{pmatrix}
\tag{3.20}
$$

Matrix Γ:

$$
\Gamma = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.
\tag{3.21}
$$

And projector matrix Π:

$$
\Pi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.
\tag{3.22}
$$

3.1 Zeroth Order Perturbation

We can now finally obtain differential equations for calculating the perturbation terms of trajectory. We compare variation of actions from 3.17 with 3.8. From zeroth order we get:

$$\left[p_i^{(0)} \delta q_i^{(0)}\right]_{z_o}^{z_i} = \delta \int_{z_o}^{z_i} M^{(0)} \mathrm{d}z \tag{3.23}$$

Which can be rewrite to the form of Lagrange equations of paraxial solution:

$$0 = \int_{z_o}^{z_i} \left(\frac{\partial M^{(0)}}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}z} \frac{\partial M^{(0)}}{\partial q_i'} \right) \delta q_i \, \mathrm{d}z \tag{3.24}$$

3.2 First Order Perturbation

If we compare linear term of λ we get:

$$\left[p_i^{(1)} \delta q_i^{(0)} + p_i^{(0)} \delta q_i^{(1)}\right]_{z_o}^{z_i} = \delta S^I + \delta \left[p_i^{(0)} q_i^{(1)}\right]_{z_o}^{z_i} \tag{3.25}$$

Which after further simplification is:

$$\delta S^I = \left[p_i^{(1)} \delta q_i^{(0)} - \delta p_i^{(0)} q_i^{(1)}\right]_{z_o}^{z_i} \tag{3.26}$$

We now assume that the initial position and momentum of the perturbed trajectory is the same as the paraxial trajectory. Thus:

$$0 = q_i^{(1)}(z_o) = p_i^{(1)}(z_o) \tag{3.27}$$

And:

$$\delta S^I = p_i^{(1)}(z_i) \delta q_i^{(0)}(z_i) - \delta p_i^{(0)}(z_i) q_i^{(1)}(z_i)$$

From which we have set of differential equations of first order perturbation:

$$\begin{aligned}
\frac{\partial S^I}{\partial q_{1,o}} &= p_1^{(1)} \frac{\partial q_1^{(0)}}{\partial q_{1,o}} + p_2^{(1)} \frac{\partial q_2^{(0)}}{\partial q_{1,o}} - q_1^{(1)} \frac{\partial p_1^{(0)}}{\partial q_{1,o}} - q_2^{(1)} \frac{\partial p_2^{(0)}}{\partial q_{1,o}} \\
\frac{\partial S^I}{\partial q_{2,o}} &= p_1^{(1)} \frac{\partial q_1^{(0)}}{\partial q_{2,o}} + p_2^{(1)} \frac{\partial q_2^{(0)}}{\partial q_{2,o}} - q_1^{(1)} \frac{\partial p_1^{(0)}}{\partial q_{2,o}} - q_2^{(1)} \frac{\partial p_2^{(0)}}{\partial q_{2,o}} \\
\frac{\partial S^I}{\partial q_{1,o}'} &= p_1^{(1)} \frac{\partial q_1^{(0)}}{\partial q_{1,o}'} + p_2^{(1)} \frac{\partial q_2^{(0)}}{\partial q_{1,o}'} - q_1^{(1)} \frac{\partial p_1^{(0)}}{\partial q_{1,o}'} - q_2^{(1)} \frac{\partial p_2^{(0)}}{\partial q_{1,o}'} \\
\frac{\partial S^I}{\partial q_{2,o}'} &= p_1^{(1)} \frac{\partial q_1^{(0)}}{\partial q_{2,o}'} + p_2^{(1)} \frac{\partial q_2^{(0)}}{\partial q_{2,o}'} - q_1^{(1)} \frac{\partial p_1^{(0)}}{\partial q_{2,o}'} - q_2^{(1)} \frac{\partial p_2^{(0)}}{\partial q_{2,o}'}
\end{aligned} \tag{3.28}$$

This can be written in more compact form:

$$\nabla_0 S^I = \nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma \cdot \boldsymbol{Q}^{(1)} \tag{3.29}$$

With solution:

$$\boldsymbol{Q}^{(1)} = (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1} \cdot \nabla_0 S^I \tag{3.30}$$

3.3 Second Order Perturbation

The second order perturbations can be derived using the same procedure. We compare quadratic terms of λ from 3.17 and 3.8:

$$\left[p_i^{(2)}\delta q_i^{(0)} + p_i^{(1)}\delta q_i^{(1)} + p_i^{(0)}\delta q_i^{(2)}\right]_{z_o}^{z_i} = \delta S^{II} + \delta\left[p_i^{(0)}q_i^{(2)} + p_i^{(1)}q_i^{(1)}\right]_{z_o}^{z_i} \tag{3.31}$$

Simplifying and using:

$$0 = q_i^{(2)}(z_o) = p_i^{(2)}(z_o) \tag{3.32}$$

We get:

$$\delta S^{II} = p_i^{(2)}(z_i)\delta q_i^{(0)}(z_i) - q_i^{(2)}(z_i)\delta p_i^{(0)}(z_i) - q_i^{(1)}(z_i)\delta p_i^{(1)}(z_i) \tag{3.33}$$

From which we get differential equations of second order perturbations:

$$\nabla_0 S^{II} = \nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma \cdot \boldsymbol{Q}^{(2)} + \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)} \tag{3.34}$$

With solution:

$$\boldsymbol{Q}^{(2)} = (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{II} - \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)}) \tag{3.35}$$

3.4 Third Order Perturbation

Finally we calculate third order perturbation:

$$\left[p_i^{(3)}\delta q_i^{(0)} + p_i^{(2)}\delta q_i^{(1)} + p_i^{(1)}\delta q_i^{(2)} + p_i^{(0)}\delta q_i^{(3)}\right]_{z_o}^{z_i} = \delta S^{III} + \delta\left[p_i^{(0)}q_i^{(3)} + p_i^{(2)}q_i^{(1)} + p_i^{(1)}q_i^{(2)}\right]_{z_o}^{z_i} \tag{3.36}$$

With same simplification as before:

$$0 = q_i^{(3)}(z_o) = p_i^{(3)}(z_o) \tag{3.37}$$

We get:

$$\begin{aligned} \delta S^{III} &= p_i^{(3)}(z_i)\delta q_i^{(0)}(z_i) - q_i^{(3)}(z_i)\delta p_i^{(0)}(z_i) \\ &+ -q_i^{(2)}(z_i)\delta p_i^{(1)}(z_i) - q_i^{(1)}(z_i)\delta p_i^{(2)}(z_i) \end{aligned} \tag{3.38}$$

From which we get differential equations of second order perturbations:

$$\nabla_0 S^{III} = \nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma \cdot \boldsymbol{Q}^{(3)} + \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(2)} + \nabla_0 \boldsymbol{Q}^{(2)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)} \tag{3.39}$$

With solution:

$$\boldsymbol{Q}^{(3)} = (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{III} - \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(2)} - \nabla_0 \boldsymbol{Q}^{(2)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)})$$

3.5 Stigmatic System

In case of the system described by Lagrangian 2.31 we can write the solution in form:

$$\begin{aligned} w^{(0)}(z) &= w_0 g(z) + w_0' h(z) \\ \bar{w}^{(0)}(z) &= \bar{w}_0 \bar{g}(z) + \bar{w}_0' \bar{h}(z) \end{aligned} \tag{3.40}$$

With corresponding momentums:

$$\begin{aligned} p^{(0)}(z) &= \frac{\sqrt{\phi_r}}{2}\left(\bar{w}_0 \bar{g}'(z) + \bar{w}_0' \bar{h}'(z)\right) \\ \bar{p}^{(0)}(z) &= \frac{\sqrt{\phi_r}}{2}\left(w_0 g'(z) + w_0' h'(z)\right) \end{aligned} \tag{3.41}$$

We can calculate matrix $(\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}$:

$$(\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1} = \begin{pmatrix} 0 & \frac{2\bar{h}}{\sqrt{\phi_r}} & 0 & -\frac{2\bar{g}}{\sqrt{\phi_r}} \\ \frac{2h}{\sqrt{\phi_r}} & 0 & -\frac{2g}{\sqrt{\phi_r}} & 0 \\ h' & 0 & -g' & 0 \\ 0 & \bar{h}' & 0 & -\bar{g}' \end{pmatrix} \tag{3.42}$$

Finally we once again sum up the equation of aberrations:

$$\begin{aligned} \boldsymbol{Q}^{(1)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1} \cdot \nabla_0 S^I \\ \boldsymbol{Q}^{(2)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{II} - \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)}) \\ \boldsymbol{Q}^{(3)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{III} - \nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(2)} - \nabla_0 \boldsymbol{Q}^{(2)} \cdot \Gamma \cdot \Pi \cdot \boldsymbol{Q}^{(1)}) \end{aligned} \tag{3.43}$$

With eikonals:

$$\begin{aligned} S^I &= \int_{z_o}^{z_i} \left(M^{(1)}\right) \mathrm{d}z \\ S^{II} &= \int_{z_o}^{z_i} \left(M^{(2)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(0)}\right) \mathrm{d}z \\ S^{III} &= \int_{z_o}^{z_i} \left(M^{(3)} - \frac{1}{2}\left(D^{(1)}\right)^2 M^{(1)} - D^{(2)} D^{(1)} M^{(0)}\right) \mathrm{d}z \end{aligned} \tag{3.44}$$

3.5.1 Alternative Formulation

There is certain freedom in actions 3.12. Sometimes it is more useful to use alternative actions and solutions:

$$\begin{aligned} \boldsymbol{Q}^{(1)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1} \cdot \nabla_0 S^I \\ \boldsymbol{Q}^{(2)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{II} - \frac{1}{2}\nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \boldsymbol{Q}^{(1)}) \\ \boldsymbol{Q}^{(3)} &= (\nabla_0 \boldsymbol{Q}^{(0)} \cdot \Gamma)^{-1}(\nabla_0 S^{III} - \frac{1}{2}\nabla_0 \boldsymbol{Q}^{(1)} \cdot \Gamma \cdot \boldsymbol{Q}^{(2)} - \frac{1}{2}\nabla_0 \boldsymbol{Q}^{(2)} \cdot \Gamma \cdot \boldsymbol{Q}^{(1)}) \end{aligned} \tag{3.45}$$

$$\begin{aligned} S^{I} &= \int_{z_o}^{z_i} \left(M^{(1)}\right) \mathrm{d}z \\ S^{II} &= \int_{z_o}^{z_i} \left(M^{(2)} + \frac{1}{2} D^{(1)} M^{(1)}\right) \mathrm{d}z \\ S^{III} &= \int_{z_o}^{z_i} \left(M^{(3)} + \frac{1}{2} D^{(1)} M^{(2)} + \frac{1}{2} D^{(2)} M^{(1)}\right) \mathrm{d}z \end{aligned} \tag{3.46}$$

4. Calculation of Aberrations for Different Fields

4.1 Magnetic Monopole

We will derive the aberration coefficients of third order of magnetic monopole. First we will start with the field. Our approximation of the field is:

$$\begin{aligned} W &= \psi_0 - \frac{1}{4}\psi_0'' w\bar{w} + \frac{1}{64}\psi_0^{(4)}\left(w\bar{w}\right)^2 \\ \Phi &= \phi_0 \end{aligned} \tag{4.1}$$

By expanding equation 2.12 (divided by $\sqrt{-2mq}$) into the second and forth order we get the lagrangian $M = M_2 + M_4$ (the zeroth order - constant - of Lagrangian is omitted):

$$M_2 = \frac{1}{2}\sqrt{\phi_r} w'\bar{w}' + \frac{1}{4} i\eta\psi_0'\left(w\bar{w}' - \bar{w}w'\right) \tag{4.2}$$

$$M_4 = -\frac{1}{8}\sqrt{\phi_r}\left(w'\bar{w}'\right)^2 - \frac{1}{32} i\eta\psi_0''' w\bar{w}\left(w\bar{w}' - \bar{w}w'\right) \tag{4.3}$$

Going to co-rotating coordinates $(\omega, \bar{\omega})$ 2.29, 2.30 the Lagrangian is then:

$$M_2 = \frac{1}{2}\sqrt{\phi_r}\omega'\bar{\omega}' - \frac{1}{8}\frac{\eta^2\psi_0'^2}{\sqrt{\phi_r}}\omega\bar{\omega} \tag{4.4}$$

$$\begin{aligned} M_4 = &-\frac{1}{4}L_1\left(\omega\bar{\omega}\right)^2 - \frac{1}{2}L_2\omega\bar{\omega}\omega'\bar{\omega}' \\ &-\frac{1}{4}L_3\left(\omega'\bar{\omega}'\right)^2 - \frac{i}{2}P\omega\bar{\omega}\left(\omega\bar{\omega}' - \bar{\omega}\omega'\right) \\ &-\frac{i}{2}Q\omega'\bar{\omega}'\left(\omega\bar{\omega}' - \bar{\omega}\omega'\right) + \frac{1}{4}R\left(\omega\bar{\omega}' - \bar{\omega}\omega'\right)^2 \end{aligned} \tag{4.5}$$

Where the functions of M_4 are[9] *:

$$\begin{aligned} L_1 &= \frac{1}{32\sqrt{\phi_r}}\left(\frac{\eta^4\psi_0'^4}{\phi_r} - 4\eta^2\psi_0'\psi_0'''\right) \\ L_2 &= \frac{1}{8}\frac{\eta^2\psi_0'^2}{\sqrt{\phi_r}} \\ L_3 &= \frac{1}{2}\sqrt{\phi_r} \\ P &= \frac{\eta}{16}\left(\frac{\eta^2\psi_0'^3}{\phi_r} - \psi_0'''\right) \\ Q &= \frac{1}{4}\eta\psi_0' \\ R &= \frac{1}{8}\frac{\eta^2\psi_0'^2}{\sqrt{\phi_r}} \end{aligned} \tag{4.6}$$

*Because we solve only magnetic monopole, not general electro-magnetic, $\sqrt{\phi_r}$ is constant and thus we can bring it directly into terms P and Q

Because the Lagrangian is separable the basis of the paraxial solution is the same for ω and $\bar{\omega}$. We choose the basis as two functions h, g which in object plane satisfy conditions:

$$\begin{aligned} g(z_o) &= 1 \qquad g'(z_o) = 0 \\ h(z_o) &= 0 \qquad h'(z_o) = 1 \end{aligned} \tag{4.7}$$

The general solution is then:

$$\begin{aligned} \omega^{(0)}(z) &= \omega_o g(z) + \omega_o' h(z) \\ \bar{\omega}^{(0)}(z) &= \bar{\omega}_o g(z) + \bar{\omega}_o' h(z) \end{aligned} \tag{4.8}$$

Where $(\omega_o, \bar{\omega}_o)$ and $(\omega_o', \bar{\omega}_o')$ are constants which correspond to the position and slope in the object plane. Now we calculate the first order perturbation by eikonal method. We calculate $M^{(1)}$ by putting 4.8 into M_4:

$$\begin{aligned} M^{(1)} \;=\; & \left[-\frac{1}{4}\left(L_1 h^4 + 2L_2 h^2 h'^2 + L_3 h'^4\right)\right] \omega_0'^2 \bar{\omega}_0'^2 \\ + & \left[-\frac{1}{2}\left(L_1 g h^3 + L_2 h h'(g h' + h g') + L_3 g' h'^3\right) + \frac{i}{2}\left(P h^2 + Q h'^2\right)\right] \bar{\omega}_0 \omega_0'^2 \bar{\omega}_0' \\ + & \left[-\frac{1}{2}\left(L_1 g h^3 + L_2 h h'(g h' + h g') + L_3 g' h'^3\right) - \frac{i}{2}\left(P h^2 + Q h'^2\right)\right] \omega_0 \omega_0' \bar{\omega}_0'^2 \\ + & \left[-\frac{1}{4}\left(L_1 g^2 h^2 + 2L_2 g h g' h' + L_3 g'^2 h'^2 - R\right) + \frac{i}{2}\left(P g h + Q g' h'\right)\right] \bar{\omega}_0^2 \omega_0'^2 \\ + & \left[-\frac{1}{2}\left(2L_1 g^2 h^2 + L_2 (g h' + h g')^2 + 2L_3 g'^2 h'^2 + R\right)\right] \omega_0 \bar{\omega}_0 \omega_0' \bar{\omega}_0' \\ + & \left[-\frac{1}{4}\left(L_1 g^2 h^2 + L_2 2 g h g' h' + L_3 g'^2 h'^2 - R\right) - \frac{i}{2}\left(P g h + Q g' h'\right)\right] \omega_0^2 \bar{\omega}_0'^2 \\ + & \left[-\frac{1}{2}\left(L_1 g^3 h + L_2 g g'(g h' + h g') + L_3 g'^3 h'\right) + \frac{i}{2}\left(P g^2 + Q g'^2\right)\right] \omega_0 \bar{\omega}_0^2 \omega_0' \\ + & \left[-\frac{1}{2}\left(L_1 g^3 h + L_2 g g'(g h' + h g') + L_3 g'^3 h'\right) - \frac{i}{2}\left(P g^2 + Q g'^2\right)\right] \omega_0^2 \bar{\omega}_0 \bar{\omega}_0' \\ + & \left[-\frac{1}{4}\left(L_1 g^4 + 2L_2 g^2 g'^2 + L_3 g'^4\right)\right] \omega_0^2 \bar{\omega}_0^2 \end{aligned} \tag{4.9}$$

Where we simplified terms by Wronskian $gh' - hg' = 1$. We write:

$$\begin{aligned}
C &= \frac{1}{\sqrt{\phi_r}} \int \left(L_1 h^4 + 2L_2 h^2 h'^2 + L_3 h'^4\right) \mathrm{d}z \\
K &= \frac{1}{\sqrt{\phi_r}} \int \left(L_1 g h^3 + L_2 h h'(gh' + hg') + L_3 g' h'^3\right) \mathrm{d}z \\
A &= \frac{1}{\sqrt{\phi_r}} \int \left(L_1 g^2 h^2 + 2L_2 g h g' h' + L_3 g'^2 h'^2 - R\right) \mathrm{d}z \\
F &= \frac{1}{\sqrt{\phi_r}} \int \left(2L_1 g^2 h^2 + L_2 (gh' + hg')^2 + 2L_3 g'^2 h'^2 + R\right) \mathrm{d}z \\
D &= \frac{1}{\sqrt{\phi_r}} \int \left(L_1 g^3 h + L_2 g g'(gh' + hg') + L_3 g'^3 h'\right) \mathrm{d}z \\
E &= \frac{1}{\sqrt{\phi_r}} \int \left(L_1 g^4 + 2L_2 g^2 g'^2 + L_3 g'^4\right) \mathrm{d}z \\
k &= \frac{1}{\sqrt{\phi_r}} \int \left(P h^2 + Q h'^2\right) \mathrm{d}z \\
a &= \frac{2}{\sqrt{\phi_r}} \int \left(P g h + Q g' h'\right) \mathrm{d}z \\
d &= \frac{1}{\sqrt{\phi_r}} \int \left(P g^2 + Q g'^2\right) \mathrm{d}z
\end{aligned} \tag{4.10}$$

Eikonal S^I then looks like:

$$\begin{aligned}
S^I = \sqrt{\phi_r}\Bigg(& -\frac{1}{4} C \omega_0'^2 \bar{\omega}_0'^2 - \frac{1}{2} F \omega_0 \bar{\omega}_0 \omega_0' \bar{\omega}_0' - \frac{1}{4} E \omega_0^2 \bar{\omega}_0^2 \\
& -\frac{1}{2}(K - ik)\bar{\omega}_0 \omega_0'^2 \bar{\omega}_0' - \frac{1}{2}(K + ik)\omega_0 \omega_0' \bar{\omega}_0'^2 \\
& -\frac{1}{4}(A - ia)\bar{\omega}_0^2 \omega_0'^2 - \frac{1}{4}(A + ia)\omega_0^2 \bar{\omega}_0'^2 \\
& -\frac{1}{2}(D - id)\omega_0 \bar{\omega}_0^2 \omega_0' - \frac{1}{2}(D + id)\omega_0^2 \bar{\omega}_0 \bar{\omega}_0' \Bigg)
\end{aligned} \tag{4.11}$$

By using equation 3.28 we get aberrations in general plane:

$$\begin{aligned}
\omega^{(1)} = & \left[\; Cg \quad -(K - ik)h \;\right] \omega_0'^2 \bar{\omega}_0' \\
+ & \left[\; (K - ik)g \quad -(A - ia)h \;\right] \bar{\omega}_0 \omega_0'^2 \\
+ & \left[\; 2(K + ik)g \quad -Fh \;\right] \omega_0 \omega_0' \bar{\omega}_0' \\
+ & \left[\; Fg \quad -2(D - id)h \;\right] \omega_0 \bar{\omega}_0 \omega_0' \\
+ & \left[\; (A + ia)g \quad (D + id)h \;\right] \omega_0^2 \bar{\omega}_0' \\
+ & \left[\; (D + id)g \quad -Eh \;\right] \omega_0^2 \bar{\omega}_0
\end{aligned} \tag{4.12}$$

In image plane $h(z_o) = 0$, and $g(z_o) = M$ where M is magnification. Thus the aberrations are:

$$\begin{aligned}
\frac{\omega^{(1)}}{M} = & \; C \omega_0'^2 \bar{\omega}_0' \\
+ & \; 2(K + ik)\omega_0 \omega_0' \bar{\omega}_0' + (K - ik)\bar{\omega}_0 \omega_0'^2 \\
+ & \; (A + ia)\omega_0^2 \bar{\omega}_0' \\
+ & \; F \omega_0 \bar{\omega}_0 \omega_0' \\
+ & \; (D + id)\omega_0^2 \bar{\omega}_0
\end{aligned} \tag{4.13}$$

4.2 Magnetic Hexapole

As in chapter with monopole we start with electromagnetic field:

$$\begin{aligned} W &= \psi_3 w^3 + \bar{\psi}_3 \bar{w}^3 \\ \Phi &= \phi_0 \end{aligned} \tag{4.14}$$

And Lagrangian series up to forth order :

$$M_2 = \frac{1}{2}\sqrt{\phi_r} w' \bar{w}' \tag{4.15}$$

$$M_3 = i\eta\left(\psi_3 w^3 - \bar{\psi}_3 \bar{w}^3\right) \tag{4.16}$$

$$M_4 = -\frac{1}{8}\sqrt{\phi_r}\left(w'\bar{w}'\right)^2 \tag{4.17}$$

Where M_3 was simplified by adding total derivative of z of $i\eta(w^3 \int \psi_3 - \bar{w}^3 \int \bar{\psi}_3)$. Unlike in monopole, there is not rotation of image in hexapole field thus we remain in standard coordinates. As before we choose two paraxial function g,h with condition 4.7. The general solution is:

$$\begin{aligned} w^{(0)}(z) = w_o g(z) + w_o' h(z) \\ \bar{w}^{(0)}(z) = \bar{w}_o g(z) + \bar{w}_o' h(z) \end{aligned} \tag{4.18}$$

We get $M^{(1)}$ by substituting 4.18 into M_3:

$$\begin{aligned} M^{(1)} = &+i\eta\left(\psi_3 h^3 w_0'^3 + 3\psi_3 h^2 g w_0 w_0'^2 + 3\psi_3 h g^2 w_0^2 w_0' + \psi_3 g^3 w_0^3\right) \\ &-i\eta\left(\bar{\psi}_3 h^3 \bar{w}_0'^3 + 3\bar{\psi}_3 h^2 g \bar{w}_0 \bar{w}_0'^2 + 3\bar{\psi}_3 h g^2 \bar{w}_0^2 \bar{w}_0' + \bar{\psi}_3 g^3 \bar{w}_0^3\right) \end{aligned} \tag{4.19}$$

We write:

$$\begin{aligned} U_0 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 h^3 \mathrm{d}z & \bar{U}_0 &= \frac{6\eta}{\sqrt{\phi_r}}\int \bar{\psi}_3 h^3 \mathrm{d}z \\ U_1 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g h^2 \mathrm{d}z & \bar{U}_1 &= \frac{6\eta}{\sqrt{\phi_r}}\int \bar{\psi}_3 g h^2 \mathrm{d}z \\ U_2 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g^2 h \mathrm{d}z & \bar{U}_2 &= \frac{6\eta}{\sqrt{\phi_r}}\int \bar{\psi}_3 g^2 h \mathrm{d}z \\ U_3 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g^3 \mathrm{d}z & \bar{U}_3 &= \frac{6\eta}{\sqrt{\phi_r}}\int \bar{\psi}_3 g^3 \mathrm{d}z \end{aligned} \tag{4.20}$$

The first aberrations are then:

$$\begin{aligned} w^{(1)} &= i(g\bar{U}_0 - h\bar{U}_1)\bar{w}_0'^2 \\ &+ 2i(g\bar{U}_1 - h\bar{U}_2)\bar{w}_0 \bar{w}_0' \\ &+ i(g\bar{U}_2 - h\bar{U}_3)\bar{w}_0^2 \end{aligned} \tag{4.21}$$

