Comments on aberration correction in symmetric imaging energy filters

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Abstract

Imaging energy filters are becoming an essential part of high-quality electron microscopes. They enhance the contrast, allow element specific imaging, and elemental decomposition by spectroscopy of inelastically scattered electrons. All filters which are commercially available are not completely corrected to second order; however, some use symmetric arrangements for the cancellation of the most destructive second order effects. However, completely corrected symmetric arrangements have been tested already. For the construction of these systems it is important to know what consequences the symmetry of the optical arrangement has: which aberrations cancel due to symmetry, which aberrations are interrelated and vanish simultaneously when implementing multipole correctors, which higher-order aberrations remain after cancellation of the leading-order aberrations. These questions can in principle be answered by the Eikonal method as well as by the transfer map method. Here we demonstrate that a combination of both methods answers these question in a very simplified fashion. This simplicity allows to draw some novel conclusions. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

Inelastically scattered electrons blur the image in an electron microscope. The reason for this disturbing effect is not only the chromatic aberration which causes the inelastically scattered electrons to be focused in a different fashion than electrons which did not suffer an energy loss. Electrons which scatter at the nuclei of the object do not suffer energy loss and therefore the elastically scattered electrons carry atomic information in the order of an angstrom. Inelastically scattered electrons excite phonons, band electrons, or plasmons, and these electrons therefore carry information on a nanometer scale. This blurring of the image cannot be corrected by eliminating the chromatic aberration of the microscope but electrons which have been scattered inelastically have to be filtered out of the electron