To calculate second order aberration we first evaluate:

$$\begin{aligned} M^{(2)} &+ \frac{1}{2}D^{(1)}M^{(1)} = \\ & \left[\frac{3\eta}{2}\left((\psi_3\bar{U}_1+\bar{\psi}_3U_1)h^3-(\psi_3\bar{U}_0+\bar{\psi}_3U_0)gh^2\right)-\frac{\sqrt{\phi_r}}{8}h'^4\right]w_0'^2\bar{w}_0'^2 \\ &+ \left[3\eta\left(\psi_3\bar{U}_2h^3-(\psi_3\bar{U}_1-\bar{\psi}_3U_1)gh^2-\bar{\psi}_3U_0g^2h\right)-\frac{\sqrt{\phi_r}}{4}g'h'^3\right]\bar{w}_0w_0'^2\bar{w}_0' \\ &+ \left[3\eta\left(\bar{\psi}_3U_2h^3-(\bar{\psi}_3U_1-\psi_3\bar{U}_1)gh^2-\psi_3\bar{U}_0g^2h\right)-\frac{\sqrt{\phi_r}}{4}g'h'^3\right]w_0w_0'\bar{w}_0'^2 \\ &+ \left[\frac{3\eta}{2}\left(\psi_3\bar{U}_3h^3-\psi_3\bar{U}_1gh^2+\bar{\psi}_3U_1g^2h-\bar{\psi}_3U_0g^3\right)-\frac{\sqrt{\phi_r}}{8}g'^2h'^2\right]\bar{w}_0^2w_0'^2 \\ &+ \left[6\eta\left((\psi_3\bar{U}_2+\bar{\psi}_3U_2)gh^2-(\psi_3\bar{U}_1+\bar{\psi}_3U_1)g^2h\right)-\frac{\sqrt{\phi_r}}{2}g'^2h'^2\right]w_0\bar{w}_0w_0'\bar{w}_0' \\ &+ \left[\frac{3\eta}{2}\left(\bar{\psi}_3U_3h^3-\bar{\psi}_3U_1gh^2+\psi_3\bar{U}_1g^2h-\psi_3\bar{U}_0g^3\right)-\frac{\sqrt{\phi_r}}{8}g'^2h'^2\right]w_0^2\bar{w}_0'^2 \\ &+ \left[3\eta\left(\psi_3\bar{U}_3gh^2-(\psi_3\bar{U}_1-\bar{\psi}_3U_2)g^2h-\bar{\psi}_3U_1g^3\right)-\frac{\sqrt{\phi_r}}{4}g'^3h'\right]w_0\bar{w}_0^2w_0' \\ &+ \left[3\eta\left(\bar{\psi}_3U_3gh^2-(\bar{\psi}_3U_1-\psi_3\bar{U}_2)g^2h-\psi_3\bar{U}_1g^3\right)-\frac{\sqrt{\phi_r}}{4}g'^3h'\right]w_0^2\bar{w}_0\bar{w}_0' \\ &+ \left[\frac{3\eta}{2}\left((\psi_3\bar{U}_3+\bar{\psi}_3U_3)g^2h-(\psi_3\bar{U}_1+\bar{\psi}_3U_1)g^3\right)-\frac{\sqrt{\phi_r}}{8}g'^4\right]w_0^2\bar{w}_0^2 \end{aligned} \tag{4.22}$$

We write:

$$\begin{aligned} C &= \frac{1}{\sqrt{\phi_r}}\int\left(\frac{\sqrt{\phi_r}}{2}h'^4-6\eta\left((\psi_3\bar{U}_1+\bar{\psi}_3U_1)h^3-(\psi_3\bar{U}_0+\bar{\psi}_3U_0)gh^2\right)\right)\mathrm{d}z \\ K &= \frac{1}{\sqrt{\phi_r}}\int\left(\frac{\sqrt{\phi_r}}{2}g'h'^3-6\eta\left(\bar{\psi}_3U_2h^3-(\bar{\psi}_3U_1-\psi_3\bar{U}_1)gh^2-\psi_3\bar{U}_0g^2h\right)\right)\mathrm{d}z \\ A &= \frac{1}{\sqrt{\phi_r}}\int\left(\frac{\sqrt{\phi_r}}{2}g'^2h'^2-6\eta\left(\bar{\psi}_3U_3h^3-\bar{\psi}_3U_1gh^2+\psi_3\bar{U}_1g^2h-\psi_3\bar{U}_0g^3\right)\right)\mathrm{d}z \\ F &= \frac{1}{\sqrt{\phi_r}}\int\left(\sqrt{\phi_r}g'^2h'^2-12\eta\left((\psi_3\bar{U}_2+\bar{\psi}_3U_2)gh^2-(\psi_3\bar{U}_1+\bar{\psi}_3U_1)g^2h\right)\right)\mathrm{d}z \\ D &= \frac{1}{\sqrt{\phi_r}}\int\left(\frac{\sqrt{\phi_r}}{2}g'^3h'-6\eta\left(\bar{\psi}_3U_3gh^2-(\bar{\psi}_3U_1-\psi_3\bar{U}_2)g^2h-\psi_3\bar{U}_1g^3\right)\right)\mathrm{d}z \\ E &= \frac{1}{\sqrt{\phi_r}}\int\left(\frac{\sqrt{\phi_r}}{2}g'^4-6\eta\left((\psi_3\bar{U}_3+\bar{\psi}_3U_3)g^2h-(\psi_3\bar{U}_1+\bar{\psi}_3U_1)g^3\right)\right)\mathrm{d}z \end{aligned} \tag{4.23}$$

And get second order eikonal S^{II}:

$$\begin{aligned} S^{II} = \sqrt{\phi_r}\Big(& -\frac{1}{4}Cw_0'^2\bar{w}_0'^2-\frac{1}{2}Fw_0\bar{w}_0w_0'\bar{w}_0'-\frac{1}{4}Ew_0^2\bar{w}_0^2 \\ & -\frac{1}{2}\bar{K}\bar{w}_0w_0'^2\bar{w}_0'-\frac{1}{2}Kw_0w_0'\bar{w}_0'^2 \\ & -\frac{1}{4}\bar{A}\bar{w}_0^2w_0'^2-\frac{1}{4}Aw_0^2\bar{w}_0'^2 \\ & -\frac{1}{2}\bar{D}w_0\bar{w}_0^2w_0'-\frac{1}{2}Dw_0^2\bar{w}_0\bar{w}_0'\Big) \end{aligned} \tag{4.24}$$

And using equations 3.43 we get second order perturbations:

$$\begin{aligned} w^{(2)} &= \Big[(C+U_0\bar{U}_1-U_1\bar{U}_0)g-(\bar{K}+U_1\bar{U}_1-U_0\bar{U}_2)h\Big]\,w_0'^2\bar{w}_0' \\ &+ \Big[(\bar{K}+U_1\bar{U}_1-U_0\bar{U}_2)g-(\bar{A}+U_1\bar{U}_1-U_0\bar{U}_3)h\Big]\,\bar{w}_0w_0'^2 \\ &+ \Big[(2K+2U_2\bar{U}_0-2U_1\bar{U}_1)g-(F+2U_2\bar{U}_1-2U_1\bar{U}_2)h\Big]\,w_0w_0'\bar{w}_0' \\ &+ \Big[(F+2U_2\bar{U}_1-2U_1\bar{U}_2)g-(2\bar{D}+2U_2\bar{U}_1-2U_1\bar{U}_3)h\Big]\,w_0\bar{w}_0w_0' \\ &+ \Big[(A+U_3\bar{U}_0-U_1\bar{U}_1)g-(D+U_3\bar{U}_1-U_1\bar{U}_2)h\Big]\,w_0^2\bar{w}_0' \\ &+ \Big[(D+U_3\bar{U}_1-U_1\bar{U}_2)g-(E+U_3\bar{U}_1-U_1\bar{U}_3)h\Big]\,w_0^2\bar{w}_0 \end{aligned} \tag{4.25}$$

5. Misalignments of Multipole Field

In this section we will derive the situation when the multipole element is shifted off axis or tilted. We will see that other multipole fields are in that case generated.

We define multipole function $\Phi_{k,f}$ of k-th order of function f as:

$$\Phi_{k,f} = \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n+k)!} (w\bar{w})^n w^k f^{(2n)} \tag{5.1}$$

And similarly complex conjugate:

$$\bar{\Phi}_{k,f} = \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n+k)!} (w\bar{w})^n \bar{w}^k f^{(2n)} \tag{5.2}$$

5.1 Shift of Multipole Field

The situation when multipole field with component ϕ_k on central is shifted off optical axis by $-\delta$ is described by substitution of coordinates $w \to w + \delta$ and $\bar{w} \to \bar{w} + \bar{\delta}$:

$$\Phi^*_{k,\phi_k} = \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n+k)!} \left((w+\delta)(\bar{w}+\bar{\delta})\right)^n (w+\delta)^k \phi_k^{(2n)} \tag{5.3}$$

By expanding the formula up to second order we get:

$$\begin{aligned}
\Phi^*_{k,\phi_k} &= \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n+k)!} (w\bar{w}))^n w^k \phi_k^{(2n)} \\
&+ \delta \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n-1+k)!} w^{n-1+k} \bar{w}^n \phi_k^{(2n)} \\
&+ \bar{\delta} \sum_{n=1}^{\infty} \frac{(-1)^n k!}{4^n (n-1)!(n+k)!} w^{n+k} \bar{w}^{n-1} \phi_k^{(2n)} \\
&+ \frac{\delta^2}{2} \sum_{n=0}^{\infty} \frac{(-1)^n k!}{4^n n!(n-2+k)!} w^{n-2+k} \bar{w}^n \phi_k^{(2n)} \\
&+ \delta\bar{\delta} \sum_{n=1}^{\infty} \frac{(-1)^n k!}{4^n (n-1)!(n-1+k)!} w^{n-1+k} \bar{w}^{n-1} \phi_k^{(2n)} \\
&+ \frac{\bar{\delta}^2}{2} \sum_{n=2}^{\infty} \frac{(-1)^n k!}{4^n (n-2)!(n+k)!} w^{n+k} \bar{w}^{n-2} \phi_k^{(2n)}
\end{aligned} \tag{5.4}$$

Where we assume that $k \geq 2$. By shifting indices it can be rewritten to more compact form:

$$\begin{aligned}
\Phi^*_{k,\phi_k} &= \Phi_{k,\phi_k} \\
&+ \delta k \Phi_{k-1,\phi_k} - \bar{\delta}\frac{1}{4(k+1)}\Phi_{k+1,\phi_k''} \\
&+ \frac{\delta^2}{2}k(k-1)\Phi_{k-2,\phi_k} - \delta\bar{\delta}\frac{1}{4}\Phi_{k,\phi_k''} + \frac{\bar{\delta}^2}{2}\frac{1}{16(k+1)(k+2)}\Phi^*_{k+2,\phi_k^{(4)}}
\end{aligned} \tag{5.5}$$

5.2 Tilt of Multipole Field

Next case is when the multipole field is tilted off axis by small angle γ. In that case the coordinates transform as:

$$\begin{aligned}
w^* &= w - \gamma z \\
\bar{w}^* &= \bar{w} - \bar{\gamma} z \\
z^* &= z + \frac{1}{2}(\gamma\bar{w} + \bar{\gamma} w)
\end{aligned} \tag{5.6}$$

The transformed field has form:

$$\Phi^*_{k,\phi_k} = \sum_{n=0}^{\infty}\frac{(-1)^n k!}{4^n n!(n+k)!}(w-\gamma z)^{n+k}(\bar{w}-\bar{\gamma}z)^n \phi_k(z + \frac{1}{2}(\gamma\bar{w}+\bar{\gamma}w))^{(2n)} \tag{5.7}$$

Which expanding to the second order of γ gives:

$$\begin{aligned}
\Phi^*_{k,\phi_k} &= \sum_{n=0}^{\infty}\frac{(-1)^n k!}{4^n n!(n+k)!}(w\bar{w}))^n w^k \phi_k^{(2n)} \\
&+ \gamma\sum_{n=0}^{\infty}\frac{(-1)^n k!}{4^n n!(n+k-1)!}w^{n-1+k}\bar{w}^n(-2n\phi_k^{(2n-1)} - z\phi_k^{(2n)}) \\
&+ \bar{\gamma}\sum_{n=0}^{\infty}\frac{(-1)^n (k+1)!}{4^n n!(n+k+1)!}w^{n+k+1}\bar{w}^n\frac{2(n+k+1)\phi_k^{(2n+1)} + z\phi_k^{(2n+2)}}{4(k+1)} \\
&+ \frac{\gamma^2}{2}\sum_{n=0}^{\infty}\frac{(-1)^n k!}{4^n n!(n+k-2)!}w^{n+k-2}\bar{w}^n\left(4(n^2-n)\phi_k^{(2n-2)} + 4nz\phi_k^{(2n-1)} + z^2\phi_k^{(2n)}\right) \\
&+ \gamma\bar{\gamma}\sum_{n=0}^{\infty}\frac{(-1)^n k!}{4^n n!(n+k)!}w^{n+k}\bar{w}^n\frac{-\left(4(kn+n^2)\phi_k^{(2n)} + (4n+2k)z\phi_k^{(2n+1)} + z^2\phi_k^{(2n+2)}\right)}{4} \\
&+ \frac{\bar{\gamma}^2}{2}\sum_{n=0}^{\infty}\frac{(-1)^n (k+2)!}{4^n (n)!(n+k+2)!}w^{n+k+2}\bar{w}^n \\
&\times\left(\frac{4(n+k+1)(n+k+2)\phi_k^{(2n+2)} + 4z(n+k+2)\phi_k^{(2n+3)} + z^2\phi_k^{(2n+4)}}{16(k+1)(k+2)}\right)
\end{aligned} \tag{5.8}$$

For simplification we will need the following formulas:

$$\begin{aligned} (zf)^{(n)} &= nf^{(n-1)} + zf^{(n)} \\ (z^2 f)^{(n)} &= n(n-1)f^{(n-2)} + +2nzf^{(n-1)} + z^2 f^{(n)} \end{aligned} \tag{5.9}$$

We can now rewrite potential as:

$$\begin{aligned} \Phi^*_{k,\phi_k} &= \Phi_{k,\phi_k} \\ &- \gamma k \Phi_{k-1,z\phi_k} + \bar{\gamma}\left[\frac{1}{4(k+1)}\Phi_{k+1,(z\phi_k)''+2k\phi'_k}\right] \\ &+ \frac{\gamma^2}{2}k(k-1)\left[\Phi_{k-2,(z^2\phi_k)-(z\phi_k)^{(-1)}-\phi_k^{(-2)}} + z\Phi_{k-2,\phi_k^{(-1)}}\right] \\ &- \gamma\bar{\gamma}\frac{1}{4}\left[\Phi_{k,(z^2\phi_k)''+(2k-3)(z\phi_k)'-(2k-1)\phi_k} - z\Phi_{k-2,\phi'_k}\right] \\ &+ \frac{\bar{\gamma}^2}{2}\frac{1}{16(k+1)(k+2)}\left[\Phi_{k,(z^2\phi_k)^{(4)}+(4k-1)(z\phi_k)'''+(4k^2-1)\phi''_k} + z\Phi_{k-2,\phi'''_k}\right] \end{aligned} \tag{5.10}$$

5.3 Ellipticity of Rotational Symmetrical Field

The last special case we derive is the elasticity effect on rotational symmetric field. We will consider just the paraxial part (without constant) of the monopole field:

$$\Phi_0 = \frac{w\bar{w}}{4}\psi''_0 \tag{5.11}$$

The ellipticity is equivalent to change of coordinate $x \to x(1+\epsilon)$, $y \to y(1-\epsilon)$ (if we assume the main axis in x, y direction). Then the field changes as:

$$\Phi^*_0 = \frac{(w+\epsilon\bar{w})(\bar{w}+\epsilon\bar{w})}{4}\psi''_0 \approx \Phi_0 + \epsilon\frac{w^2+\bar{w}^2}{4}\psi''_0 \tag{5.12}$$

Where the second term is additional quadrupole field.

6. Hexapole Corrector

In this chapter we will introduce main topic of the thesis – hexapole corrector. The first part introduces the ideal hexapole corrector and its working principle without any misalignments. The parasitic aberration caused by misalignments are calculated in the second part.

6.1 Ideal Case

We start with idealized corrector in STEM set-up. The corrector consist of two hexapoles with same fields and two lenses, with fields of different signs to eliminate rotation, which create double symmetry (lens doublet). For proper working in STEM mode we have one transfer lens before and one after the corrector. The second transfer lens image the specimen plane in the centre of the corrector and focal plane of the objective lens in the centre of the hexapoles to transfer the coma free plane from the objective and minimize spherical aberration of the fifth order[4]. The set-up with paraxial rays g, h with the parametrization in the specimen plane $g(z_i) = 1, g'(z_i) = 0, h(z_i) = 0, h'(z_i) = 0$ * , is shown in the figure 6.1.

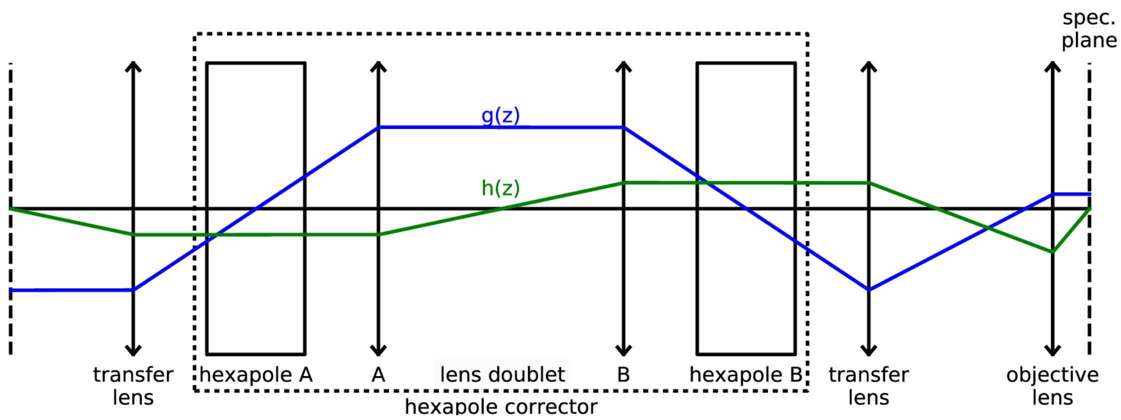


Figure 6.1: STEM set-up of hexapole corrector with paraxial rays g, h

The arrangement is in such way that the object focal plane of the first lens is in the centre of the first hexapole and the image focal plane of the second lens in the middle of the second hexapole. The image focal plane of the first lens and the object focal plane of the second lens coincide in the centre of the corrector. In this ideal case we will assume that there are thin lenses without any aberrations.

The plots in this section are done with several assumptions. We assume that the hexapole field is constant in the hexapole and zero outside. For calculation of the field of the lens we use the ψ_0' in the form:

$$\psi_0'(z) = \frac{B_{max}}{1 + \left(\frac{z-z_0}{a}\right)^2} \tag{6.1}$$

*In previous chapters we used the parametrization in the object plane.

with width of the field a small – thin lens approximation. For better visualization we have unrealistic objective lens – thin lens with specimen plane far away and low (only around 3×) magnification. The paraxial rays are thus more visible on plots. However, the formulas are written without any approximation.

The double symmetry of the corrector is crucial to eliminates all of the second aberrations. All of the integrals which has impact on the aberrations of the second order are zero outside the corrector:

$$\begin{aligned} U_0 &= \frac{6\eta}{\sqrt{\phi_r}} \int \psi_3 h^3 \mathrm{d}z \\ U_1 &= \frac{6\eta}{\sqrt{\phi_r}} \int \psi_3 g h^2 \mathrm{d}z \\ U_2 &= \frac{6\eta}{\sqrt{\phi_r}} \int \psi_3 g^2 h \mathrm{d}z \\ U_3 &= \frac{6\eta}{\sqrt{\phi_r}} \int \psi_3 g^3 \mathrm{d}z \end{aligned} \tag{6.2}$$

Integrals U_1 and U_3 are zero over one hexapole due to symmetry of ϕ_3, h^2 and antisymmetry g or g^3. The integrals U_0, U_2 are zero after propagation through both hexapoles due to change of sign of h or h^3 (figure 6.2)

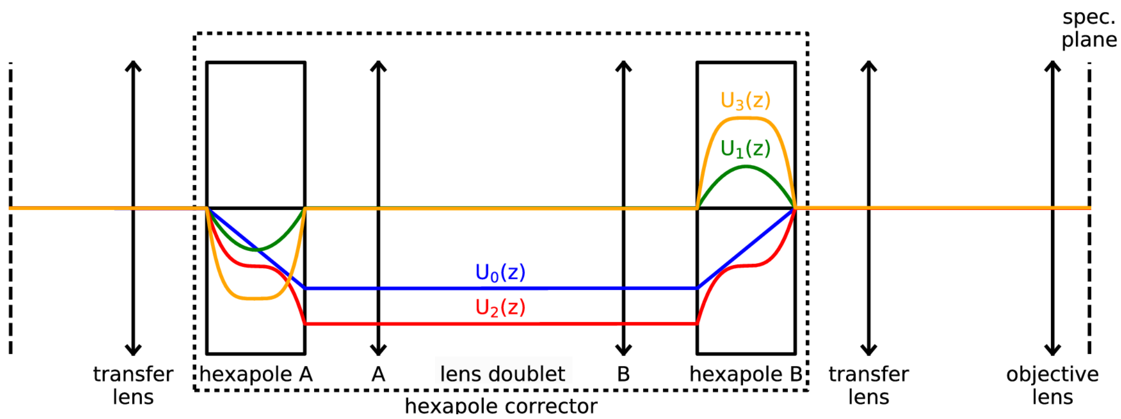


Figure 6.2: Functions U_0, U_1, U_2, U_3 in hexapole corrector with $\psi_3(z) = 1$ inside hexapole

On the other hand the aberrations of third order are not zero. The aberrations in the image plane are summation of the hexapole and monopole aberrations which has the form:

$$\begin{aligned} w^{(2)} &= C w_i'^2 \bar{w}_i' + \bar{K} \bar{w}_i w_i'^2 + 2K w_i w_i' \bar{w}_i' \\ &+ F w_i \bar{w}_i w_i' + A w_i^2 \bar{w}_i' + D w_i^2 \bar{w}_i \end{aligned} \tag{6.3}$$

The most important is the spherical aberration:

$$\begin{aligned} C &= \frac{1}{2}\int h'^4 \mathrm{d}z \\ &+\frac{1}{\sqrt{\phi_r}}\int\left(\frac{1}{32\sqrt{\phi_r}}\left(\frac{\eta^4\psi_0'^4}{\phi_r}-4\eta^2\psi_0'\psi_0'''\right)h^4+\frac{1}{4}\frac{\eta^2\psi_0'^2}{\sqrt{\phi_r}}h^2h'^2\right)\mathrm{d}z \\ &-\frac{6\eta}{\sqrt{\phi_r}}\int\left((\psi_3\bar{U}_1+\bar{\psi}_3U_1)h^3-(\psi_3\bar{U}_0+\bar{\psi}_3U_0)gh^2\right)\mathrm{d}z \end{aligned} \tag{6.4}$$

The first row is non-negligible only in the objective lens. In the area further to the left h' is smaller then $1/M$ where M is magnification of the objective lens. The integral is in the order of $1/M^4$ thus very small. Second term is the summation of the spherical aberration of the lenses and is always positive. The last term can be further simplified in the form:

$$C_H = -\int\left(U_0'\bar{U}_1-U_0\bar{U}_1'+\bar{U}_0'U_1-\bar{U}_0U_1'\right)\mathrm{d}z \tag{6.5}$$

And using integration by part:

$$C_H = -2\int\left(U_1\bar{U}_0'+\bar{U}_1U_0'\right)\mathrm{d}z \tag{6.6}$$

Let's choose orientation of the ψ_3 as a real than the sign U_1 is always the same as the sign of U_0' in the corrector and thus the spherical aberration of hexapole field is negative. The same would be valid for any orientation of ψ_3.

Spherical aberration through the hexapole corrector is shown in the figure 6.3

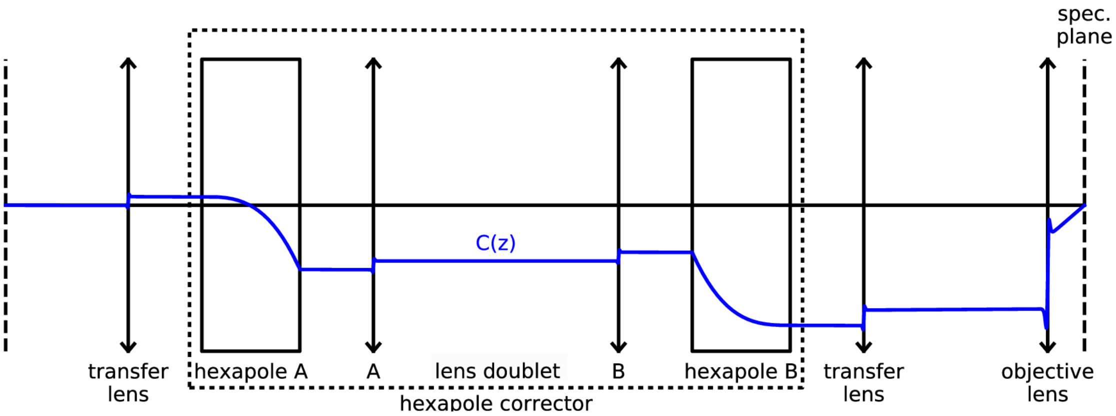


Figure 6.3: Spherical aberration in hexapole corrector. The strength of hexapoles is set in such a way that the spherical aberration in the specimen plane is zero

The next coefficient, which than play role in the axial aberration of the third order of misaligned corrector is coma:

$$\begin{aligned} K &= \frac{1}{\sqrt{\phi_r}}\int\frac{\sqrt{\phi_r}}{2}g'h'^3\mathrm{d}z \\ &+\frac{1}{\sqrt{\phi_r}}\int\left(\frac{1}{32\sqrt{\phi_r}}\left(\frac{\eta^4\psi_0'^4}{\phi_r}-4\eta^2\psi_0'\psi_0'''\right)gh^3+\frac{1}{4}\frac{\eta^2\psi_0'^2}{\sqrt{\phi_r}}hh'(gh'+hg')\right)\mathrm{d}z \\ &+\frac{1}{\sqrt{\phi_r}}\int\left(-6\eta\left(\bar{\psi}_3U_2h^3-(\bar{\psi}_3U_1-\psi_3\bar{U}_1)gh^2-\psi_3\bar{U}_0g^2h\right)\right)\mathrm{d}z \end{aligned} \tag{6.7}$$

we can simplify hexapole term:

$$K_H = -\int \left(U_2 \bar{U}_0{}' - \bar{U}_1{}' U_1 + U_1' \bar{U}_1 - U_2' \bar{U}_0 \right) \mathrm{d}z \tag{6.8}$$

Which due to symmetry is zero outside of the corrector:

6.1.1 Evaluation of Spherical Aberration

It is useful to evaluate integral 6.6 with optical parameters. In set-up described in figure 6.1 g, h trajectories in first hexapole are:

$$\begin{aligned} h &= \frac{f_T}{M_o} \\ g &= -\frac{M_o}{f_T} z \end{aligned} \tag{6.9}$$

where f_T focal length of the second transfer lens just before objective, M_o magnification of objective lens. We also assume local coordinate system: z is zero in the middle of hexapole, in the second hexapole the situation is similar with just different signs of functions g, h. Now we assume that the hexapole field is constant inside hexapole with length L and zero outside. In that case spherical aberration of two hexapole is:

$$C_H = -\frac{24\eta^2 |\psi_3|^2}{\phi_r} \left(\frac{f_T}{M_o} \right)^4 L^3 \tag{6.10}$$

If we have high magnification of the objective lens the spherical aberration of objective is the most significant. To have a image without spherical aberration of the third order the spherical aberration of hexapoles should be comparable (higher) to the spherical aberration of the objective we also evaluate the integral U_0 over one hexapole:

$$U_{0A} = \frac{6\eta\psi_3}{\sqrt{\phi_r}} \left(\frac{f_T}{M_o} \right)^3 L \tag{6.11}$$

By evaluating absolute value of U_{0A} as a function of C_H we get:

$$|U_{0A}| = \sqrt{\frac{3C_H}{2L} \frac{f_T}{M_o}} \tag{6.12}$$

This value is quite big in-between the hexapoles. In fact the first hexapole create very distorted beam and the second hexapole improve it back.

6.1.2 Symmetry in Corrector

In this part we introduce the symmetry concept in hexapole corrector. Generally, we can split any function in the symmetric and asymmetric part with respect to a plane. In hexapole corrector we have two sets of planes – the centre of entire corrector and centres of hexapoles. If we mark symmetric part of the function by S and asymmetric by A we can define algebra with following operations of addition:

$$\begin{aligned} A + A &= A \\ S + S &= S \end{aligned} \tag{6.13}$$

multiplication:

$$\begin{aligned} A \cdot A &= S \\ A \cdot S &= A \\ S \cdot A &= A \\ S \cdot S &= S \end{aligned} \tag{6.14}$$

derivative and integration:

$$\begin{aligned} A' &= S \\ S' &= A \\ \int A &= S \\ \int S &= A + S_{const.} \end{aligned} \tag{6.15}$$

In Table 6.1, there is a list of symmetry of the most important functions in ideal hexapole corrector.

Table 6.1: Symmetry of functions in ideal hexapole corrector

function	centre of corrector	centres of hexapoles
$g, \bar{g}$	S	A
$h, \bar{h}$	A	S
θ	S	0
ψ_0'	A	0
ψ_3	S	S
U_0, U_2	S	$A + S_{const.}$
U_1, U_3	A	S
C	$A + S_{const.}$	$A + S$
K	S	$A + S$

6.2 Parasitic Aberrations

In reality hexapole corrector is never ideal. Quite opposite, it is very sensitive to all misalignments since we require to correct third order aberrations. In this section we will cover all major misalignments and its induced aberrations in image.

Every element in corrector can be shifted and tilted off axis, hexapoles can be also rotated around z. Also it can be shifted in z-axis and have imperfect poles. In this text we will at first focus on axial misalignments - we will see that the most important is the mis-rotation of the two hexapoles. Than we will deal with off-axial misalignments. Generally we can distinguish between the shifts and tilts and errors of the pole pieces of the hexapoles and lenses. However, the errors has exactly the same behaviour as the shift and tilt (in case of hexapole) so it will be treated implicitly. For the lens we will assume additional quadrupole field due to the ellipticity.

6.2.1 Axial Misalignments

Let us look at the different rotation of the hexapoles. If the hexapole fields are misaligned with angle θ around z-axis we can write:

$$\psi_3 = \psi_{3A} = \psi_{3B} e^{i\theta} \tag{6.16}$$

In this case integrals U_1, U_3 are still zero but not U_0, U_2:

$$\begin{aligned} U_0 &= \frac{6\eta}{\sqrt{\phi_r}} \left(1 - e^{-i\theta}\right) \int_A \psi_3 h_A^3 \mathrm{d}z \\ U_2 &= \frac{6\eta}{\sqrt{\phi_r}} \left(1 - e^{-i\theta}\right) \int_A \psi_3 g_A^2 h_A \mathrm{d}z \end{aligned} \tag{6.17}$$

Where integral the double symmetry is already used for simplification and it is integrated just over A hexapole. We can eliminate this by asymmetric excitation of the lenses which produces rotation angle $\theta/3$. This, however, results in magnification of the rays g, h and we need to modify strength of hexapoles as we will see further.

The similar effect is the z-position of elements and rotation of the hexapoles. The ideal focus length of lenses is defined such as there is the common focal plane in between of lenses. This, however, means that the centres of the hexapoles do not have to be in the focal plane of the lenses. If it is the case integrals U_1, U_2, U_3 do not necessary vanish. The trajectories of g, h with image rotation θ are shown in figure 6.4

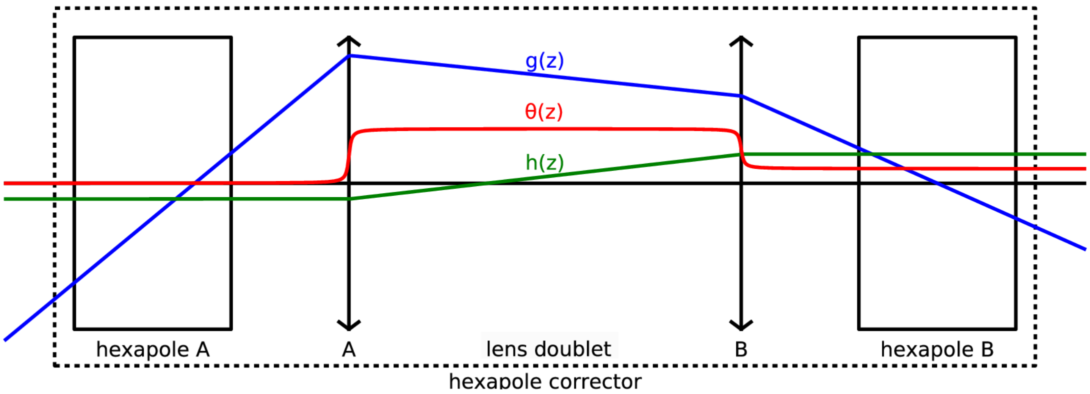


Figure 6.4: Correction of different orientation of hexapoles - g, h rays and image rotation θ

We have two degrees of freedom - two excitations of the lens doublets. They are used in such way that the rotation around z-axis is $\theta/3$ and that they have common central focal plane in-between. In that case the ray h in two hexapoles is:

$$h_B = M h_A e^{i\theta/3} \tag{6.18}$$

Where h_A is trajectory h in the first hexapole, h_B in the second and M is the magnification of the doublet:

$$M = -\frac{f_B}{f_A} \approx -1 - \frac{\Delta_f}{f} \tag{6.19}$$

where f_B, f_A are focal lengths of lenses, Δ_f is the difference and f is an average of f_B, f_A. As a consequence g ray is not necessary antisymmetric and we get residual non-vanishing U_1, U_2, U_3. We still would like to eliminate U_0:

$$U_0 = \frac{6\eta}{\sqrt{\phi_r}}\left(\int_A \psi_{3A} h^3 \mathrm{d}z - M^3 \int_B \psi_{3B} e^{-i\theta} h^3 \mathrm{d}z\right) \tag{6.20}$$

To do so we set excitations ψ_{3A}, ψ_{3B} such as:

$$|\psi_{3B}| = |\psi_{3A}|/M^3 \tag{6.21}$$

6.2.2 Monopole Off-axial Misalignments

Now we will explore off-axis misalignments. We will start with misalignments of lenses. Both shift and tilt will induce additional dipole field as we saw from section 5. We will assume that δ and $\gamma z \approx 2\gamma f$ are smaller than $w, \bar{w}$ of realized trajectories in lenses. In that case we will just use first expansion of the modified monopole field and neglect the terms of second and higher order of δ and γ. We Thus get additional dipole fields:

$$\begin{aligned} \psi_{1\bar{\delta}} &= -\frac{1}{4}\bar{\delta}\psi_0'' \\ \psi_{1\bar{\gamma}} &= \frac{1}{4}\bar{\gamma}\left(z\psi_0\right)'' \quad \dagger \end{aligned} \tag{6.22}$$

The lens can also be elliptic so we have additional dipole field ψ_{2L} which can be split into symmetric and antisymmetric part with respect to the centre of the corrector -$\psi_2 = \psi_{2+} + \psi_{2-}$.

The important feature is also symmetry of the misalignments. We define off axial shift of first and second lens as δ_A, δ_B and tilt γ_A, γ_B. In that case we can split dipole and quadrupole generated fields to symmetric and antisymmetric parts (Table 6.2).

† Every time we write this, we mean local coordinates in optical element - $z\psi_0$ means $(z - z_A)\psi_{0A}$ in lens A and $(z - z_B)\psi_{0B}$ where z_A, z_B are z-coordinates of centre of the lens A, B

Table 6.2: Symmetry of misalignments of lens doublet

function	centre of corrector	centres of hexapoles
$\psi_{1\bar{\delta}-} = (\delta_A + \delta_B)\psi_0''/2$	A	0
$\psi_{1\bar{\delta}+} = (\delta_A - \delta_B)(\psi_{0A}'' - \psi_{0B}'')/2$	S	0
$\psi_{1\bar{\gamma}-} = (\gamma_A - \gamma_B)(z\psi_0)''/2$	A	0
$\psi_{1\bar{\gamma}+} = (\gamma_A + \gamma_B)((z\psi_{0A})'' - (z\psi_{0B})'')/2$	S	0
ψ_{2L-}	A	0
ψ_{2L+}	S	0

6.2.3 Hexapole Off-axial Misalignments

In case of hexapole we get additional quadrupole and octupole field. Also now we cannot neglect dipole field term:

$$\begin{aligned}
\psi_{1\delta^2} &= 3\delta^2\psi_3 \\
\psi_{2\delta} &= 3\delta\psi_3 \\
\psi_{4\bar{\delta}} &= -\frac{1}{16}\bar{\delta}\psi_3'' \\
\\
\psi_{1\gamma^2} &= 3\gamma^2 z^2\psi_3 \qquad (\ddagger) \\
\psi_{2\gamma} &= 3\gamma z\psi_3 \\
\psi_{4\bar{\gamma}} &= -\frac{1}{16}\bar{\gamma}\left((z\psi_3)'' + 6\psi_3'\right)
\end{aligned} \tag{6.23}$$

Similarly as with misalignments of lens we can split it into symmetric and antisymmetric parts (Table 6.3).

6.2.4 Lagrangians

The Lagrangian for hexapole corrector then looks like:

$$\begin{aligned}
M_2 &= -\frac{\sqrt{\phi_r}}{2}w'\bar{w}' \\
&\quad -\frac{i\eta}{4}\psi_0'\left(w\bar{w}' - \bar{w}w'\right)
\end{aligned} \tag{6.24}$$

$$M_{2b} = i\eta\epsilon\left(\psi_{1L}w - \bar{\psi}_{1L}\bar{w}\right) \tag{6.25}$$

$$\begin{aligned}
M_3 &= i\eta\left(\psi_3 w^3 - \bar{\psi}_3\bar{w}^3\right) \\
&\quad + i\eta\epsilon\left(\psi_2 w^2 - \bar{\psi}_2\bar{w}^2\right) \\
&\quad + i\eta\epsilon^2\left(\psi_1 w - \bar{\psi}_1\bar{w}\right)
\end{aligned} \tag{6.26}$$

‡It is true just for the first expansion term $\psi_1 w$, but we will not need more

Table 6.3: Symmetry of misalignments of hexapoles

function	centre of corrector	centres of hexapoles
$\psi_{1\bar{\delta}^2+} = 3/2(\delta_A^2 + \delta_B^2)\psi_3$	S	S
$\psi_{1\bar{\delta}^2-} = 3/2(\delta_A^2 - \delta_B^2)(\psi_{3A} - \psi_{3B})$	A	S
$\psi_{1\bar{\gamma}^2+} = 3/2(\gamma_A^2 + \gamma_B^2)z^2\psi_3$	S	S
$\psi_{1\bar{\gamma}^2-} = 3/2(\gamma_A^2 - \gamma_B^2)z^2(\psi_{3A} - \psi_{3B})$	A	S
$\psi_{2\bar{\delta}+} = 3/2(\delta_A + \delta_B)\psi_3$	S	S
$\psi_{2\bar{\delta}-} = 3/2(\delta_A - \delta_B)(\psi_{3A} - \psi_{3B})$	A	S
$\psi_{2\bar{\gamma}+} = 3/2(\gamma_A - \gamma_B)z\psi_3$	S	A
$\psi_{2\bar{\gamma}-} = 3/2(\gamma_A + \gamma_B)z(\psi_{3A} - \psi_{3B})$	A	A
$\psi_{4\bar{\delta}+} = -1/32(\bar{\delta}_A + \bar{\delta}_B)\psi_3''$	S	S
$\psi_{4\bar{\delta}-} = -1/32(\bar{\delta}_A - \bar{\delta}_B)(\psi_{3A}'' - \psi_{3B})''$	A	S
$\psi_{4\bar{\gamma}+} = -1/32(\bar{\gamma}_A - \bar{\gamma}_B)\left((z\psi_3)'' + 6\psi_3'\right)$	S	A
$\psi_{4\bar{\gamma}-} = -1/32(\bar{\gamma}_A + \bar{\gamma}_B)\left((z\psi_3)'' + 6\psi_3'\right)_{A-B}$	A	A

$$\begin{aligned} M_4 &= -\frac{\sqrt{\phi_r}}{8}w'^2\bar{w}'^2 \\ &+\frac{i\eta}{32}\psi_0'''w\bar{w}\left(w\bar{w}' - \bar{w}w'\right) \\ &+\frac{i\eta}{8}\epsilon\left(2w\bar{w}\left(\psi_{1L}'w' - \bar{\psi}_{1L}'\bar{w}'\right) - \left(\psi_{1L}'\bar{w}'w^2 - \bar{\psi}_{1L}'w'\bar{w}^2\right)\right) \end{aligned} \tag{6.27}$$

$$\begin{aligned} M_5 &= i\eta\epsilon\left(\psi_4 w^4 - \bar{\psi}_4\bar{w}^4\right) \\ &+\frac{i\eta}{16}\left(4w\bar{w}\left(\psi_3'w^2w' - \bar{\psi}_3'\bar{w}^2\bar{w}'\right) - \left(\psi_3'\bar{w}'w^4 - \bar{\psi}_3'w'\bar{w}^4\right)\right) \\ &+\frac{i\eta}{12}\epsilon\left(3w\bar{w}\left(\psi_2'ww' - \bar{\psi}_2'\bar{w}\bar{w}'\right) - \left(\psi_2'\bar{w}'w^3 - \bar{\psi}_2'w'\bar{w}^3\right)\right) \end{aligned} \tag{6.28}$$

Where in M_2 there is paraxial solution including just lenses. M_{2b} is correction of paraxial solution due to shift and tilt of the lenses. M_3 includes hexapole field and it's quadrupole and dipole field due to shift and tilt (we do not higher expansion term of dipole field in higher order Lagrangians because it is very weak) and also quadrupole field of the ellipticity of the lenses. In M_4 are aberrations of the lenses and it's dipole field. Finally in M_5 there higher order terms of hexapole field - hexapole and weak octupole with quadrupole. We use factor ϵ to deal with weak fields (at the end of calculation we will put $\epsilon = 1$).

6.2.5 Paraxial Solution

Let's define paraxial equation of magnetic lens:

$$\omega'' + \frac{\eta^2\psi_0'^2}{4\phi_r}\omega = 0 \tag{6.29}$$

with solutions $\tilde{g}, \tilde{h}$ which satisfy the conditions in the specimen plane:

$$\begin{array}{ll} \tilde{g}(z_i) = 1 & \tilde{g}'(z_i) = 0 \\ \tilde{h}(z_i) = 0 & \tilde{h}'(z_i) = 1 \end{array} \tag{6.30}$$

Then solutions of Lagrangian M_2:

$$M_2 = -\frac{\sqrt{\phi_r}}{2} w'\bar{w}' - \frac{i\eta}{4}\psi_0' \left(w\bar{w}' - \bar{w}w'\right) \tag{6.31}$$

are:

$$\begin{aligned} w^{(0)} &= w_i g + w_i' h \\ \bar{w}^{(0)} &= \bar{w}_i \bar{g} + \bar{w}_i' \bar{h} \end{aligned} \tag{6.32}$$

where $g, h, \bar{g}, \bar{h}$ are rotated solutions:

$$\begin{aligned} g &= \tilde{g}e^{i\theta} \\ \bar{g} &= \tilde{g}e^{-i\theta} \\ h &= \tilde{h}e^{i\theta} \\ \bar{h} &= \tilde{h}e^{-i\theta} \end{aligned} \tag{6.33}$$

and rotation of image θ is defined as:

$$\theta = \frac{\eta\psi_0}{2\sqrt{\phi_r}} \tag{6.34}$$

6.2.6 Correction of Paraxial Solution

The Lagrangian of paraxial correction is:

$$M_{2b} = i\eta\epsilon\left(\psi_{1L} w - \bar{\psi}_{1L}\bar{w}\right) \tag{6.35}$$

and calculated correction trajectory:

$$o(z) = \frac{i\eta\epsilon\bar{g}}{2\sqrt{\phi_r}} \int \bar{\psi}_{1L}\bar{h}\,\mathrm{d}z - \frac{i\eta\epsilon\bar{h}}{2\sqrt{\phi_r}} \int \bar{\psi}_{1L}\bar{g}\,\mathrm{d}z \tag{6.36}$$

Then:

$$\begin{aligned} w^{(0)} &= w_i g + w_i' h + o \\ \bar{w}^{(0)} &= \bar{w}_i \bar{g} + \bar{w}_i' \bar{h} + \bar{o} \end{aligned} \tag{6.37}$$

is exact solution of corrected paraxial equation of Lagrangian $M_2 + M_{2b}$

Let's look at the correction in details we express the dipole field as the shift and tilt of the first and second lenses in the image plane:

$$o(z_i) = \frac{i\eta}{4\sqrt{\phi_r}}\left(-\delta_A \int_A \psi_0''\bar{h}\,\mathrm{d}z - \delta_B \int_B \psi_0''\bar{h}\,\mathrm{d}z + \gamma_A \int_A (z\psi_0)''\bar{h}\,\mathrm{d}z + \gamma_B \int_B (z\psi_0)''\bar{h}\,\mathrm{d}z\right)$$

Due to symmetry of the corrector we can write:

$$o(z_i) \quad = \quad \frac{i\eta}{4\sqrt{\phi_r}}\left(-(\delta_A+\delta_B)\int_A \psi_0''\bar{h}\,\mathrm{d}z + (\gamma_A-\gamma_B)\int_A (z\psi_0)''\bar{h}\,\mathrm{d}z\right) \tag{6.38}$$

Further more integrating paraxial equation we can get formula:

$$\frac{i\eta}{2\sqrt{\phi_r}}\int \psi_0''w\,\mathrm{d}z = \left[w' + \frac{i\eta}{\sqrt{\phi_r}}\psi_0'w\right]_{z_0}^{z} \tag{6.39}$$

Which gives for $\bar{h}$:

$$\frac{i\eta}{2\sqrt{\phi_r}}\int \psi_0''\bar{h}\,\mathrm{d}z = \left[\bar{h}' + \frac{i\eta}{\sqrt{\phi_r}}\psi_0'\bar{h}\right]_{z_0}^{z} = h'(\bar{z_i}) - h'(\bar{z_o}) = \frac{M-1}{M} \tag{6.40}$$

where $M = h'(z_i)/h'(z_o)$ is the magnification of the transfer and objective lens. We can simplify 6.38 as:

$$o(z_i) \quad = \quad \frac{M-1}{M}\frac{\delta_A+\delta_B}{2} + \frac{i\eta(\gamma_A-\gamma_B)}{4\sqrt{\phi_r}}\int_A (z\psi_0)''\bar{h}\,\mathrm{d}z$$

The meaning of this is obvious - there can be only seen the relative shift of the two lenses and it's sum of tilts in the image plane. The shift of the image due to the misalignments of lenses can be compensated by deflection system. The pure shift does not influence resolution but the misalignments produce additional aberrations of higher order and thus it is desirable to correct it.

6.2.7 First Order Aberrations

We put paraxial solution to the Lagrangian M_3 and calculate eikonal S^I. We define functions:

$$\begin{aligned} U_0 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 h^3\mathrm{d}z \\ U_1 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g h^2\mathrm{d}z \\ U_2 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g^2 h\mathrm{d}z \\ U_3 &= \frac{6\eta}{\sqrt{\phi_r}}\int \psi_3 g^3\mathrm{d}z \end{aligned} \tag{6.41}$$

$$\begin{aligned} V_0 &= \frac{\eta}{\sqrt{\phi_r}}\int \left(6\psi_3 o + 2\psi_2\right) h^2\mathrm{d}z \\ V_1 &= \frac{\eta}{\sqrt{\phi_r}}\int \left(6\psi_3 o + 2\psi_2\right) gh\mathrm{d}z \\ V_2 &= \frac{\eta}{\sqrt{\phi_r}}\int \left(6\psi_3 o + 2\psi_2\right) g^2\mathrm{d}z \end{aligned} \tag{6.42}$$

$$W_0 = \frac{\eta}{\sqrt{\phi_r}} \int \left(6\psi_3 o^2 + 4\psi_2 o + 2\psi_1\right) h\mathrm{d}z \tag{6.43}$$
$$W_1 = \frac{\eta}{\sqrt{\phi_r}} \int \left(6\psi_3 o^2 + 4\psi_2 o + 2\psi_1\right) g\mathrm{d}z$$

$$o_3 = \frac{2\eta}{\sqrt{\phi_r}} \int \left(\psi_3 o^3 + \psi_2 o^2 + \psi_1 o\right) \mathrm{d}z \tag{6.44}$$

Eikonal S^I then looks like:

$$\begin{aligned} S^I = & \frac{i\sqrt{\phi_r}}{2}\left(\frac{U_0}{3} w_0'^3 + U_1 w_0'^2 w_i + U_2 w_0' w_i^2 + \frac{U_3}{3} w_i^3\right) \\ & + \frac{i\sqrt{\phi_r}}{2}\epsilon\left(V_0 w_0'^2 + V_1 w_0' w_i + V_2 w_i^2\right) \\ & + \frac{i\sqrt{\phi_r}}{2}\epsilon^2\left(w_i w_0' + W_1 w_i\right) \\ & + \frac{i\sqrt{\phi_r}}{2}\epsilon^3 O_3 \\ & + c.c. \end{aligned} \tag{6.45}$$

And the first order aberrations looks like:

$$\begin{aligned} w^{(1)} = & i\left(\bar{g}\bar{U}_0 - \bar{h}\bar{U}_0\right)\bar{w}_0'^2 \\ & + i\left(2\bar{g}\bar{U}_1 - 2\bar{h}\bar{U}_2\right)\bar{w}_0'\bar{w}_i \\ & + i\left(\bar{g}\bar{U}_2 - \bar{h}\bar{U}_3\right)\bar{w}_0^2 \\ & + i\left(2\bar{g}\bar{V}_0 - \bar{h}\bar{V}_1\right)\bar{w}_0' \\ & + i\left(\bar{g}\bar{V}_1 - 2\bar{h}\bar{V}_2\right)\bar{w}_i \\ & + i\left(\bar{g}\bar{w}_i - \bar{h}\bar{W}_1\right) \end{aligned} \tag{6.46}$$

In the image plane all first three row with just dependence on hexapole field integrals vanish due to symmetry as was written before, the rest is:

$$w^{(1)}(z_i) = 2i\bar{V}_0\bar{w}_0' + i\bar{V}_1\bar{w}_i + i\bar{w}_i \tag{6.47}$$

Monopole Astigmatism

Second thing what we have to consider is ellipticity of the lenses. Let's define common quadrupole field of lenses ψ_{2L} we can split it in the symmetric and antisymmetric part with respect to centre of the corrector $\psi_{2L} = \psi_{2L+} + \psi_{2L-}$. In that case we can write for V_0, V_1, w_i:

$$
\begin{aligned}
V_0 &= \frac{4\eta}{\sqrt{\phi_r}} \int_A \psi_{2L+} h^2 \mathrm{d}z \\
V_1 &= \frac{4\eta}{\sqrt{\phi_r}} \int_A \psi_{2L-} g h \mathrm{d}z \\
W_0 &= \frac{\eta}{\sqrt{\phi_r}} \int \psi_{2L} o h \mathrm{d}z
\end{aligned} \tag{6.48}
$$

And aberrations in image plane:

$$
\begin{aligned}
w_L^{(1)}(z_i) &= \left(\frac{4\eta}{\sqrt{\phi_r}} \int_A \psi_{2L+} h^2 \mathrm{d}z \right) \bar{w}_0' \\
&+ \left(\frac{4\eta}{\sqrt{\phi_r}} \int_A \psi_{2L-} g h \mathrm{d}z \right) \bar{w}_i \\
&+ \left(\frac{\eta}{\sqrt{\phi_r}} \int \psi_{2L} o h \right)
\end{aligned} \tag{6.49}
$$

Hexapole Misalignments

We start with evaluating the misalignments of hexapole and it's influence on first order aberrations. Let's look at the integral V_0 over corrector, the function o is zero in the first hexapole and $o(z)$ linear in the second. The integration with symmetric function $\psi_3 h^2$ with respect to the centre of hexapole gives:

$$
V_0 = \frac{6\eta o(z_{HB})}{\sqrt{\phi_r}} \int_B \psi_3 h^2 \mathrm{d}z + \frac{2\eta}{\sqrt{\phi_r}} \int \psi_2 h^2 \mathrm{d}z \tag{6.50}
$$

Where $o(z_{HB})$ is calculated in the middle of the second hexapole:

$$
o(z_{HB}) = -\frac{i\epsilon \bar{h}(z_{HB})}{2\sqrt{\phi_r}} \int \bar{\psi}_{1L} \bar{g} \, \mathrm{d}z \tag{6.51}
$$

For simplicity we will write just $o_B = o(z_H B)$ and $o_B' = o'(z_H B)$. By expanding quadrupole term $\psi_2 = 3\delta\psi_3 + 3\gamma z \psi_3$ with using local coordinate systems of optical elements with $z = 0$ in the centre:

$$
\begin{aligned}
V_0 &= \frac{6\eta o_B}{\sqrt{\phi_r}} \int_B \psi_3 h^2 \mathrm{d}z \\
&+ \frac{6\eta}{\sqrt{\phi_r}} \left(\delta_A \int_A \psi_3 h^2 \mathrm{d}z + \delta_B \int_B \psi_3 h^2 \mathrm{d}z + \gamma_A \int_A z\psi_3 h^2 \mathrm{d}z + \gamma_B \int_B z\psi_3 h^2 \mathrm{d}z \right)
\end{aligned} \tag{6.52}
$$

The integrals $\int z\psi_3 h^2 \mathrm{d}z$ are zero due to the symmetry and integrals $\int_A \psi_3 h^2 \mathrm{d}z$, $\int_B \psi_3 h^2 \mathrm{d}z$ are same, thus:

$$
V_0 = (o_B + \delta_A + \delta_B) \frac{6\eta}{\sqrt{\phi_r}} \int_A \psi_3 h^2 \mathrm{d}z \tag{6.53}
$$

We can obtain similar results for V_1:

$$V_1 = (o'_B + \gamma_A + \gamma_B) \frac{6\eta}{\sqrt{\phi_r}} \int_A z\psi_3 gh \mathrm{d}z \tag{6.54}$$

To expand integral w_i we substitute dipole field as well $\psi_1 = 3\delta^2\psi_3 + 3\gamma^2 z\psi_3$ and use symmetry:

$$\begin{aligned} W_0 &= \frac{6\eta o_B^2}{\sqrt{\phi_r}} \int_B \psi_3 h \mathrm{d}z + \frac{6\eta o_B'^2}{\sqrt{\phi_r}} \int_B z^2\psi_3 h \mathrm{d}z \\ &+ \frac{12\eta}{\sqrt{\phi_r}} \left(o_B\delta_B \int_B \psi_3 h \mathrm{d}z + o'_B\gamma_B \int_B z^2\psi_3 h \mathrm{d}z \right) \\ &+ \frac{6\eta}{\sqrt{\phi_r}} \left(\delta_A^2 \int_A \psi_3 h \mathrm{d}z + \delta_B^2 \int_B \psi_3 h \mathrm{d}z + \gamma_A^2 \int_A z^2\psi_3 h \mathrm{d}z + \gamma_B^2 \int_B z^2\psi_3 h \mathrm{d}z \right) \end{aligned} \tag{6.55}$$

Which gives:

$$\begin{aligned} W_0 &= \frac{6\eta}{\sqrt{\phi_r}} \left(\delta_A^2 - (o_B + \delta_B)^2\right) \int_A \psi_3 h \mathrm{d}z \\ &+ \frac{6\eta}{\sqrt{\phi_r}} \left(\gamma_A^2 - (o'_B + \gamma_B)^2\right) \int_A \psi_3 z^2 h \mathrm{d}z \end{aligned} \tag{6.56}$$

Putting it all together and using equality $z = h = \bar{h}$,$g = \bar{g} = 1$ in first hexapole:

$$\begin{aligned} w_H^{(1)}(z_i) &= \left((\bar{o}_B + \bar{\delta}_A + \bar{\delta}_B) \frac{6i\eta}{\sqrt{\phi_r}} \int_A \bar{\psi}_3 h^2 \mathrm{d}z \right) \bar{w}'_0 \\ &+ \left((\bar{o'}_B + \bar{\gamma}_A + \bar{\gamma}_B) \frac{6i\eta}{\sqrt{\phi_r}} \int_A z\bar{\psi}_3 gh \mathrm{d}z \right) \bar{w}_i \\ &+ \left(\bar{\delta}_A^2 - (\bar{o}_B + \bar{\delta}_B)^2\right) \frac{6\eta}{\sqrt{\phi_r}} \int_A \psi_3 h \mathrm{d}z \\ &+ \left(\bar{\gamma}_A^2 - (\bar{o}'_B + \bar{\gamma}_B)^2\right) \frac{6\eta}{\sqrt{\phi_r}} \int_A \psi_3 z^2 h \mathrm{d}z \end{aligned} \tag{6.57}$$

The last term is already in the second order of parasitic aberrations (ϵ^2) and does not influence resolution. It is not negligible when comparing with spherical aberration, so we written it down, however any higher aberration which are order ϵ^2 or higher will be smaller thus we neglect it.

To graphically interpret the equation above we can look in Figure 6.5. If we have asymmetric shifts of hexapole fields and ellipticity of doublet we get zero V_0 at the end of corrector. We can use it to correct V_0 in the image induced by lenses (figure 6.6).

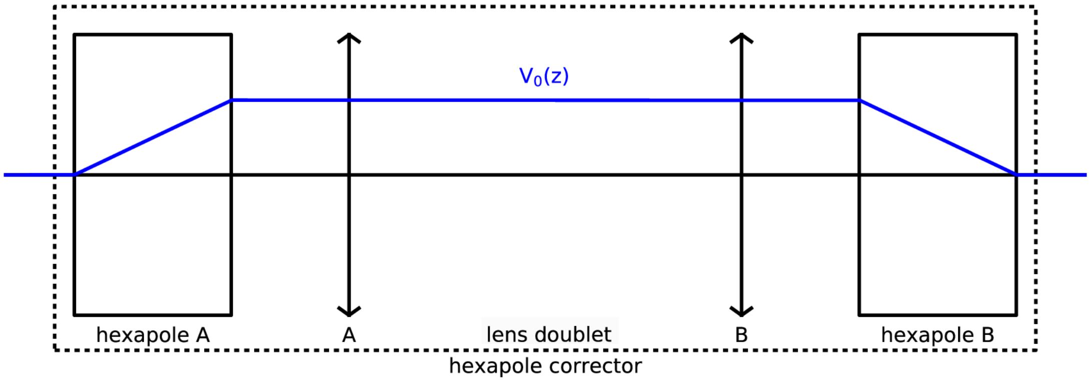


Figure 6.5: The function V_0, V_1 through hexapole corrector with $\delta_A = -\delta_B$, $o = 0$, $\gamma_A = 0$, $\gamma_B = 0$ and $\psi_{2L} = 0$

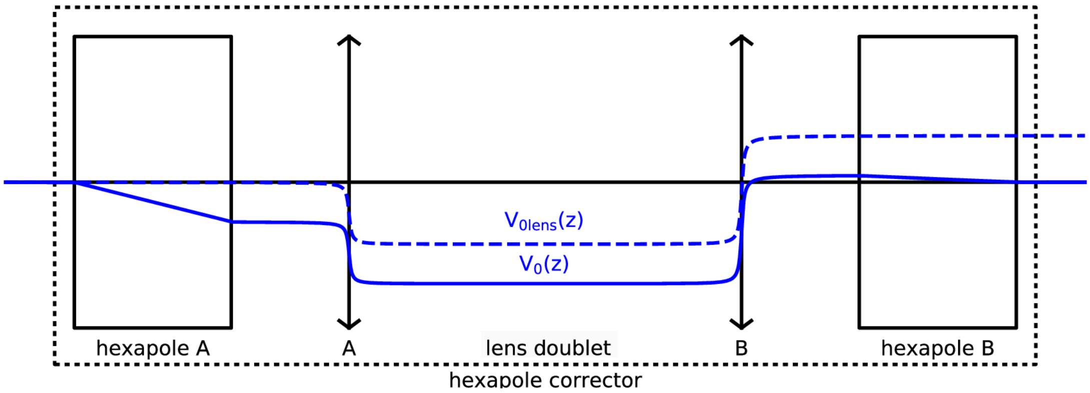


Figure 6.6: V_0 of lens doublet and it's correction by hexapole shifts $\delta_A = \delta_B$

6.2.8 Second Order Aberrations

The second order aberrations are becoming more complicated. We start with calculation of integral of M_4:

$$
\begin{aligned}
M_4 \quad = \quad & -\frac{\sqrt{\phi_r}}{8} w'^2 \bar{w}'^2 \\
& + \frac{i\eta}{32} \psi_0''' w\bar{w} \left(w\bar{w}' - \bar{w}w' \right) \\
& + \frac{i\eta}{8} \epsilon \left(2w\bar{w} \left(\psi_{1L}' w' - \bar{\psi}_{1L}' \bar{w}' \right) - \left(\psi_{1L}' \bar{w}' w^2 - \bar{\psi}_{1L}' w' \bar{w}^2 \right) \right)
\end{aligned}
\tag{6.58}
$$

The eikonal S^{II} has form:

$$\begin{aligned} S^{II} \;=\; -\sqrt{\phi_r}\,\Big(& \frac{C}{4}\bar{w}_0'^2 w_0'^2 + \frac{F}{2}w_0\bar{w}_0\bar{w}_0'w_0' + \frac{E}{4}w_0^2\bar{w}_0^2 \\ & +\frac{K}{2}w_0\bar{w}_0'^2w_0' + \frac{\bar{K}}{2}\bar{w}_0\bar{w}_0'w_0'^2 \\ & +\frac{A}{4}w_0^2\bar{w}_0'^2 + \frac{\bar{A}}{4}\bar{w}_0^2w_0'^2 \\ & +\frac{D}{2}\bar{w}_0w_0^2\bar{w}_0' + \frac{\bar{D}}{2}w_0\bar{w}_0^2w_0'\Big) \\ -\sqrt{\phi_r}\epsilon\,\Big(& \frac{B_2}{2}w_0'\bar{w}_0'^2 + \frac{A_2}{2}\bar{w}_0\bar{w}_0'w_0' + \frac{C_2}{2}w_0\bar{w}_0'^2 + \frac{D_2}{2}w_0'\bar{w}_0^2 + \frac{E_2}{2}w_0\bar{w}_0\bar{w}_0' + \frac{F_2}{2}w_0\bar{w}_0^2 \\ & +\frac{\bar{B}_2}{2}\bar{w}_0'w_0'^2 + \frac{\bar{A}_2}{2}w_0\bar{w}_0'w_0' + \frac{\bar{C}_2}{2}\bar{w}_0w_0'^2 + \frac{\bar{D}_2}{2}\bar{w}_0'w_0^2 + \frac{\bar{E}_2}{2}w_0\bar{w}_0w_0' + \frac{\bar{F}_2}{2}\bar{w}_0w_0^2\Big) \end{aligned} \tag{6.59}$$

Where the coefficients are sum of free field, monopole, dipole, hexapole and quadrupole-hexapole coupling coefficients defined in the appendix. The general second order trajectory is complicated (see appendix). It simplify in the image plane as:

$$\begin{aligned} w^2(z) \;=\; & C\bar{w}_0'{w'}_0^2 + \bar{K}\bar{w}_0{w'}_0^2 + 2Kw_0\bar{w}_0'{w'}_0 + Fw_0\bar{w}_0{w'}_0 + Aw_0^2\bar{w}_0' + Dw_0^2\bar{w}_0 \\ + \;& \epsilon\left(\bar{B}_2{w'}_0^2 + 2B_2\bar{w}_0'{w'}_0 + \bar{A}_2w_0{w'}_0 + A_2\bar{w}_0{w'}_0 + 2C_2w_0\bar{w}_0' + \bar{D}_2w_0^2 + E_2w_0\bar{w}_0\right) \end{aligned} \tag{6.60}$$

We will now focus on error axial coefficients B_2. It consists of four integrals:

$$\begin{aligned} B_{2F} &= \int \frac{1}{2}\bar{h}'^2h'o'\mathrm{d}z \\ B_{2M} &= \frac{i\eta}{16\sqrt{\phi_r}}\int \left(h\bar{h}^2o' - 2h\bar{h}\bar{h}'o + \bar{h}^2h'o\right)\psi_0'''\mathrm{d}z \\ B_{2D} &= \frac{i\eta}{4\sqrt{\phi_r}}\int \left(2h\bar{h}\bar{h}' - \bar{h}^2h'\right)\bar{\psi}'_{1L}\mathrm{d}z \\ B_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0\bar{g}ho\psi_3 - U_1h\bar{h}o\psi_3\mathrm{d}z \\ B_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 2U_0\eta\bar{g}h\psi_2 - 2U_1\eta h\bar{h}\psi_2 + 6\bar{V}_0\eta g\bar{h}^2\bar{\psi}_3 - 3\bar{V}_1\eta h\bar{h}^2\bar{\psi}_3\mathrm{d}z \end{aligned} \tag{6.61}$$

We simplify last hexapole-quadrupole coupling integral. We split quadrupole field to hexapole and monopole part $\psi_2 = \psi_{2H} + \psi_{2L}$ as well as integration limits:

$$\begin{aligned} B_{2Q} \;=\; -\tfrac{\eta}{\sqrt{\phi_r}}\Big(& 2\int_H U_0\bar{g}h\psi_{2H}\mathrm{d}z + 2\int_L U_0\bar{g}h\psi_{2L}\mathrm{d}z \\ - \;& 2\int_H U_1h\bar{h}\psi_{2H}\mathrm{d}z - 2\int_L U_1h\bar{h}\psi_{2L}\mathrm{d}z \\ + \;& 6\int_H \bar{V}_0g\bar{h}^2\bar{\psi}_3\mathrm{d}z - 3\int_H \bar{V}_1h\bar{h}^2\bar{\psi}_3\mathrm{d}z\Big) \end{aligned} \tag{6.62}$$

where index H means integration over both hexapoles HA, HB first and second hexapole respectively and L integration over lenses. U_1 is zero in lens area, U_0 is constant, also in hexapoles $g = \bar{g}$ and $h = \bar{h}$. Thus we can write:

$$\begin{aligned} B_{2Q} &= -U_{0A}\frac{2\eta}{\sqrt{\phi_r}}\left(\int_L h\bar{h}\psi_{2L}\mathrm{d}z\right) \\ &- \int_H U_0V_1' - U_1V_0' + \bar{V}_0\bar{U}_1' - \frac{1}{2}\bar{V}_1\bar{U}_0'\mathrm{d}z \\ &+ \frac{6\eta}{\sqrt{\phi_r}}\int_H \left(U_0gh - U_1h^2\right)o\psi_3\mathrm{d}z \end{aligned} \tag{6.63}$$

and integrating by parts:

$$\begin{aligned} B_{2Q} &= -U_{0A}\frac{2\eta}{\sqrt{\phi_r}}\left(\int_L h\bar{g}\psi_{2L}\mathrm{d}z\right) \\ &+ \int_H U_1V_0' + \bar{U}_1\bar{V}_0' - U_0V_1' - \frac{1}{2}\bar{U}_0\bar{V}_1'\mathrm{d}z - \bar{U}_{0A}\frac{\eta}{\sqrt{\phi_r}}\int_L gh\bar{\psi}_{2L}\mathrm{d}z \\ &+ \frac{6\eta}{\sqrt{\phi_r}}\int_H \left(U_0gh - U_1h^2\right)o\psi_3\mathrm{d}z \end{aligned} \tag{6.64}$$

Since gh is antisymmetric with respect to the centre of corrector the non-vanishing term is ψ_{2L-}. We can split V_0', V_1' to part only dependant on quadrupole field and the dependence on shift of the optical axis in second hexapole o. We can write:

$$\begin{aligned} B_{2Q} + B_{2H} &= -U_{0A}\frac{2\eta}{\sqrt{\phi_r}}\int_L h\bar{g}\psi_{2L-}\mathrm{d}z - \bar{U}_{0A}\frac{\eta}{\sqrt{\phi_r}}\int_L gh\bar{\psi}_{2L-}\mathrm{d}z \\ &+ \frac{2\eta}{\sqrt{\phi_r}}\int_H U_1\psi_2h^2 + \bar{U}_1\bar{\psi}_2\bar{h}^2 - U_0\psi_2gh - \frac{1}{2}\bar{U}_0\bar{\psi}_2\bar{g}\bar{h}\mathrm{d}z \\ &+ \frac{6\eta}{\sqrt{\phi_r}}\int_{HB} U_1\psi_3oh^2 + \bar{U}_1\bar{\psi}_3\bar{o}\bar{h}^2 - U_0\psi_3ogh - \frac{1}{2}\bar{U}_0\bar{\psi}_3\bar{o}\bar{g}\bar{h}\mathrm{d}z \end{aligned} \tag{6.65}$$

U_1h^2 and U_0gh are antisymmetric with respect to centre of corrector thus only non-zero addition of ψ_2 is ψ_{2-}. Thus:

$$\begin{aligned} B_{2Q} + B_{2H} &= -U_{0A}\frac{2\eta}{\sqrt{\phi_r}}\int_L h\bar{g}\psi_{2L-}\mathrm{d}z - \bar{U}_{0A}\frac{\eta}{\sqrt{\phi_r}}\int_L gh\bar{\psi}_{2L-}\mathrm{d}z \\ &+ \frac{6\eta(\delta_A - \delta_B - o_B)}{\sqrt{\phi_r}}\int_{HA} U_1\psi_3h^2 - U_0\psi_3gh\mathrm{d}z \\ &+ \frac{6\eta(\bar{\delta}_A - \bar{\delta}_B - \bar{o}_B)}{\sqrt{\phi_r}}\int_{HA} \bar{U}_1\bar{\psi}_3\bar{h}^2 - \frac{1}{2}\bar{U}_0\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \\ &+ \frac{6\eta(\gamma_A + \gamma_B + o_B')}{\sqrt{\phi_r}}\int_{HA} U_1z\psi_3h^2 - U_0z\psi_3gh\mathrm{d}z \\ &+ \frac{6\eta(\bar{\gamma}_A + \bar{\gamma}_B + \bar{o}_B')}{\sqrt{\phi_r}}\int_{HA} \bar{U}_1z\bar{\psi}_3\bar{h}^2 - \frac{1}{2}\bar{U}_0z\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \end{aligned} \tag{6.66}$$

The last two rows can be further simplified using symmetry with respect to hexapole field and we get final formula of B_2:

$$
\begin{aligned}
B_2 \;=\; & \int \frac{1}{2}\bar{h}'^2 h' o'_{-} \mathrm{d}z \\
& + \frac{i\eta}{16\sqrt{\phi_r}} \int \left(h\bar{h}^2 o'_{-} - 2h\bar{h}\bar{h}' o_{-} + \bar{h}^2 h' o_{-} \right) \psi_0{}''' \mathrm{d}z \\
& + \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2h\bar{h}\bar{h}' - \bar{h}^2 h' \right) \bar{\psi}'{}_{1L-} \mathrm{d}z \\
& - U_{0A} \frac{2\eta}{\sqrt{\phi_r}} \int_L h\bar{g}\psi_{2L-} \mathrm{d}z - \bar{U}_{0A} \frac{\eta}{\sqrt{\phi_r}} \int_L gh\bar{\psi}_{2L-} \mathrm{d}z \\
& + \frac{6\eta(\delta_A - \delta_B - o_B)}{\sqrt{\phi_r}} \int_{HA} U_1 \psi_3 h^2 - U_0 \psi_3 gh \mathrm{d}z \\
& + \frac{6\eta(\bar{\delta}_A - \bar{\delta}_B - \bar{o}_B)}{\sqrt{\phi_r}} \int_{HA} \bar{U}_1 \bar{\psi}_3 \bar{h}^2 - \frac{1}{2} \bar{U}_0 \bar{\psi}_3 \bar{g}\bar{h} \mathrm{d}z \\
& - \frac{3\eta(\gamma_A + \gamma_B + o'_B)}{\sqrt{\phi_r}} U_{0A} \int_{HA} z\psi_3 gh \mathrm{d}z \\
& - \frac{3\eta(\bar{\gamma}_A + \bar{\gamma}_B + \bar{o}'_B)}{2\sqrt{\phi_r}} \bar{U}_{0A} \int_{HA} z\bar{\psi}_3 \bar{g}\bar{h} \mathrm{d}z
\end{aligned}
\tag{6.67}
$$

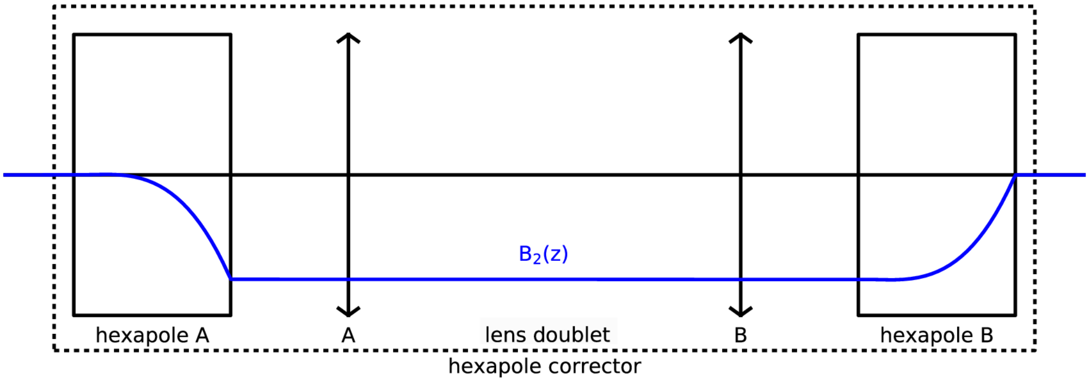


Figure 6.7: The function B_2 through hexapole corrector with $\delta_A = \delta_B$, $o = 0$, $\gamma_A = 0$, $\gamma_B = 0$, and $\psi_{2L} = 0$

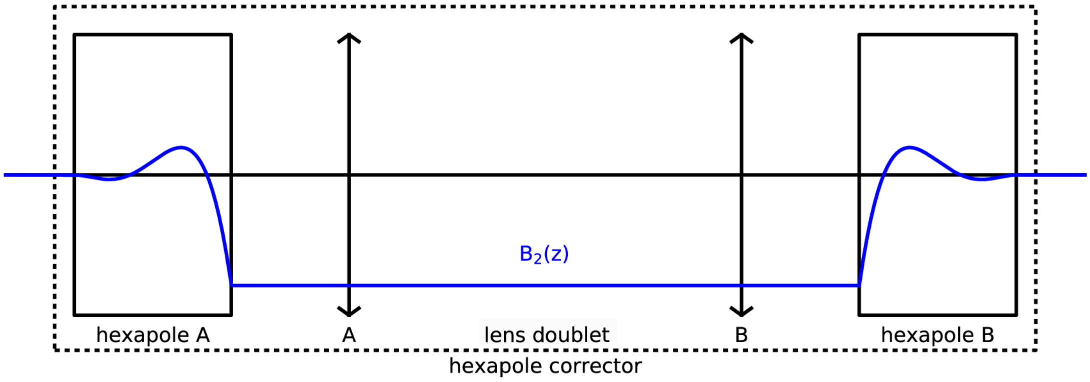


Figure 6.8: The function B_2 through hexapole corrector with $\gamma_A = -\gamma_B$, $o = 0$, $\delta_A = 0$, $\delta_B = 0$, and $\psi_{2L} = 0$

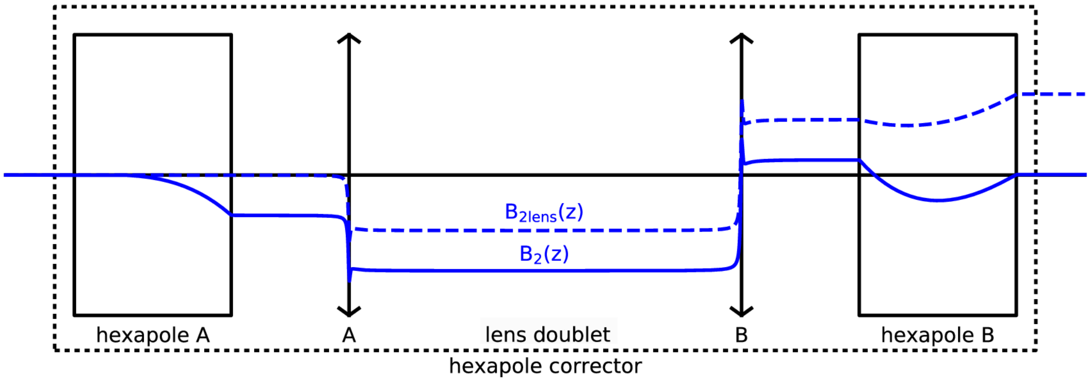


Figure 6.9: Correcting doublet B_2 using $\delta_A = -\delta_B$

6.2.9 Third Order Aberrations

At third we evaluate derivative of the third order eikonal $S^{III} = \int M_5 + \frac{1}{2}D^{(1)}M_4 + \frac{1}{2}D^{(2)}M_3 \mathrm{d}z$:

$$\begin{aligned}
\frac{\mathrm{d}S^{III}}{\mathrm{d}z} = & \sqrt{\phi_r}\left(-\frac{w'^{(0)}w'^{(1)}}{8}\bar{w}'^{(0)^2} - \frac{\bar{w}'^{(0)}\bar{w}'^{(1)}}{8}w'^{(0)^2}\right) \\
& +\frac{i\eta}{64}\left[2\bar{w}^{(0)}w^{(0)}\left(\bar{w}'^{(0)}w^{(1)} - \bar{w}^{(1)}w'^{(0)}\right)\right. \\
& \quad + \left(\bar{w}'^{(0)}\bar{w}^{(1)} + \bar{w}'^{(1)}\bar{w}^{(0)}\right)w^{(0)^2} \\
& \quad \left. - \left(w'^{(0)}w^{(1)} + w'^{(1)}w^{(0)}\right)\bar{w}^{(0)^2}\right]\psi'''_0 \\
& +\frac{i\eta}{2}\left(w^{(2)}\psi_1 - \bar{w}^{(2)}\bar{\psi}_1\right) \\
& +\frac{3i\eta}{2}\left(w^{(0)^2}w^{(2)}\psi_3 - \bar{w}^{(0)^2}\bar{w}^{(2)}\bar{\psi}_3\right) \\
& +\frac{i\eta}{16}\left(4\bar{w}^{(0)}w'^{(0)}w^{(0)^3} - \bar{w}'^{(0)}w^{(0)^4}\right)\psi'_3 - \frac{i\eta}{16}\left(4\bar{w}'^{(0)}\bar{w}^{(0)^3}w^{(0)} - \bar{w}^{(0)^4}w'^{(0)}\right)\bar{\psi}'_3 \\
& \epsilon\left[\frac{i\eta}{16}\left(4\bar{w}^{(0)}w^{(0)}w^{(1)} + 2\bar{w}^{(1)}w^{(0)^2} - 2\bar{w}'^{(0)}w^{(0)}w^{(1)} - \bar{w}'^{(1)}w^{(0)^2}\right)\psi'_{1L}\right. \\
& \quad -\frac{i\eta}{16}\left(4\bar{w}^{(0)}\bar{w}^{(1)}w^{(0)} + 2\bar{w}^{(0)^2}w^{(1)} - 2\bar{w}^{(0)}\bar{w}^{(1)}w'^{(0)} - \bar{w}^{(0)^2}w'^{(1)}\right)\bar{\psi}'_{1L} \\
& \quad +i\eta\left(w^{(0)}w^{(2)}\psi_2 - \bar{w}^{(0)}\bar{w}^{(2)}\bar{\psi}_2\right) \\
& \quad +\frac{i\eta}{12}\left(3\bar{w}^{(0)}w'^{(0)}w^{(0)^2} - \bar{w}'^{(0)}w^{(0)^3}\right)\psi'_2 - \frac{i\eta}{12}\left(3\bar{w}'^{(0)}\bar{w}^{(0)^2}w^{(0)} - \bar{w}^{(0)^3}w'^{(0)}\right)\bar{\psi}'_2 \\
& \quad \left. +i\eta\left(w^{(0)^4}\psi_4 - \bar{w}^{(0)^4}\bar{\psi}_4\right)\right]
\end{aligned} \tag{6.68}$$

We will be now interested in the axial aberrations in the image plane. In that case we have to just consider derivative of eikonal with respect to w'_0 and $\bar{w}'_0$. Furthermore we will use trajectories $w^{(0)}, w^{(1)}, w^{(2)}$ in the form:

$$\begin{aligned}
w^{(0)} &= h(z)w'_0 + o(z)\epsilon \\
w^{(1)} &= C_{02}(z)\bar{w}'^2_0 + E_{01}(z)\epsilon\bar{w}'_0 \\
w^{(2)} &= C_{21}(z)w'^2_0\bar{w}'_0 + E_{20}(z)\epsilon w'^2_0 + E_{11}(z)\epsilon w'_0\bar{w}'_0
\end{aligned} \tag{6.69}$$

Where $C_{02}(z), E_{01}(z), C_{21}(z), E_{20}(z), E_{11}(z)$ are function to corresponding coefficient defined as:

$$\begin{aligned}
C_{02}(z) &= i\bar{g}\bar{U}_0 - i\bar{h}\bar{U}_1 \\
E_{01}(z) &= i2\bar{g}\bar{V}_0 - i\bar{h}\bar{V}_1 \\
C_{21}(z) &= C\bar{g} - \bar{K}\bar{h} + U_0\bar{U}_0\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + U_0\bar{U}_1\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&\quad +U_1\bar{U}_0\left(g\bar{g}h' + gg'\bar{h} - 2\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{U}_1\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&\quad +U_2\bar{U}_0\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + U_2\bar{U}_1\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right) \\
E_{20}(z) &= \bar{B}_2\bar{g} - \bar{C}_2\bar{h} + \bar{U}_0V_0\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + \bar{U}_0V_1\left(\frac{1}{2}g\bar{g}h' + \frac{1}{2}gg'\bar{h} - \bar{g}\bar{g}'\bar{h}\right) \\
&\quad +\bar{U}_0V_2\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + \bar{U}_1V_0\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&\quad +\bar{U}_1V_1\left(-\frac{1}{2}\bar{g}hh' + \bar{g}\bar{h}\bar{h}' - \frac{1}{2}g'h\bar{h}\right) + \bar{U}_1V_2\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right) \\
E_{11}(z) &= -A_2\bar{h} + 2B_2\bar{g} + U_0\bar{V}_0\left(-2g\bar{g}g' + 2\bar{g}^2\bar{g}'\right) + U_0\bar{V}_1\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&\quad +U_1\bar{V}_0\left(2g\bar{g}h' + 2gg'\bar{h} - 4\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{V}_1\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&\quad +U_2\bar{V}_0\left(-2g\bar{h}h' + 2\bar{g}'\bar{h}^2\right) + U_2\bar{V}_1\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)
\end{aligned} \tag{6.70}$$

We define integrals:

$$\begin{aligned}
L_4 &= -\frac{4\eta}{\sqrt{\phi_r}}\int \frac{i\sqrt{\phi_r}}{4\eta}C'_{02}\bar{h}'^2h' + \frac{1}{32}\left(-C'_{02}h\bar{h}^2 + 2C_{02}h\bar{h}\bar{h}' - C_{02}\bar{h}^2h'\right){\psi'''}_0 \\
&\quad -3\bar{C}_{21}\bar{h}^2\bar{\psi}_3 + \frac{1}{8}\left(\bar{h}^4h' - 4h\bar{h}^3\bar{h}'\right){\bar{\psi}'}_3\mathrm{d}z \\
S_3 &= -\frac{4\eta}{\sqrt{\phi_r}}\int \frac{i\sqrt{\phi_r}}{2\eta}C'_{02}\bar{h}'h'\bar{o}' + \frac{i\sqrt{\phi_r}}{4\eta}E_{01}\bar{h}'^2h' \\
&\quad +\frac{1}{16}\left(-C'_{02}h\bar{h}\bar{o} + C_{02}h\bar{h}\bar{o}' + C_{02}h\bar{h}'\bar{o} - C_{02}\bar{h}h'\bar{o}\right){\psi'''}_0 \\
&\quad +\frac{1}{32}\left(-E_{01}h\bar{h}^2 + 2E_{01}h\bar{h}\bar{h}' - E_{01}\bar{h}^2h'\right){\psi'''}_0 \\
&\quad +\frac{1}{4}\left({C_{02}}'h\bar{h} + C_{02}h'\bar{h} - C_{02}h\bar{h}'\right){\psi'}_{1L} - 2\bar{C}_{21}\bar{h}\bar{\psi}_2 + \left(-\frac{1}{2}h\bar{h}^2\bar{h}' + \frac{1}{6}\bar{h}^3h'\right){\bar{\psi}'}_2 \\
&\quad +\left(-\frac{1}{2}h\bar{h}^3\bar{o}' - \frac{3}{2}h\bar{h}^2\bar{h}'\bar{o} + \frac{1}{2}\bar{h}^3h'\bar{o}\right){\bar{\psi}'}_3 - 6\bar{C}_{21}\bar{h}\bar{o}\bar{\psi}_3 - 3\bar{E}_{11}\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
A_3 &= -\frac{16\eta}{\sqrt{\phi_r}}\int \frac{i\sqrt{\phi_r}}{4\eta}C'_{02}\bar{h}'^2o' + \frac{1}{32}\left(-C'_{02}\bar{h}^2o - C_{02}\bar{h}^2o' + 2C_{02}\bar{h}\bar{h}'o\right){\psi'''}_0 \\
&\quad +\left(\frac{1}{8}C'_{02}\bar{h}^2 - \frac{1}{4}C_{02}\bar{h}\bar{h}'\right){\bar{\psi}'}_{1L} + \left(\frac{1}{8}\bar{h}^4o' - \frac{1}{2}\bar{h}^3\bar{h}'o\right){\bar{\psi}'}_3 \\
&\quad -3\bar{E}_{20}\bar{h}^2\bar{\psi}_3 - 2\bar{h}^4\bar{\psi}_4\mathrm{d}z
\end{aligned} \tag{6.71}$$

Then eikonal looks like:

$$\begin{aligned}
S^{III} &= 2\sqrt{\phi_r}\left(-\frac{1}{4}L_4\bar{w}'^4_0w'_0 - \frac{1}{4}\bar{L}_4\bar{w}'_0w'^4_0\right) \\
&\quad +2\epsilon\sqrt{\phi_r}\left(-\frac{i}{16}A_3\bar{w}'^4_0 - \frac{i}{4}S_3\bar{w}'^3_0w'_0 + \frac{i}{4}\bar{S}_3\bar{w}'_0w'^3_0 + \frac{i}{16}\bar{A}_3w'^4_0\right)
\end{aligned} \tag{6.72}$$

The canonical momentums are in the image plane just linear combination of positions:

$$p^{(j)} = \frac{\sqrt{\phi_r}g'}{2g}\bar{w}^{(j)} \tag{6.73}$$

Thus any vector:

$$\nabla_0 \boldsymbol{Q}^{(j)}\Gamma\boldsymbol{Q}^{(k)} \tag{6.74}$$

is zero. Thus the third order axial aberrations are in the image plane:

$$w^{(3)}(z_i) = -i\bar{L}_4 {w'}_0^4 + 4iL_4 \bar{w}'^3_0 w'_0 + iA_3\epsilon\bar{w}'^3_0 + 3iS_3\epsilon\bar{w}'^2_0 w'_0 - i\bar{S}_3\epsilon {w'}^3_0 \tag{6.75}$$

Now we use symmetry with respect to centre of the corrector. C_{02} is symmetric, C_{21} antisymmetric with constant symmetric part (only from term Cg). Symmetric parts of E_{01}, E_{20}, E_{11} are:

$$\begin{aligned}
E_{01+} &= i2\bar{g}\bar{V}_{0+} - i\bar{h}\bar{V}_{1-} \qquad (6.76)\\
E_{20+} &= \bar{B}_{2+}\bar{g} - \bar{C}_{2-}\bar{h} + \bar{U}_0V_{0-}\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + \bar{U}_0V_{1+}\left(\frac{1}{2}g\bar{g}h' + \frac{1}{2}gg'\bar{h} - \bar{g}\bar{g}'\bar{h}\right)\\
&+\bar{U}_0V_{2-}\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + \bar{U}_1V_{0-}\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right)\\
&+\bar{U}_1V_{1+}\left(-\frac{1}{2}\bar{g}hh' + \bar{g}\bar{h}\bar{h}' - \frac{1}{2}g'h\bar{h}\right) + \bar{U}_1V_{2-}\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\\
E_{11+} &= -A_{2-}\bar{h} + 2B_{2+}\bar{g} + U_0\bar{V}_{0-}\left(-2g\bar{g}g' + 2\bar{g}^2\bar{g}'\right) + U_0\bar{V}_{1+}\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right)\\
&+U_1\bar{V}_{0-}\left(2g\bar{g}h' + 2gg'\bar{h} - 4\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{V}_{1+}\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right)\\
&+U_2\bar{V}_{0-}\left(-2g\bar{h}h' + 2\bar{g}'\bar{h}^2\right) + U_2\bar{V}_{1+}\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)
\end{aligned}$$

The antisymmetric parts are with opposite signs. We can now write non-vanishing parts of L_4, S_3, A_3 outside corrector:

$$\begin{aligned}
L_4 &= \frac{12\eta}{\sqrt{\phi_r}}\int Cg\bar{h}^2\bar{\psi}_3\mathrm{d}z = C\bar{U}_1 = 0 \qquad (6.77)\\
S_3 &= -\frac{4\eta}{\sqrt{\phi_r}}\int \frac{i\sqrt{\phi_r}}{2\eta}C'_{02}\bar{h}'h'{\bar{o}_+}' + \frac{i\sqrt{\phi_r}}{4\eta}E_{01+}\bar{h}'^2h'\\
&+\frac{1}{16}\left(-C'_{02}h\bar{h}\bar{o}_+ + C_{02}h\bar{h}{\bar{o}_+}' + C_{02}h\bar{h}'\bar{o}_+ - C_{02}\bar{h}h'\bar{o}_+\right){\psi'''}_0\\
&+\frac{1}{32}\left(-E_{01-}h\bar{h}^2 + 2E_{01-}h\bar{h}\bar{h}' - E_{01-}\bar{h}^2h'\right){\psi'''}_0\\
&+\frac{1}{4}\left({C_{02}}'h\bar{h} + C_{02}h'\bar{h} - C_{02}h\bar{h}'\right){\psi'}_{1L+} - 2\bar{C}_{21}\bar{h}\bar{\psi}_2 + \left(-\frac{1}{2}h\bar{h}^2\bar{h}' + \frac{1}{6}\bar{h}^3h'\right){\bar{\psi}'}_{2-}\\
&+\left(-\frac{1}{2}h\bar{h}^3{\bar{o}_+}' - \frac{3}{2}h\bar{h}^2\bar{h}'\bar{o}_+ + \frac{1}{2}\bar{h}^3h'\bar{o}_+\right){\bar{\psi}'}_3 - 6\bar{C}_{21}\bar{h}\bar{o}\bar{\psi}_3 - 3\bar{E}_{11+}\bar{h}^2\bar{\psi}_3\mathrm{d}z\\
A_3 &= -\frac{16\eta}{\sqrt{\phi_r}}\int \frac{i\sqrt{\phi_r}}{4\eta}C'_{02}\bar{h}'^2o'_+ + \frac{1}{32}\left(-C'_{02}\bar{h}^2o_+ - C_{02}\bar{h}^2o'_+ + 2C_{02}\bar{h}\bar{h}'o_+\right){\psi'''}_0\\
&+\left(\frac{1}{8}C'_{02}\bar{h}^2 - \frac{1}{4}C_{02}\bar{h}\bar{h}'\right){\bar{\psi}'}_{1L+} + \left(\frac{1}{8}\bar{h}^4o'_+ - \frac{1}{2}\bar{h}^3\bar{h}'o_+\right){\bar{\psi}'}_3\\
&-3\bar{E}_{20+}\bar{h}^2\bar{\psi}_3 - 2\bar{h}^4\bar{\psi}_{4+}\mathrm{d}z
\end{aligned}$$

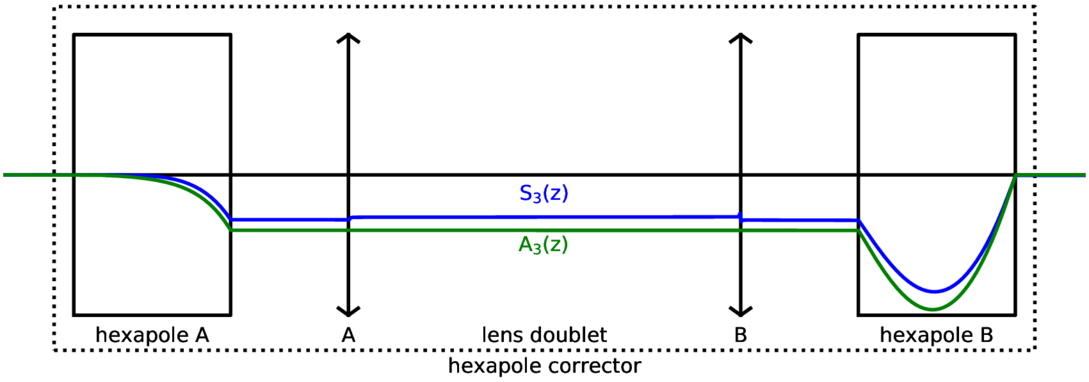


Figure 6.10: The function A_3, S_3 through hexapole corrector with $\delta_A = -\delta_B$, $o = 0$, $\gamma_A = 0$, $\gamma_B = 0$, and $\psi_{2L} = 0$ (S_3 is very small after corrector but not zero)

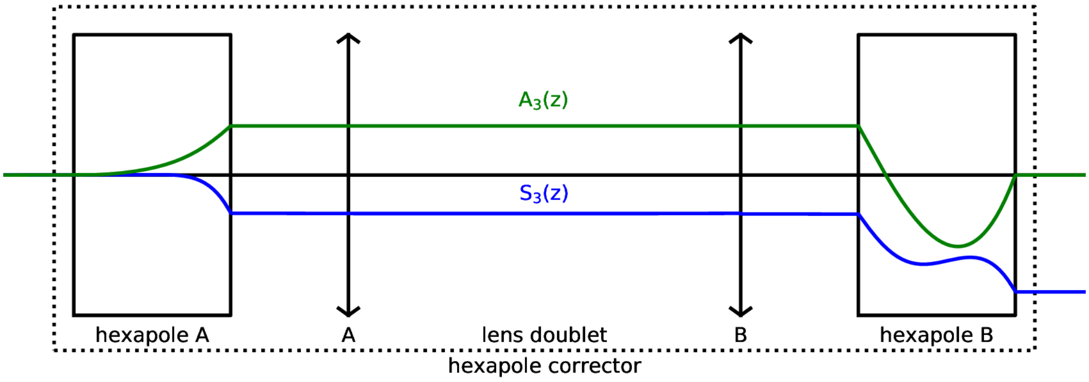


Figure 6.11: The function A_3, S_3 through hexapole corrector with $\gamma_A = \gamma_B$, $o = 0$, $\delta_A = 0$, $\delta_B = 0$, and $\psi_{2L} = 0$

6.3 Chromatic Aberration

In previous part we dealt with geometrical aberrations of the hexapole corrector. However, due to the lens doublet the hexapole corrector gives to the contribution to the first order chromatic aberration as well. To calculate chromatic aberration we expand the Relativistic potential in Lagrangian. The addition to the paraxial Lagrangian has form:

$$M_{2c} = \frac{1}{4}\sqrt{\phi_r} w' \bar{w}' \frac{\Delta E}{E} \tag{6.78}$$

Where $\frac{\Delta E}{E}$ is relative dispersion of the beam. The derivative of eikonal is:

$$\frac{\mathrm{d}S^c}{\mathrm{d}z} = \frac{\Delta E}{4E}\sqrt{\phi_r}(w_i \bar{w}_i g' \bar{g}' + w_i' \bar{w}_i h' \bar{g}' + w_i \bar{w}_i' g' \bar{h}' + w_i' \bar{w}_i' h' \bar{h}') \tag{6.79}$$

And addition to the trajectory:

$$w^{(0c)} = \frac{\Delta E}{2E}\left(\bar{h}\int h'\bar{g}'\mathrm{d}z - \bar{g}\int h'\bar{h}'\mathrm{d}z\right)w_i' + \frac{\Delta E}{2E}\left(\bar{h}\int g'\bar{g}'\mathrm{d}z - \bar{g}\int g'\bar{h}'\mathrm{d}z\right)w_i \tag{6.80}$$

We define coefficient of chromatic aberration as:

$$C_c = \frac{1}{2}\int h'\bar{h}'\mathrm{d}z \tag{6.81}$$

This can be using rotated coordinates and using integration by parts rewritten in the form:

$$C_c = \int h\bar{h}\left(\frac{\eta\psi_0'}{2\sqrt{\phi_r}}\right)^2\mathrm{d}z \tag{6.82}$$

For thin/weak lens approximation (h is constant inside lens) we get solution:

$$C_c = |h|^2\int\left(\frac{\eta\psi_0'}{2\sqrt{\phi_r}}\right)^2\mathrm{d}z = \frac{|h|^2}{f} \tag{6.83}$$

Where f is the focal length of the lens.

7. Resolution

7.1 Intensity in Image Plane

To calculate resolution of the hexapole corrector system we start with diffraction integral [9] to calculate wave function in the image point $\boldsymbol{q}_i$:

$$\psi(\boldsymbol{q}_i) \propto \int_{\mathbb{R}^2} \psi(\boldsymbol{q}_o) e^{-\frac{i}{\hbar}S(\boldsymbol{q}_o,\boldsymbol{q}_i)} \mathrm{d}\boldsymbol{q}_o \tag{7.1}$$

where S is eikonal and it is integrated over the coordinates $\boldsymbol{q}_o$ in the object plane. If we have system with an aperture than the diffraction integral changes as:

$$\psi(\boldsymbol{q}_i) \propto \int_A \left(\int_{\mathbb{R}^2} \psi(\boldsymbol{q}_o) e^{-\frac{i}{\hbar}S(\boldsymbol{q}_o,\boldsymbol{q}_a)} \mathrm{d}\boldsymbol{q}_o \right) e^{-\frac{i}{\hbar}S(\boldsymbol{q}_a,\boldsymbol{q}_i)} \mathrm{d}\boldsymbol{q}_a \tag{7.2}$$

where it is additionally integrated over aperture A. We would like to know point spread function. Thus we use $\psi(\boldsymbol{q}_o) = \delta(\boldsymbol{q}_o)$ and simplify equation to:

$$\psi(\boldsymbol{q}_i) \propto \int_A e^{-\frac{i}{\hbar}(S(\boldsymbol{q}_o,\boldsymbol{q}_a)+S(\boldsymbol{q}_a,\boldsymbol{q}_i))} \mathrm{d}\boldsymbol{q}_a \tag{7.3}$$

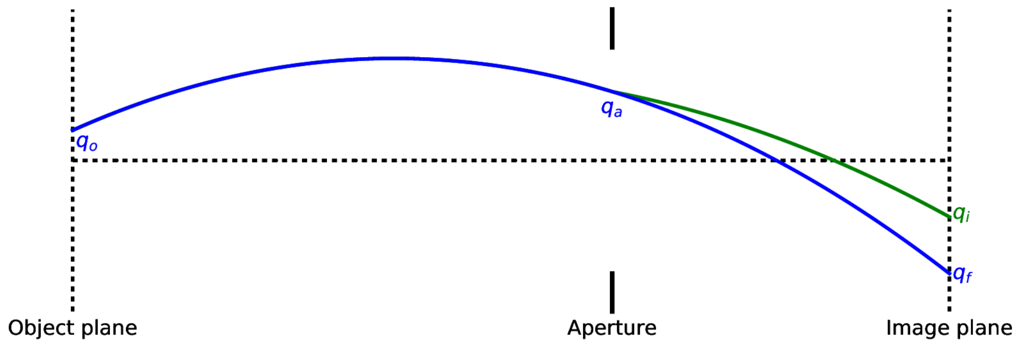


Figure 7.1: Trajectories in system with aperture. Blue – paraxial trajectory, green – trajectory from $\boldsymbol{q}_a$ to examined point q_i

Generally $S(\boldsymbol{q}_o,\boldsymbol{q}_a) + S(\boldsymbol{q}_a,\boldsymbol{q}_i)! = S(\boldsymbol{q}_o,\boldsymbol{q}_i)$, however, we are interested only in the close surrounding around the image point $\boldsymbol{q}_f$ (Figure 7.1). In that case we can assume that $\boldsymbol{q}_i - \boldsymbol{q}_f$ is small * and we can use Taylor expansion and write:

$$\begin{aligned} S(\boldsymbol{q}_o,\boldsymbol{q}_a) + S(\boldsymbol{q}_a,\boldsymbol{q}_i) &\approx S(\boldsymbol{q}_o,\boldsymbol{q}_a) + S(\boldsymbol{q}_a,\boldsymbol{q}_f) + \boldsymbol{p}_f(\boldsymbol{q}_i - \boldsymbol{q}_f) \\ &= S(\boldsymbol{q}_o,\boldsymbol{q}_f) + \boldsymbol{p}_f(\boldsymbol{q}_i - \boldsymbol{q}_f) \end{aligned} \tag{7.4}$$

*On the other hand we still have to satisfy the condition for WKB approximation such as the size $|\boldsymbol{q}_i - \boldsymbol{q}_f|$ is bigger than wave length of the electron: $|\boldsymbol{q}_i - \boldsymbol{q}_f| \gg \lambda_{el.}$

Where there is $\boldsymbol{q}_f(\boldsymbol{q}_a)$ is given by trajectory equation. We can now re-parametrize eikonal by Legendre transformation $\boldsymbol{q}_f \mapsto \boldsymbol{p}_f$:

$$S(\boldsymbol{q}_o, \boldsymbol{q}_f) + \boldsymbol{p}_f(\boldsymbol{q}_i - \boldsymbol{q}_f) = \boldsymbol{p}_f \boldsymbol{q}_f - \tilde{S}(\boldsymbol{q}_o, \boldsymbol{p}_f) + \boldsymbol{p}_f(\boldsymbol{q}_i - \boldsymbol{q}_f) = -\tilde{S}(\boldsymbol{q}_o, \boldsymbol{p}_f) + \boldsymbol{p}_f \boldsymbol{q}_i \quad (7.5)$$

And we can calculate relative intensity as:

$$\psi(\boldsymbol{q}_i) \propto \int_{A,ang.} e^{\frac{i}{\hbar}\tilde{S}(\boldsymbol{q}_o,\boldsymbol{p}_f)} e^{-\frac{i}{\hbar}\boldsymbol{p}_f \boldsymbol{q}_i} \mathrm{d}\boldsymbol{p}_f \quad (7.6)$$

The canonical momentum $\boldsymbol{p}_f$ and direction of the ray $\boldsymbol{q}_f'$ are related by formula:

$$\boldsymbol{p}_f = g\boldsymbol{q}_f' + \boldsymbol{A} \quad (7.7)$$

Where $g = \sqrt{-2mq\phi_r}$ is kinetic momentum for magnetic system. $\boldsymbol{A}$ gives just phase shift to the wave function and does not contribute to the intensity and therefore we can write:

$$\psi(\boldsymbol{q}_i) \propto \int_{A,ang.} e^{\frac{i}{\hbar}\tilde{S}(\boldsymbol{q}_o,\boldsymbol{q}_f')} e^{-\frac{ig}{\hbar}\boldsymbol{q}_f' \boldsymbol{q}_i} \mathrm{d}\boldsymbol{q}_f' \quad (7.8)$$

We define wave number of electron:

$$k = \frac{g}{\hbar} = \frac{2\pi}{\lambda} \quad (7.9)$$

and function of wave deviation χ as :

$$\chi = \frac{\tilde{S}}{g} \quad (7.10)$$

We can calculate intensity as:

$$I(\boldsymbol{q}_i) \propto \left| \int_{A,ang.} e^{ik\chi(\boldsymbol{q}_o,\boldsymbol{q}_f')} e^{-ik\boldsymbol{q}_f' \boldsymbol{q}_i} \mathrm{d}\boldsymbol{q}_f' \right|^2 \quad (7.11)$$

In case of radial symmetric χ we evaluate 7.11 for $\boldsymbol{q}_i = q_i \boldsymbol{e}_y$ in polar coordinates and integrate partly over angle:

$$\begin{aligned} I(q_i) &\propto \left| \int_{A,ang.} e^{ik\chi(\boldsymbol{q}_o,q_f')} \int_{-\pi}^{\pi} e^{-ikq_i q_f' \sin\phi} \mathrm{d}\phi q_f' \mathrm{d}q_f' \right|^2 \\ &= \left| 2\pi \int_{A,ang.} e^{ik\chi(\boldsymbol{q}_o,q_f')} J_0(kq_i q_f') q_f' \mathrm{d}q_f' \right|^2 \end{aligned} \quad (7.12)$$

where J_0 is Bessel function.

To calculate chromatic aberration which is present due to the energy dispersion of the beam we can assume that the electrons with different energy are in-coherent. In that case we can calculate the intensity of polychromatic beam as the convolution of the intensities as a function of defocus with the Gaussian distribution of standard deviation equal to:

$$\sigma = \frac{\Delta E}{\sqrt{8\ln 2}E} C_c \alpha \quad (7.13)$$

where ΔE is FWHM of the dispersion of the beam with energy E, C_c is chromatic aberration and α is maximal aperture angle.

7.2 Axial Aberrations of Hexapole Corrector

In the STEM set-up of hexapole corrector we are interested just in axial aberrations $\boldsymbol{q}_o = 0$. Up to third order the wave deviation has the form:

$$\begin{aligned}\chi &= -\frac{F}{2}w_0'\bar{w}'_0 + \left(\frac{iV_0}{2}\right)w_0'^2 - \left(\frac{i\bar{V}_0}{2}\right)\bar{w}_0'^2 \\ &+ \left(\frac{iU_0}{6}\right)w_0'^3 - \left(\frac{i\bar{U}_0}{6}\right)\bar{w}_0'^3 - \left(\frac{B_2}{2}\right)w_0'\bar{w}'^2_0 - \left(\frac{\bar{B}_2}{2}\right)\bar{w}_0'w_0'^2 \\ &- \frac{C}{4}w_0'^2\bar{w}'^2_0 - \left(\frac{iA_3}{16}\right)\bar{w}'^4 + \left(\frac{i\bar{A}_3}{16}\right)w'^4 - \left(\frac{iS_3}{4}\right)w'\bar{w}'^3 + \left(i\frac{\bar{S}_3}{4}\right)w'^3\bar{w}'\end{aligned} \tag{7.14}$$

Where F, C are main aberrations – defocus and spherical aberration and rest is due to the misalignments. The probe intensity in image plane for different aberrations are in figures 7.2 and 7.3

Table 7.1: Aberration notation

Aberration coefficient	Used the thesis	Uhlemann and Haider[21]	Krivanek[11]
Two-fold astigmatism	$2i\bar{V}_0$	A_1	$C_{1,2}$
Defocus	F	C_1	$C_{1,0}$
Three-fold astigmatism	$i\bar{U}_0$	A_2	$C_{2,3}$
Axial coma	$\bar{B}_2$	B_2	$\frac{1}{3}\bar{C}_{2,1}$
Four-fold astigmatism	$-\frac{i}{2}A_3$	A_3	$C_{3,4}$
Axial star aberration	$-\frac{i}{2}S_3$	S_3	$\frac{1}{3}\bar{C}_{3,2}$
Spherical aberration	C	C_3	$C_{3,0}$

To describe the resolution we can use the width of the peak in half of its intensity – FWHM. This has the advantage that it can be easily calculated even for aberrations with large support, however, it may gives us misleading information if the intensity peak is not sharp. In that case it is better to use parameter d_{50}, which is the diameter of the circle at which there is 50% of the intensity. That is also equivalent to the beam current as we will show. The current in image plane $\boldsymbol{j}$ is defined as:

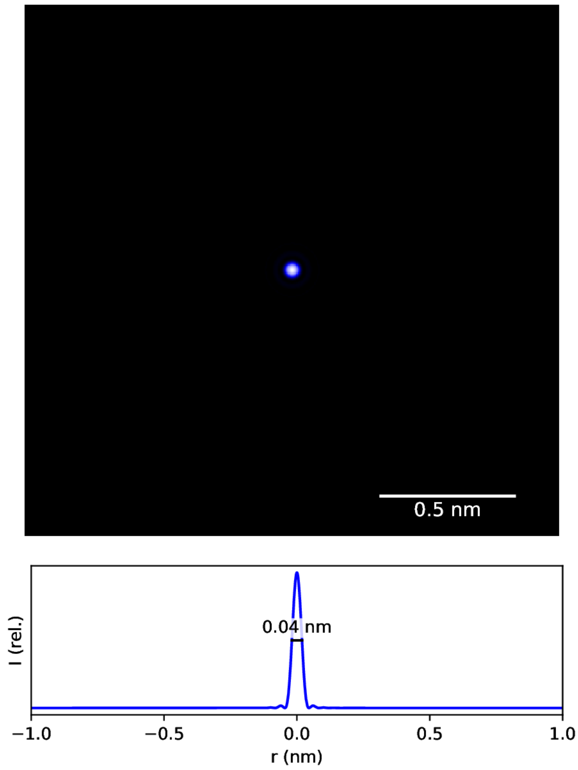
$$\boldsymbol{j} = \frac{q\hbar}{2mi}(\bar{\psi}\nabla\psi - \psi\nabla\bar{\psi}) - \frac{q}{m}|\psi|^2\boldsymbol{A} \tag{7.15}$$

where ψ is the wave function in the image plane:

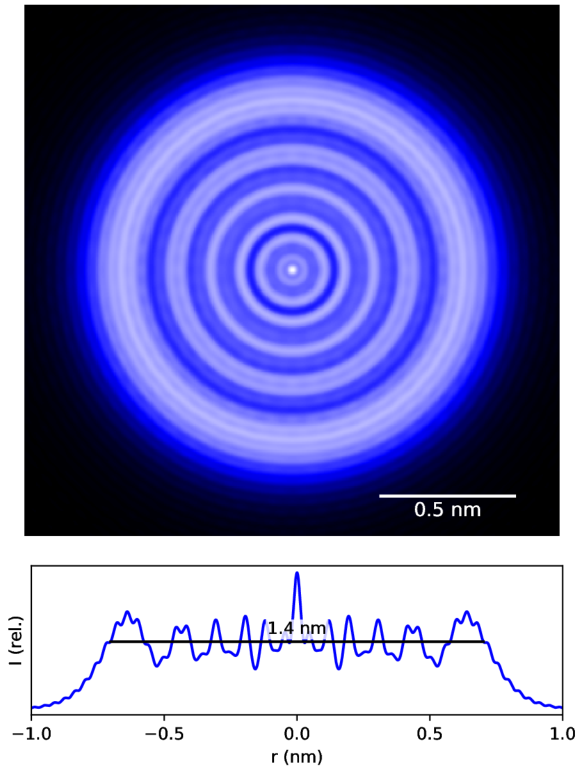
$$\psi = \sqrt{\rho}e^{\frac{iS}{\hbar}} \tag{7.16}$$

with probability density ρ and Hamilton's principal function S. If we expand 7.15 and calculate z-component we get:

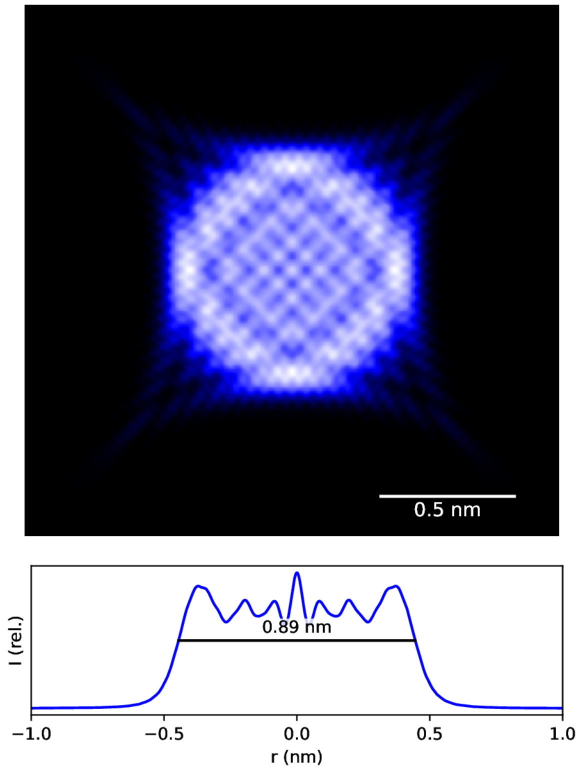
$$j_z = \frac{q}{m}\rho\left(\frac{\partial S}{\partial z} - qA_z\right) = \rho\frac{qg_z}{m} \tag{7.17}$$



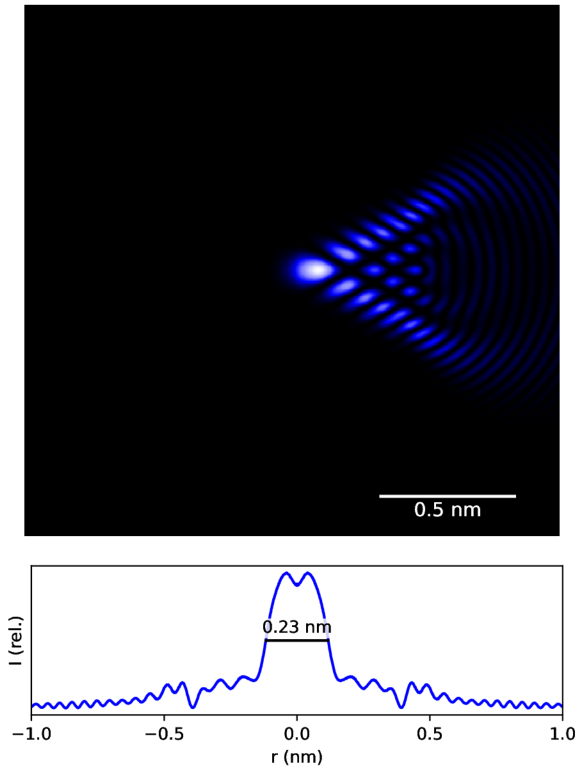
(a) Diffraction on 50 mrad aperture



(b) Defocus $F = 17$ nm

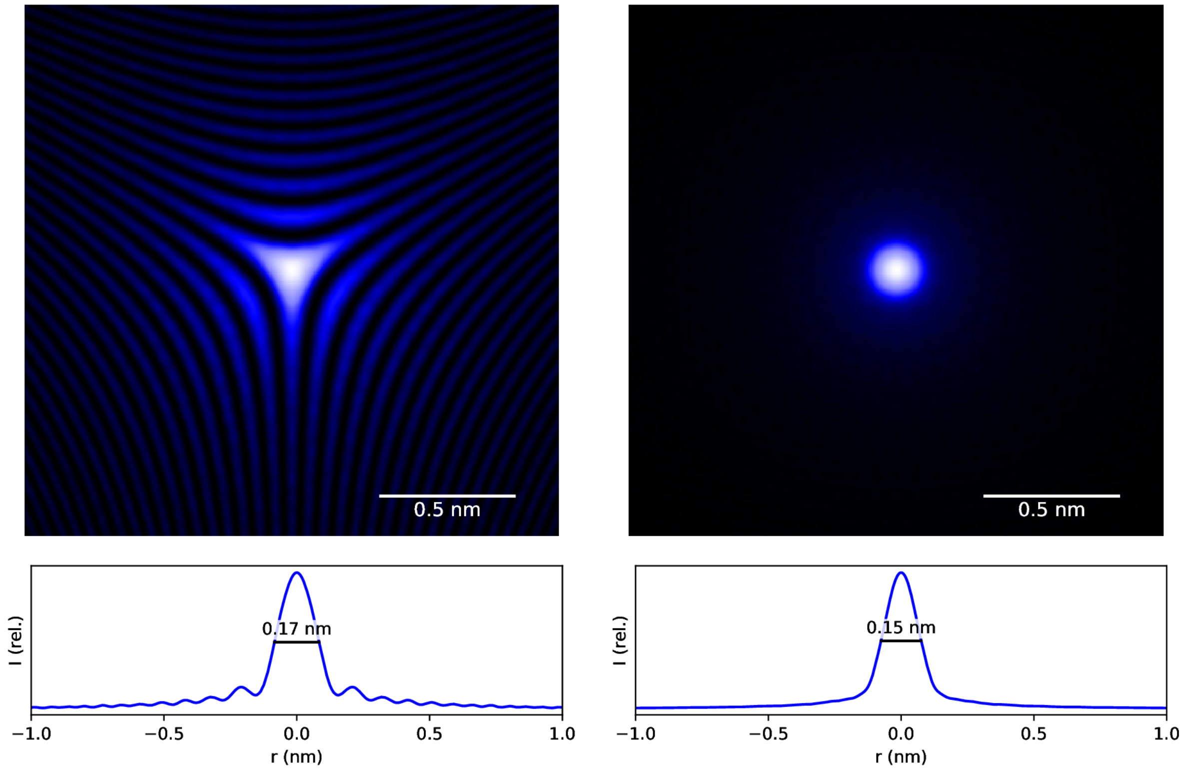


(c) Two fold astigmatism $V_0 = 5$ nm

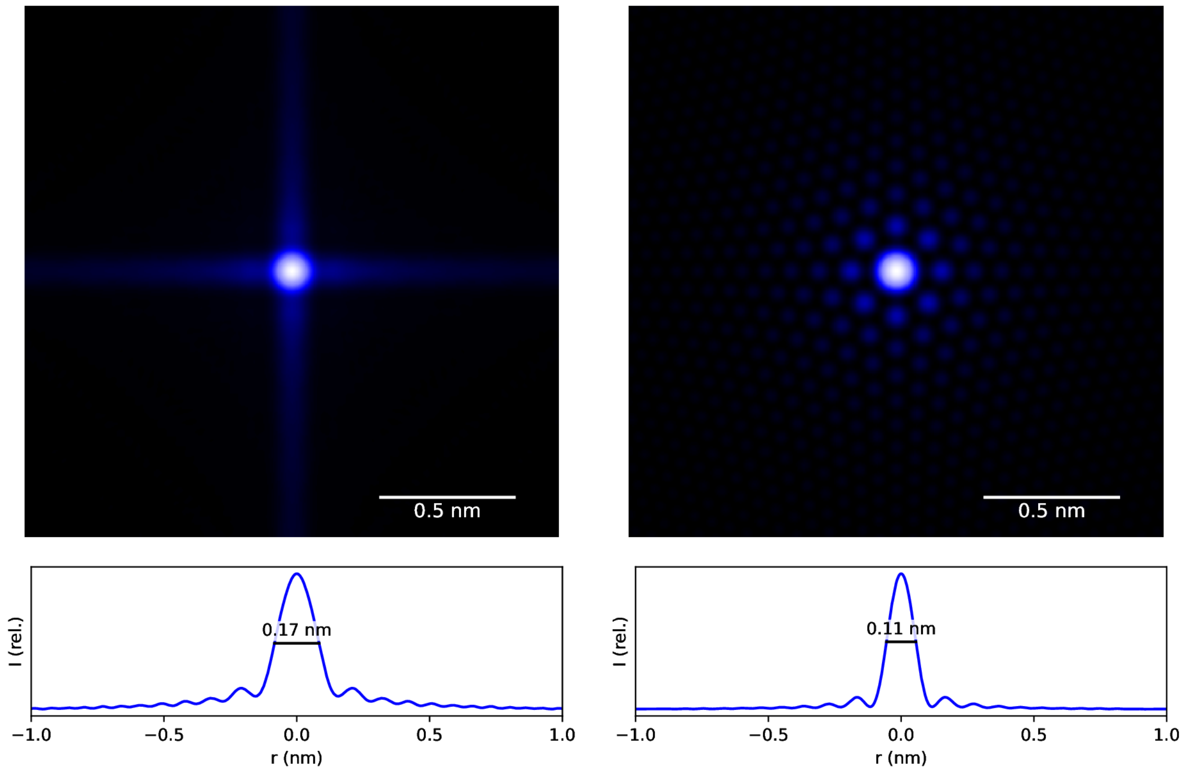


(d) Third order axial coma $B_2 = 0.2\ \mu$m

Figure 7.2: Probe intensity and radial averaged intensity for different aberrations with aperture maximum angles 50 mrad for 100keV electron (part 1.)



(a) Three fold astigmatism $U_0 = 1\ \mu$m **(b)** Spherical aberration $C = 50\ \mu$m



(c) Star aberration $S_3 = 10\ \mu$m **(d)** Four fould astigmatism $C = 50\ \mu$m

Figure 7.3: Probe intensity and radial averaged intensity for different aberrations with aperture maximum angles 50 mrad for 100 keV electron (part 2.)

For small angles we can say that g_z is constant and thus the current is proportional to the intensity (probability density).

7.2.1 Resolution without Corrector

The system without corrector is limited mainly by spherical aberration of the third order. In Figure 7.4. There is a calculation of the spherical aberration of the third order with chromatic aberration within the optimal defocus as a function of the aperture angle. If the spherical aberration is present than the additional increase due to the chromatic aberration is negligible. If we apply the hexapole corrector we can zero the spherical aberration and in that case the resolution is limited by the chromatic aberration.

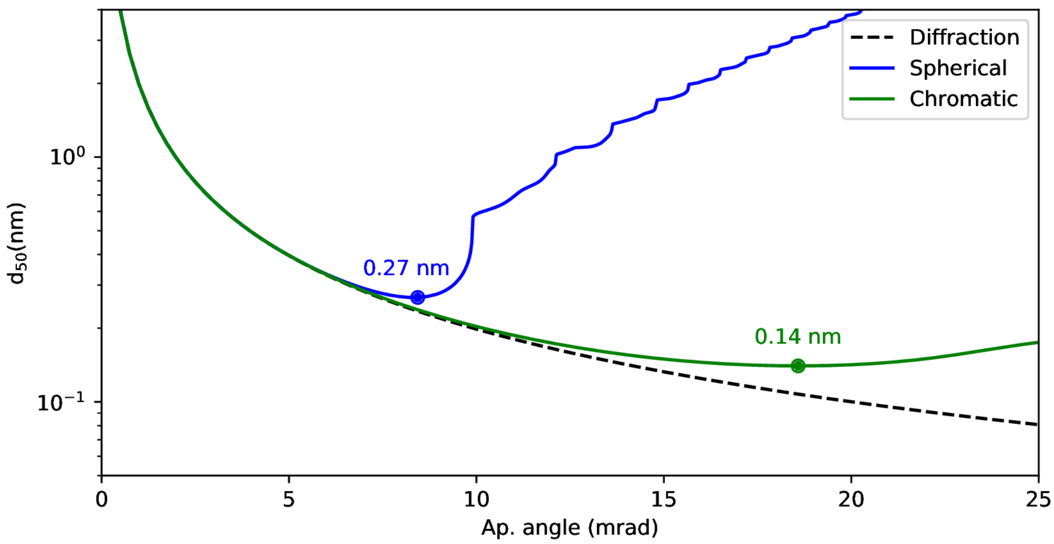
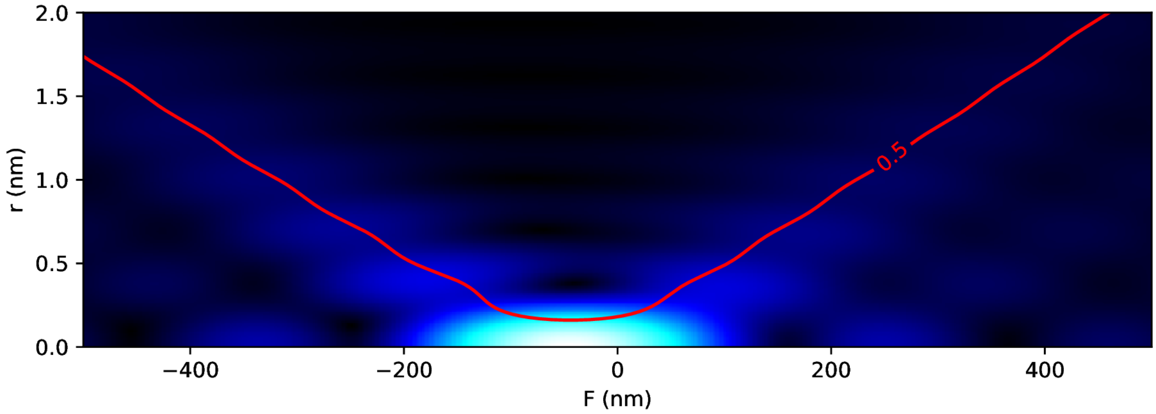
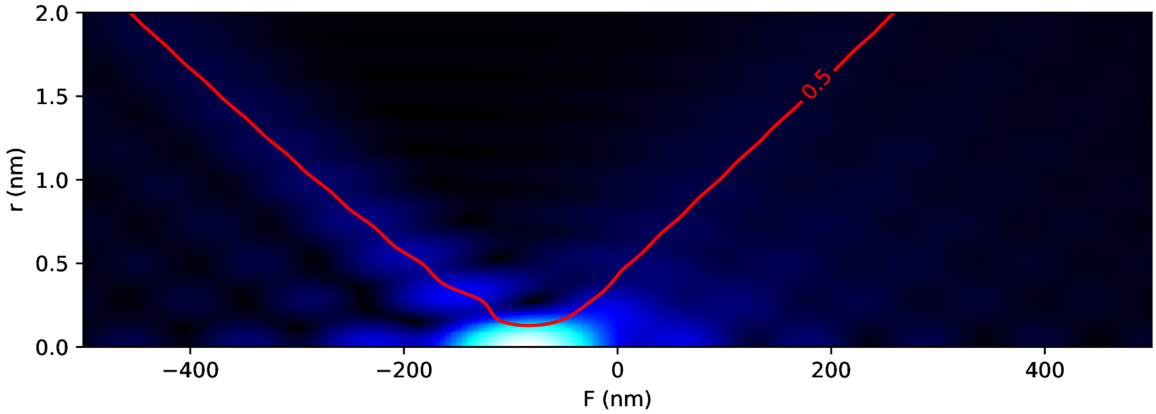


Figure 7.4: Dependence of the resolution on aperture angle in optimal defocus for spherical aberration $C = 2.5$ mm and for chromatic aberration $C_c = 2.5$ mm (100 keV electrons) If we combine spherical aberration and chromatic aberration the result is almost indistinguishable from the spherical resolution alone

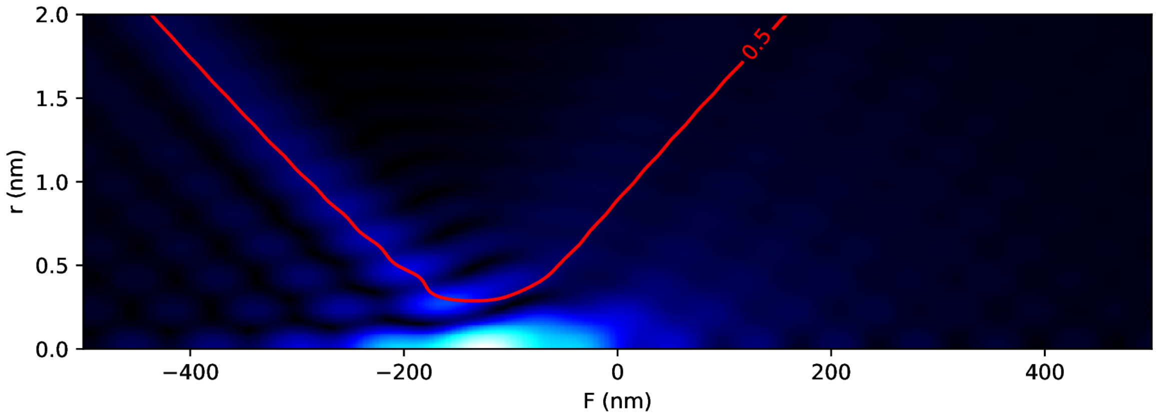
As we see we can get the maximal resolution ($d_{50} = 0.27$ nm) for apertures angles 8.4 mrad. In Figure 7.5 there is a radial distribution of the intensity for different defocus if we are limited by diffraction, in optimal aperture or limited by spherical aberration.



(a) 6 mrad, $d = 0.32\,\mathrm{nm}$, $f_{opt} = -44\,\mathrm{nm}$



(b) optimal 8.4 mrad, $d = 0.27\,\mathrm{nm}$, $f_{opt} = -83\,\mathrm{nm}$



(c) 10 mrad, $d = 0.57\,\mathrm{nm}$, $f_{opt} = -134\,\mathrm{nm}$

Figure 7.5: Radial probe intensity through focus for 100 keV at different maximal angles of aperture with spherical aberration $C = 2.5\,\mathrm{mm}$

7.2.2 Resolution with Corrector

Now we would like to add hexapole corrector to eliminate all axial aberrations up to third order. As we saw it is now limited by chromatic aberration. Furthermore the hexapole corrector increases the chromatic aberration due to the lens doublet and transfer lens. We can estimate the additional chromatic aberration by the transfer lens using the formula 6.83:

$$C_{c,H} = 2\frac{|h_H|^2}{f_d} + \frac{|h_H|^2}{f_t} = \frac{f_t}{|M_o|^2}\left(1 + \frac{2f_t}{f_d}\right) \tag{7.18}$$

where $|h_H| = \frac{f_t}{M_o}$ is the value of the h ray in the hexapole f_d is focal lens of the doublet lens,f_t the focal length of the transfer lens before the objective lens and M_o magnification of the objective lens. For values $f_T = f_D = 40$ mm, $|M_o| = 20$ is additional chromatic aberration $C_{c,H} = 0.3$ mm. In Figure 7.4 we already increased the chromatic aberration. The real value for the objective alone is about 2 mm.

To further proceed we will assume that our system with hexapole corrector is only limited by chromatic aberration $C_c = 2.5$ mm. We choose the aperture angles 18.3 mrad (see Figure 7.4) to get the best resolution. We will now estimate what the maximal allowed residual aberrations to keep resolution under 0.16 nm. The results will be similar to the published in [6]. The limiting values for each coefficients were made by calculation of the d_{50} of probe intensity (Figure 7.6).

We omit defocus effect since it can be modified with any lens and just gives required precision on electrical source of the excitation. The hexapole field in the corrector is strong so we consider only the leading terms of aberration dependent on hexapole field. The astigmatism caused by hexapoles is:

$$V_0 \quad = \quad (o_B + \delta_A + \delta_B)\,\frac{6\eta}{\sqrt{\phi_r}}\int_A \psi_3 h^2 \mathrm{d}z \tag{7.19}$$

Using the approximation of constant hexapole field, we get the absolute value of astigmatism as a function of spherical aberration of the objective C_o and optical parameters:

$$|V_0| \quad = \quad \frac{|o_B + \delta_A + \delta_B|}{|h_F|}|U_{0A}| = |o_B + \delta_A + \delta_B|\sqrt{\frac{3C_o}{2L}} \tag{7.20}$$

Where $h_F = \frac{f_T}{|M_o|}$ is h ray in the hexapole L is length of the hexapole f_T is focal length of the transfer lens just before the objective lens and M_o is magnification of the objective. For parameters $L = 40\,\mathrm{mm}, C_o = 2.5\,\mathrm{mm}, |V_{0,limit}| = 2\,\mathrm{nm}$ (Figure 7.6) we get requirement for $|o_B + \delta_A + \delta_B|$:

$$|o_B + \delta_A + \delta_B| < |V_{0,limit}|\sqrt{\frac{2L}{3C_o}} \approx 7\ \mathrm{nm} \tag{7.21}$$

This, however, is not critical, because the astigmatism can be additionally eliminated by stigmator.

Aberration of Second Order

We have additional three-fold astigmatism U_0 due to axial mis-rotation of the hexapole correctors. For small values of mis-rotation and $|U_{0,limit}| = 350\mathrm{nm}$, $f_T = 40\mathrm{mm}$,$|M_o| = 20$

we get the requirement as:

$$|\theta| < \frac{|U_{0,limit}|}{|U_{0A}|} = \frac{|U_{0,limit}||M_o|}{f_T}\sqrt{\frac{2L}{3C_H}} \approx 1\,\text{mrad} \tag{7.22}$$

In case of axial coma B_2 we have the leading terms:

$$\begin{aligned} B_2 \;=\;& \frac{6\eta(\delta_A - \delta_B - o_B)}{\sqrt{\phi_r}} \int_{HA} U_1\psi_3 h^2 - U_0\psi_3 g h \mathrm{d}z \\ &+ \frac{6\eta(\bar{\delta}_A - \bar{\delta}_B - \bar{o}_B)}{\sqrt{\phi_r}} \int_{HA} \bar{U}_1\bar{\psi}_3\bar{h}^2 - \frac{1}{2}\bar{U}_0\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \\ &- \frac{3\eta(\gamma_A + \gamma_B + o'_B)}{\sqrt{\phi_r}} U_{0A} \int_{HA} z\psi_3 g h \mathrm{d}z \\ &- \frac{3\eta(\bar{\gamma}_A + \bar{\gamma}_B + \bar{o}'_B)}{2\sqrt{\phi_r}} \bar{U}_{0A} \int_{HA} z\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \end{aligned} \tag{7.23}$$

Assuming all components real we can get two evaluate $|B_2|$ due to the shifts:

$$|B_2| \;=\; |\delta_A - \delta_B - o_B|\frac{3C_oM_o}{8f_T} \tag{7.24}$$

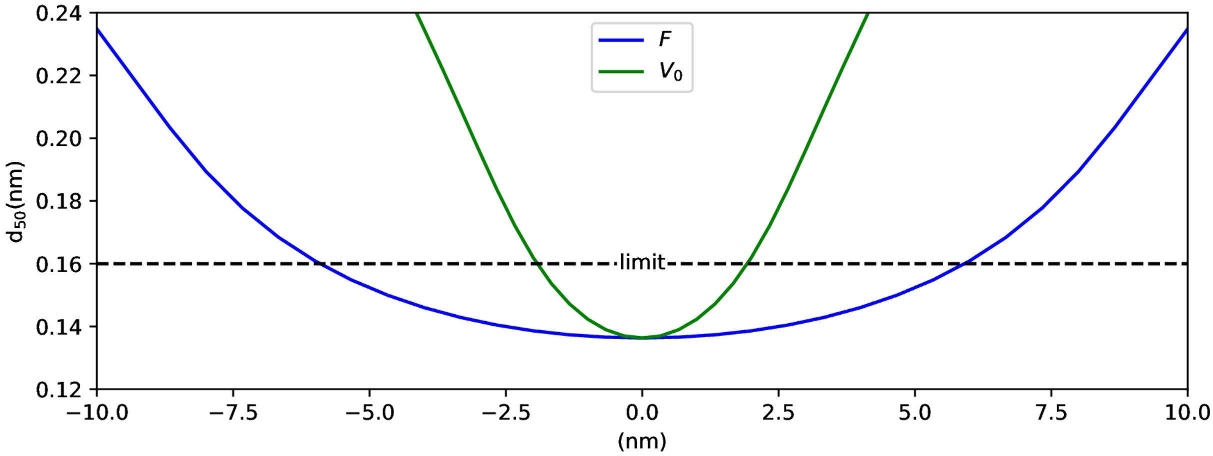
And due to the tilts:

$$|B_2| \;=\; |\gamma_A + \gamma_B + o'_B|\frac{3C_oM_o}{32f_T}L \tag{7.25}$$

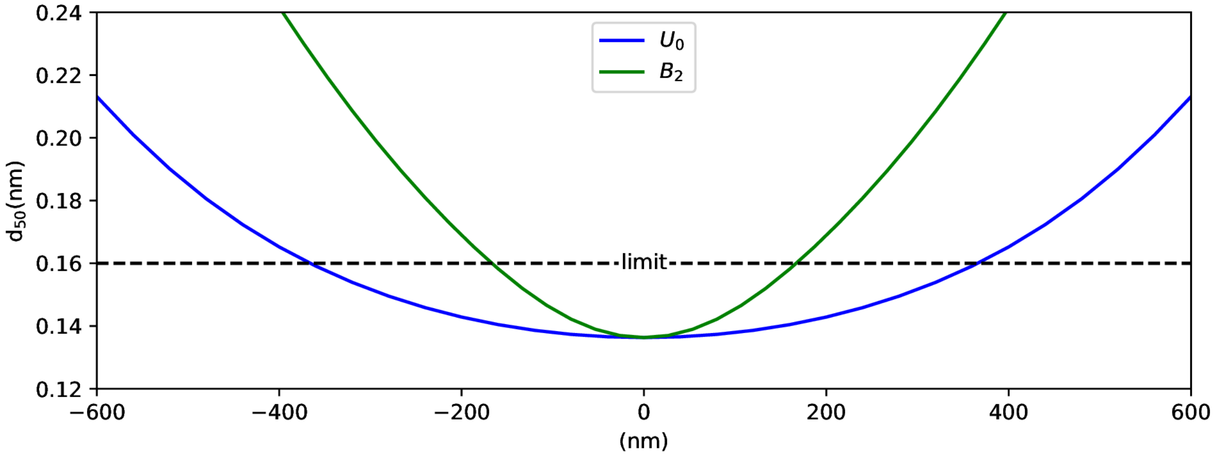
For limiting value $|B_{2,lim}| = 150\,\text{nm}$:

$$\begin{aligned} |\delta_A - \delta_B - o_B| \;&<\; |B_{2,lim}|\frac{8f_T}{3C_oM_o} \approx 320\,\text{nm} \\ |\gamma_A + \gamma_B + o'_B| \;&<\; |B_{2,lim}|\frac{32f_T}{3C_oM_oL} \approx 0.03\,\text{mrad} \end{aligned} \tag{7.26}$$

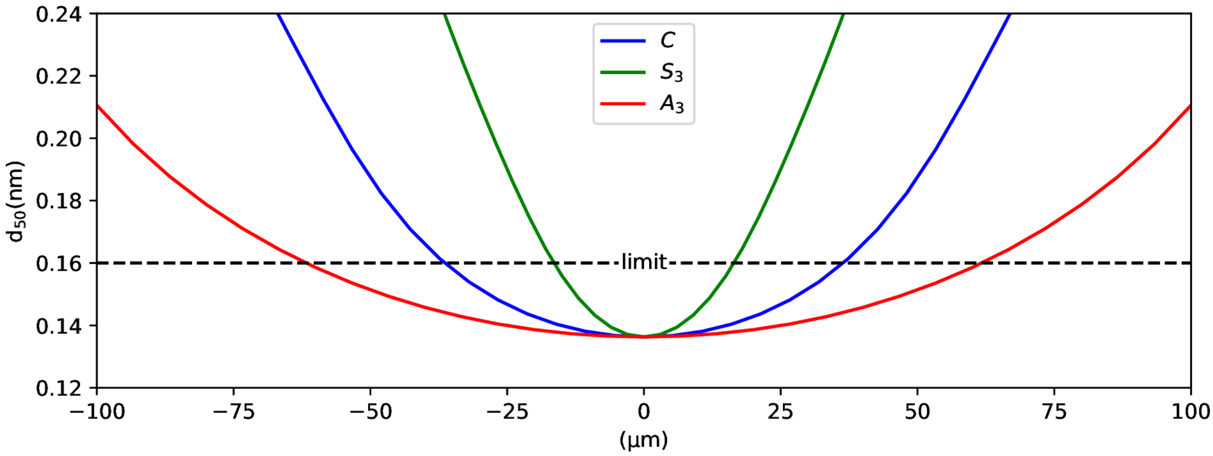
Of course in reality we do not have to eliminate both tilt and shift but just a linear combination of these two.



(a) Defocus F and astigmatisms V_0



(b) Axial coma B_2 and three-fold astigmatisms U_0



(c) Spherical aberration C, Star aberration S_3 and four-fold astigmatism A_3

Figure 7.6: Sensitivity of resolution on aberration coefficients for maximal aperture angle 30 mrad and 100 keV electron

Aberration of Third Order

To keep the resolution under limit we need to control the spherical aberration with precision:

$$|C| < 35\,\mu\text{m} \tag{7.27}$$

Which gives the request on electronics of the hexapole excitation.

We now consider only the leading term which are third power of the hexapole field:

$$\begin{aligned} S_3 &= -\frac{4i\eta}{\sqrt{\phi_r}}\int -2\bar{C}_{21}\bar{h}\bar{\psi}_2 - 6\bar{C}_{21}\bar{h}\bar{o}\bar{\psi}_3 - 3\bar{E}_{11+}\bar{h}^2\bar{\psi}_3\mathrm{d}z \\ A_3 &= -\frac{16i\eta}{\sqrt{\phi_r}}\int -3\bar{E}_{20+}\bar{h}^2\bar{\psi}_3\mathrm{d}z \end{aligned} \tag{7.28}$$

In hexapoles functions C_{21}, E_{20+}, E_{11+} can be written as:

$$\begin{aligned} C_{21} &= (C - U_0\bar{U}_1 + U_1\bar{U}_0)g - (\bar{K} - U_1\bar{U}_1 + U_2\bar{U}_0)h \\ E_{20+} &= (\bar{B}_{2+} + \frac{1}{2}\bar{U}_0V_{1+} - \bar{U}_1V_{0-})g - (\bar{C}_{2-} + \bar{U}_0V_{2-} - \bar{U}_1V_{1+})h \\ E_{11+} &= (2B_{2+} - U_0\bar{V}_{1+} + 2U_1\bar{V}_{0-})g - (A_{2-} - U_1\bar{V}_{1+} + 2U_2\bar{V}_{0-})h \end{aligned} \tag{7.29}$$

In this situation we will not provide exact calculation and just estimate scaling:

$$S_3, A_3 \propto (\delta + \gamma L)C_o^{3/2}L^{1/2}\frac{M_o^2}{f_T^2} \tag{7.30}$$

where δ is some combination of shifts of hexapoles and γ some combination of tilts. for δ and γ we have limitations in order of:

$$\begin{aligned} |\delta| &\approx 8\,\mu\text{m} \\ |\gamma| &\approx 0.2\,\text{mrad} \end{aligned} \tag{7.31}$$

which is in the same order or better as consideration for B_2.

7.2.3 Summary

If we would like to achieve better efficiency of the corrector as well as minimize additional aberration B_2, A_3, S_3 it is needed to maximize h ray in the hexapole. On the other hand this negatively influence three-fold astigmatism due to mis-rotation of the hexapoles.

8. Adjustment of Corrector

As we saw in previous chapter to eliminate parasitic aberration it is crucial to be able to control tilt and shift of the hexapoles. The shift, tilt and ellipticity of the doublet influence the residual aberrations as well, however, their effect is much smaller than of the strong hexapole field. Therefore we can align the corrector by just using two double deflector systems [7]. The standard placement of the deflectors is in Figure 8.1. By using the first (blue) deflector we create symmetrical shift $\delta_A = \delta_B$ and anti-symmetrical tilt $\gamma_A = -\gamma_B$. By linear combination with the second (green) deflector we can produce also the anti-symmetrical shift and symmetrical tilt.

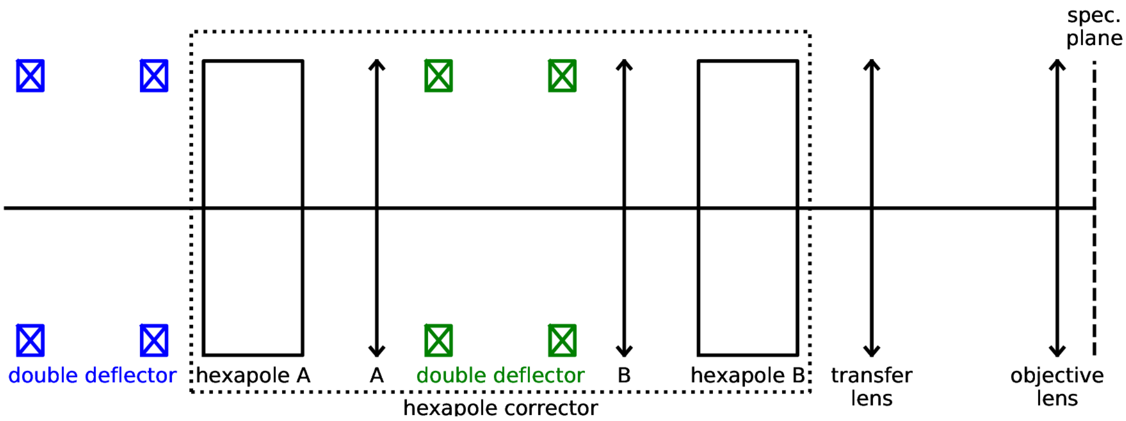


Figure 8.1: Placement of two double deflectors in the hexapole corrector

To compensate the residual aberration it is necessary to be able to measure it. It is usually done by two approaches - by Zemlin tableau[23] or by using Ronchigram [12]. The measurement and calculation of the aberration coefficients is rather complicated and is not subject of this thesis. Once we know the coefficient of the aberration we can start a procedure to eliminate them.

8.1 Three-fold Astigmatism

Probably the first step is to eliminate the three-fold astigmatism produced by mis-rotation of the hexapoles. The procedure of its elimination is already described in section 6.2.1. The main idea is to change excitation of the lens doublet to generate image rotation which minimize the absolute value of U_0 than we change the relative strength of the hexapoles such to again minimize the U_0, we should be able to get it to zero, if not we can repeat the process with lens rotation and strength of the hexapoles to get the coma under desired limit.

Now we can focus on eliminated aberrations, mainly caused by misalignments of the hexapoles.

8.2 Astigmatism of Hexapoles

We start with aberrations of the first order. The defocus is obviously eliminated by changing of excitation of a lens. The astigmatisms is also well known in standard electron microscopy and it can be eliminated by stigmator. However, it is useful to eliminate the astigmatisms produced by the hexapoles because it negatively influences the star aberration and four-fold aberration. At first we align the lenses of the corrector and zero its astigmatism with hexapoles switched off. Than we switch off the hexapoles and eliminate the produced astigmatism by changing $\delta_A = \delta_B$ since the astigmatism is dependant on the value:

$$V_0 = (o_B + \delta_A + \delta_B)\frac{6\eta}{\sqrt{\phi_r}}\int_A \psi_3 h^2 \mathrm{d}z \tag{8.1}$$

In that case we can say that $\delta_A + \delta_B + o_B$ is zero and therefore minimize the star aberration and four-fold aberration.

8.3 Axial Coma

The axial coma is generally dependant on $\delta_A - \delta_B$ and $\gamma_A - \gamma_B$. We can use change of both to eliminate it, however, it is better to use just $\delta_A = -\delta_B$ since the coma is more sensitive on shifts than on tilts.

$$\begin{aligned} B_2 = {} & \frac{6\eta(\delta_A - \delta_B - o_B)}{\sqrt{\phi_r}}\int_{HA} U_1\psi_3 h^2 - U_0\psi_3 g h \mathrm{d}z \\ & + \frac{6\eta(\bar{\delta}_A - \bar{\delta}_B - \bar{o}_B)}{\sqrt{\phi_r}}\int_{HA} \bar{U}_1\bar{\psi}_3\bar{h}^2 - \frac{1}{2}\bar{U}_0\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \\ & - \frac{3\eta(\gamma_A + \gamma_B + o'_B)}{\sqrt{\phi_r}}U_{0A}\int_{HA} z\psi_3 g h \mathrm{d}z \\ & - \frac{3\eta(\bar{\gamma}_A + \bar{\gamma}_B + \bar{o}'_B)}{2\sqrt{\phi_r}}\bar{U}_{0A}\int_{HA} z\bar{\psi}_3\bar{g}\bar{h}\mathrm{d}z \end{aligned} \tag{8.2}$$

We also noticed that there is certain combination of $\delta_A - \delta_B$ and $\gamma_A + \gamma_B$ for which the coma does not change. We can use this combination to eliminate the aberration of higher order. Theoretically, the needed combination can be calculated from the formula above separating it to the imaginary and real part. Nevertheless, in practice it might be easier to directly measure the combinations of $\delta_A - \delta_B$ and $\gamma_A + \gamma_B$ which does not influence B_2.

8.4 Aberration of Third Order

The last two aberrations, we eliminate, are four-fold astigmatism and star aberration. The dependence on hexapole tilt and shift is through the formulas:

$$\begin{aligned} S_3 &= -\frac{4i\eta}{\sqrt{\phi_r}} \int -2\bar{C}_{21}\bar{h}\bar{\psi}_2 - 6\bar{C}_{21}\bar{h}\bar{o}\bar{\psi}_3 - 3\bar{E}_{11+}\bar{h}^2\bar{\psi}_3 \mathrm{d}z \\ A_3 &= -\frac{16i\eta}{\sqrt{\phi_r}} \int -3\bar{E}_{20+}\bar{h}^2\bar{\psi}_3 \mathrm{d}z \end{aligned} \tag{8.3}$$

The four-fold astigmatism depends through the function $\bar{E}_{20+}$ only on $\delta_A + \delta_B$ and $\gamma_A - \gamma_B$. On the other hand the function $\bar{C}_{21}$ has symmetric as well as antisymmetric part with respect to the centre of the corrector thus the star aberration depends on any of $(\delta_A + \delta_B)$,$(\delta_A - \delta_B)$,$(\gamma_A + \gamma_B)$,$(\gamma_A - \gamma_B)$.

The correct solution is thus to use $\gamma_A = -\gamma_B$ to eliminate the four-fold astigmatism and the linear combination of $\delta_A - \delta_B$ and $\gamma_A + \gamma_B$ which does not change B_2 to eliminate the star aberration.

Another possibility would be to use $\delta_A = \delta_B$ and $\gamma_A = -\gamma_B$ to eliminate both A_3 and S_3 and use additional quadrupole stigmator to get rid of two-fold astigmatism.

The procedure above is based on the assumption that we do not change the hexapole strength to change spherical aberration. To change it, it is needed to do the aligning procedure with dependency on the hexapole strenght or to use additional weak lens before objective to be able to change the spherical aberration.

Conclusion

The thesis provide a deep insight into the origin of the parasitic aberration and gives a proposition on how to improve the alignment procedure for the system with the hexapole corrector. The formalism used in the thesis for calculation of the aberrations can be also used as an example for calculation of similar problems. The eikonal method, which has been used, can be easily applied on harder problems and the use of symmetry of the system is more straightforward. Also the transition to quantum mechanics and wave optics is quite direct.

The parasitic aberrations of the hexapole corrector due to misalignments and mechanical imperfections has been studied. The exact analytical expressions of the axial aberration coefficients up to the third order have been found. It was proved that two-fold astigmatism is mainly dependant on the symmetrical off-axial shift of the hexapoles ($\delta_A = \delta_B$). The another of its source comes from the ellipticity of the lenses.

The second order axial aberrations are: three-fold astigmatism and axial coma. The residual three-fold astigmatism originates from the uneven orientation of the multipoles and it can be corrected by the excitation of the doublet lenses which produce the adequate image rotation. The axial coma originates from the anti-symmetrical shift of the hexapoles ($\delta_A = -\delta_B$) or their symmetrical tilt ($\gamma_A = \gamma_B$). Additionally the aberrations are also influenced by the misalignments of the doublet but this effect is much weaker than the effect of hexapoles.

The expression of the third order residual axial aberrations – four-fold astigmatism and star aberration – has been derived as well, however, those are quite complicated. The star aberration depends on any combination of shifts and tilts of the hexapoles, the four-fold astigmatism depends just on the symmetrical shift ($\delta_A = \delta_B$) and the anti-symmetrical tilt ($\gamma_A = -\gamma_B$).

The theoretical resolution of a standard system with the hexapole corrector limited by chromatic aberration has been estimated as 0.14 nm at energy 100 keV. The maximal limitation on the residual aberration which does not deteriorate the resolution has been found. At the end the general idea about the alignment procedure has been presented.

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A. Second Order Aberrations of Misaligned Corrector

A.1 Aberration Coefficients

The aberration coefficients of third order consist of three parts - free field propagation, aberrations of lenses and aberrations of misalignments of lenses. We start with free field aberration. We define integrals:

$$
\begin{aligned}
C_F &= \int \frac{1}{2}\bar{h}'^2 h'^2 \mathrm{d}z \\
K_F &= \int \frac{1}{2} g' \bar{h}'^2 h' \mathrm{d}z \\
F_F &= \int \bar{g}' g' \bar{h}' h' \mathrm{d}z \\
A_F &= \int \frac{1}{2} g'^2 \bar{h}'^2 \mathrm{d}z \\
D_F &= \int \frac{1}{2} \bar{g}' g'^2 \bar{h}' \mathrm{d}z \\
E_F &= \int \frac{1}{2} \bar{g}'^2 g'^2 \mathrm{d}z
\end{aligned}
\tag{A.1}
$$

$$
\begin{aligned}
B_{2F} &= \int \frac{1}{2}\bar{h}'^2 h' o' \mathrm{d}z \\
A_{2F} &= \int \bar{g}' \bar{h}' h' o' \mathrm{d}z \\
C_{2F} &= \int \frac{1}{2} g' \bar{h}'^2 o' \mathrm{d}z \\
D_{2F} &= \int \frac{1}{2} \bar{g}'^2 h' o' \mathrm{d}z \\
E_{2F} &= \int \bar{g}' g' \bar{h}' o' \mathrm{d}z \\
F_{2F} &= \int \frac{1}{2} \bar{g}'^2 g' o' \mathrm{d}z
\end{aligned}
\tag{A.2}
$$

For monopole part we have:

$$C_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-2h^2\bar{h}\bar{h}' + 2h\bar{h}^2h'\right) {\psi_0}'''\mathrm{d}z \tag{A.3}$$
$$K_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-2gh\bar{h}\bar{h}' + g\bar{h}^2h' + g'h\bar{h}^2\right) {\psi_0}'''\mathrm{d}z$$
$$F_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-2g\bar{g}h\bar{h}' + 2g\bar{g}\bar{h}h' - 2g\bar{g}'h\bar{h} + 2\bar{g}g'h\bar{h}\right) {\psi_0}'''\mathrm{d}z$$
$$A_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-2g^2\bar{h}\bar{h}' + 2gg'\bar{h}^2\right) {\psi_0}'''\mathrm{d}z$$
$$D_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-g^2\bar{g}\bar{h}' - g^2\bar{g}'\bar{h} + 2g\bar{g}g'\bar{h}\right) {\psi_0}'''\mathrm{d}z$$
$$E_M = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(-2g^2\bar{g}\bar{g}' + 2g\bar{g}^2g'\right) {\psi_0}'''\mathrm{d}z$$

$$B_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(h\bar{h}^2o' - 2h\bar{h}\bar{h}'o + \bar{h}^2h'o\right) {\psi_0}'''\mathrm{d}z \tag{A.4}$$
$$A_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(2\bar{g}h\bar{h}o' - 2\bar{g}h\bar{h}'o + 2\bar{g}\bar{h}h'o - 2\bar{g}'h\bar{h}o\right) {\psi_0}'''\mathrm{d}z$$
$$C_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(g\bar{h}^2o' - 2g\bar{h}\bar{h}'o + g'\bar{h}^2o\right) {\psi_0}'''\mathrm{d}z$$
$$D_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(\bar{g}^2ho' + \bar{g}^2h'o - 2\bar{g}\bar{g}'ho\right) {\psi_0}'''\mathrm{d}z$$
$$E_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(2g\bar{g}\bar{h}o' - 2g\bar{g}\bar{h}'o - 2g\bar{g}'\bar{h}o + 2\bar{g}g'\bar{h}o\right) {\psi_0}'''\mathrm{d}z$$
$$F_{2M} = \frac{i\eta}{16\sqrt{\phi_r}} \int \left(g\bar{g}^2o' - 2g\bar{g}\bar{g}'o + \bar{g}^2g'o\right) {\psi_0}'''\mathrm{d}z$$

And dipole part:

$$B_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2h\bar{h}\bar{h}' - \bar{h}^2h'\right) \bar{\psi}'_{1L}\mathrm{d}z \tag{A.5}$$
$$A_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2\bar{g}h\bar{h}' - 2\bar{g}\bar{h}h' + 2\bar{g}'h\bar{h}\right) \bar{\psi}'_{1L}\mathrm{d}z$$
$$C_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2g\bar{h}\bar{h}' - g'\bar{h}^2\right) \bar{\psi}'_{1L}\mathrm{d}z$$
$$D_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(-\bar{g}^2h' + 2\bar{g}\bar{g}'h\right) \bar{\psi}'_{1L}\mathrm{d}z$$
$$E_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2g\bar{g}\bar{h}' + 2g\bar{g}'\bar{h} - 2\bar{g}g'\bar{h}\right) \bar{\psi}'_{1L}\mathrm{d}z$$
$$F_{2D} = \frac{i\eta}{4\sqrt{\phi_r}} \int \left(2g\bar{g}\bar{g}' - \bar{g}^2g'\right) \bar{\psi}'_{1L}\mathrm{d}z$$

The next part in eikonal is $\int D^{(1)}M^{(0)}$. We can split that into pure hexapole field and coupling of hexapole with quadrupole field, hexapole integrals look like:

$$
\begin{aligned}
C_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0\bar{g}h^2\psi_3 - U_1h^2\bar{h}\psi_3 + \bar{U}_0g\bar{h}^2\bar{\psi}_3 - \bar{U}_1h\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
K_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0g\bar{g}h\psi_3 - U_1gh\bar{h}\psi_3 + \bar{U}_1g\bar{h}^2\bar{\psi}_3 - \bar{U}_2h\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
F_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int 2U_1g\bar{g}h\psi_3 - 2U_2gh\bar{h}\psi_3 + 2\bar{U}_1g\bar{g}\bar{h}\bar{\psi}_3 - 2\bar{U}_2\bar{g}h\bar{h}\bar{\psi}_3\mathrm{d}z \\
A_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0g^2\bar{g}\psi_3 - U_1g^2\bar{h}\psi_3 + \bar{U}_2g\bar{h}^2\bar{\psi}_3 - \bar{U}_3h\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
D_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_1g^2\bar{g}\psi_3 - U_2g^2\bar{h}\psi_3 + \bar{U}_2g\bar{g}\bar{h}\bar{\psi}_3 - \bar{U}_3\bar{g}h\bar{h}\bar{\psi}_3\mathrm{d}z \\
E_H &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_2g^2\bar{g}\psi_3 - U_3g^2\bar{h}\psi_3 + \bar{U}_2g\bar{g}^2\bar{\psi}_3 - \bar{U}_3\bar{g}^2h\bar{\psi}_3\mathrm{d}z
\end{aligned}
\tag{A.6}
$$

$$
\begin{aligned}
B_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0\bar{g}ho\psi_3 - U_1h\bar{h}o\psi_3\mathrm{d}z \\
A_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int 2U_1\bar{g}ho\psi_3 - 2U_2h\bar{h}o\psi_3\mathrm{d}z \\
C_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_0g\bar{g}o\psi_3 - U_1g\bar{h}o\psi_3\mathrm{d}z \\
D_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_2\bar{g}ho\psi_3 - U_3h\bar{h}o\psi_3\mathrm{d}z \\
E_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int 2U_1g\bar{g}o\psi_3 - 2U_2g\bar{h}o\psi_3\mathrm{d}z \\
F_{2H} &= -\frac{6\eta}{\sqrt{\phi_r}}\int U_2g\bar{g}o\psi_3 - U_3g\bar{h}o\psi_3\mathrm{d}z
\end{aligned}
\tag{A.7}
$$

and coupling of quadrupole with hexapole field:

$$
\begin{aligned}
B_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 2U_0\eta\bar{g}h\psi_2 - 2U_1\eta h\bar{h}\psi_2 + 6\bar{V}_0\eta g\bar{h}^2\bar{\psi}_3 - 3\bar{V}_1\eta h\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
A_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 4U_1\eta\bar{g}h\psi_2 - 4U_2\eta h\bar{h}\psi_2 + 12\bar{V}_0\eta g\bar{g}\bar{h}\bar{\psi}_3 - 6\bar{V}_1\eta\bar{g}h\bar{h}\bar{\psi}_3\mathrm{d}z \\
C_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 2U_0\eta g\bar{g}\psi_2 - 2U_1\eta g\bar{h}\psi_2 + 3\bar{V}_1\eta g\bar{h}^2\bar{\psi}_3 - 6\bar{V}_2\eta h\bar{h}^2\bar{\psi}_3\mathrm{d}z \\
D_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 2U_2\eta\bar{g}h\psi_2 - 2U_3\eta h\bar{h}\psi_2 + 6\bar{V}_0\eta g\bar{g}^2\bar{\psi}_3 - 3\bar{V}_1\eta\bar{g}^2h\bar{\psi}_3\mathrm{d}z \\
E_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 4U_1\eta g\bar{g}\psi_2 - 4U_2\eta g\bar{h}\psi_2 + 6\bar{V}_1\eta g\bar{g}\bar{h}\bar{\psi}_3 - 12\bar{V}_2\eta\bar{g}h\bar{h}\bar{\psi}_3\mathrm{d}z \\
F_{2Q} &= -\frac{1}{\sqrt{\phi_r}}\int 2U_2\eta g\bar{g}\psi_2 - 2U_3\eta g\bar{h}\psi_2 + 3\bar{V}_1\eta g\bar{g}^2\bar{\psi}_3 - 6\bar{V}_2\eta\bar{g}^2h\bar{\psi}_3\mathrm{d}z
\end{aligned}
\tag{A.8}
$$

A.2 Trajectory

The second order aberrations are:

$$
\begin{aligned}
w^{(2)} = &\big[C\bar{g} - \bar{K}\bar{h} + U_0\bar{U}_0\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + U_0\bar{U}_1\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&+U_1\bar{U}_0\left(g\bar{g}h' + gg'\bar{h} - 2\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{U}_1\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&+U_2\bar{U}_0\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + U_2\bar{U}_1\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\big]\,\bar{w}_0'{w'}_0^2 \\
&+\big[-\bar{A}\bar{h} + \bar{K}\bar{g} + U_1\bar{U}_0\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + U_1\bar{U}_1\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&+U_2\bar{U}_0\left(g\bar{g}h' + gg'\bar{h} - 2\bar{g}\bar{g}'\bar{h}\right) + U_2\bar{U}_1\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&+U_3\bar{U}_0\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + U_3\bar{U}_1\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\big]\,\bar{w}_0{w'}_0^2 \\
&+\big[-F\bar{h} + 2K\bar{g} + U_0\bar{U}_1\left(-2g\bar{g}g' + 2\bar{g}^2\bar{g}'\right) + U_0\bar{U}_2\left(-2\bar{g}^2\bar{h}' + 2\bar{g}g'h\right) \\
&+U_1\bar{U}_1\left(2g\bar{g}h' + 2gg'\bar{h} - 4\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{U}_2\left(-2\bar{g}hh' + 4\bar{g}\bar{h}\bar{h}' - 2g'h\bar{h}\right) \\
&+U_2\bar{U}_1\left(-2g\bar{h}h' + 2\bar{g}'\bar{h}^2\right) + U_2\bar{U}_2\left(2h\bar{h}h' - 2\bar{h}^2\bar{h}'\right)\big]\,w_0\bar{w}_0'{w'}_0 \\
&+\big[-2\bar{D}\bar{h} + F\bar{g} + U_1\bar{U}_1\left(-2g\bar{g}g' + 2\bar{g}^2\bar{g}'\right) + U_1\bar{U}_2\left(-2\bar{g}^2\bar{h}' + 2\bar{g}g'h\right) \\
&+U_2\bar{U}_1\left(2g\bar{g}h' + 2gg'\bar{h} - 4\bar{g}\bar{g}'\bar{h}\right) + U_2\bar{U}_2\left(-2\bar{g}hh' + 4\bar{g}\bar{h}\bar{h}' - 2g'h\bar{h}\right) \\
&+U_3\bar{U}_1\left(-2g\bar{h}h' + 2\bar{g}'\bar{h}^2\right) + U_3\bar{U}_2\left(2h\bar{h}h' - 2\bar{h}^2\bar{h}'\right)\big]\,w_0\bar{w}_0{w'}_0 \\
&+\big[A\bar{g} - D\bar{h} + U_0\bar{U}_2\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + U_0\bar{U}_3\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&+U_1\bar{U}_2\left(g\bar{g}h' + gg'\bar{h} - 2\bar{g}\bar{g}'\bar{h}\right) + U_1\bar{U}_3\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&+U_2\bar{U}_2\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + U_2\bar{U}_3\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\big]\,w_0^2\bar{w}_0' \\
&+\big[D\bar{g} - E\bar{h} + U_1\bar{U}_2\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + U_1\bar{U}_3\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&+U_2\bar{U}_2\left(g\bar{g}h' + gg'\bar{h} - 2\bar{g}\bar{g}'\bar{h}\right) + U_2\bar{U}_3\left(-\bar{g}hh' + 2\bar{g}\bar{h}\bar{h}' - g'h\bar{h}\right) \\
&+U_3\bar{U}_2\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + U_3\bar{U}_3\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\big]\,w_0^2\bar{w}_0 \\
&+\Bigg[\bar{B}_2\bar{g} - \bar{C}_2\bar{h} + \bar{U}_0V_0\left(-g\bar{g}g' + \bar{g}^2\bar{g}'\right) + \bar{U}_0V_1\left(\frac{1}{2}g\bar{g}h' + \frac{1}{2}gg'\bar{h} - \bar{g}\bar{g}'\bar{h}\right) \\
&+\bar{U}_0V_2\left(-g\bar{h}h' + \bar{g}'\bar{h}^2\right) + \bar{U}_1V_0\left(-\bar{g}^2\bar{h}' + \bar{g}g'h\right) \\
&+\bar{U}_1V_1\left(-\frac{1}{2}\bar{g}hh' + \bar{g}\bar{h}\bar{h}' - \frac{1}{2}g'h\bar{h}\right) + \bar{U}_1V_2\left(h\bar{h}h' - \bar{h}^2\bar{h}'\right)\Bigg]\,\epsilon{w'}_0^2
\end{aligned}
\tag{A.9}
$$

$$
\begin{aligned}
&+\left[-A_2\bar{h}+2B_2\bar{g}+U_0\bar{V}_0\left(-2g\bar{g}g'+2\bar{g}^2\bar{g}'\right)+U_0\bar{V}_1\left(-\bar{g}^2\bar{h}'+\bar{g}g'h\right)\right.\\
&+U_1\bar{V}_0\left(2g\bar{g}h'+2gg'\bar{h}-4\bar{g}\bar{g}'\bar{h}\right)+U_1\bar{V}_1\left(-\bar{g}hh'+2\bar{g}\bar{h}\bar{h}'-g'h\bar{h}\right)\\
&\left.+U_2\bar{V}_0\left(-2g\bar{h}h'+2\bar{g}'\bar{h}^2\right)+U_2\bar{V}_1\left(h\bar{h}h'-\bar{h}^2\bar{h}'\right)\right]\epsilon\bar{w}_0'w'_0
\end{aligned}
$$

$$
\begin{aligned}
&+\left[\bar{A}_2\bar{g}-\bar{E}_2\bar{h}+\bar{U}_1V_0\left(-2g\bar{g}g'+2\bar{g}^2\bar{g}'\right)+\bar{U}_1V_1\left(g\bar{g}h'+gg'\bar{h}-2\bar{g}\bar{g}'\bar{h}\right)\right.\\
&+\bar{U}_1V_2\left(-2g\bar{h}h'+2\bar{g}'\bar{h}^2\right)+\bar{U}_2V_0\left(-2\bar{g}^2\bar{h}'+2\bar{g}g'h\right)\\
&\left.+\bar{U}_2V_1\left(-\bar{g}hh'+2\bar{g}\bar{h}\bar{h}'-g'h\bar{h}\right)+\bar{U}_2V_2\left(2h\bar{h}h'-2\bar{h}^2\bar{h}'\right)\right]\epsilon w_0w'_0
\end{aligned}
$$

$$
\begin{aligned}
&+\left[A_2\bar{g}-2D_2\bar{h}+U_1\bar{V}_0\left(-2g\bar{g}g'+2\bar{g}^2\bar{g}'\right)+U_1\bar{V}_1\left(-\bar{g}^2\bar{h}'+\bar{g}g'h\right)\right.\\
&+U_2\bar{V}_0\left(2g\bar{g}h'+2gg'\bar{h}-4\bar{g}\bar{g}'\bar{h}\right)+U_2\bar{V}_1\left(-\bar{g}hh'+2\bar{g}\bar{h}\bar{h}'-g'h\bar{h}\right)\\
&\left.+U_3\bar{V}_0\left(-2g\bar{h}h'+2\bar{g}'\bar{h}^2\right)+U_3\bar{V}_1\left(h\bar{h}h'-\bar{h}^2\bar{h}'\right)\right]\epsilon\bar{w}_0w'_0
\end{aligned}
$$

$$
\begin{aligned}
&+\left[2C_2\bar{g}-E_2\bar{h}+U_0\bar{V}_1\left(-g\bar{g}g'+\bar{g}^2\bar{g}'\right)+U_0\bar{V}_2\left(-2\bar{g}^2\bar{h}'+2\bar{g}g'h\right)\right.\\
&+U_1\bar{V}_1\left(g\bar{g}h'+gg'\bar{h}-2\bar{g}\bar{g}'\bar{h}\right)+U_1\bar{V}_2\left(-2\bar{g}hh'+4\bar{g}\bar{h}\bar{h}'-2g'h\bar{h}\right)\\
&\left.+U_2\bar{V}_1\left(-g\bar{h}h'+\bar{g}'\bar{h}^2\right)+U_2\bar{V}_2\left(2h\bar{h}h'-2\bar{h}^2\bar{h}'\right)\right]\epsilon w_0\bar{w}_0'
\end{aligned}
$$

$$
\begin{aligned}
&+\left[\bar{D}_2\bar{g}-\bar{F}_2\bar{h}+\bar{U}_2V_0\left(-g\bar{g}g'+\bar{g}^2\bar{g}'\right)+\bar{U}_2V_1\left(\frac{1}{2}g\bar{g}h'+\frac{1}{2}gg'\bar{h}-\bar{g}\bar{g}'\bar{h}\right)\right.\\
&+\bar{U}_2V_2\left(-g\bar{h}h'+\bar{g}'\bar{h}^2\right)+\bar{U}_3V_0\left(-\bar{g}^2\bar{h}'+\bar{g}g'h\right)\\
&\left.+\bar{U}_3V_1\left(-\frac{1}{2}\bar{g}hh'+\bar{g}\bar{h}\bar{h}'-\frac{1}{2}g'h\bar{h}\right)+\bar{U}_3V_2\left(h\bar{h}h'-\bar{h}^2\bar{h}'\right)\right]\epsilon w_0^2
\end{aligned}
$$

$$
\begin{aligned}
&+\left[E_2\bar{g}-2F_2\bar{h}+U_1\bar{V}_1\left(-g\bar{g}g'+\bar{g}^2\bar{g}'\right)+U_1\bar{V}_2\left(-2\bar{g}^2\bar{h}'+2\bar{g}g'h\right)\right.\\
&+U_2\bar{V}_1\left(g\bar{g}h'+gg'\bar{h}-2\bar{g}\bar{g}'\bar{h}\right)+U_2\bar{V}_2\left(-2\bar{g}hh'+4\bar{g}\bar{h}\bar{h}'-2g'h\bar{h}\right)\\
&\left.+U_3\bar{V}_1\left(-g\bar{h}h'+\bar{g}'\bar{h}^2\right)+U_3\bar{V}_2\left(2h\bar{h}h'-2\bar{h}^2\bar{h}'\right)\right]\epsilon w_0\bar{w}_0
\end{aligned}
$$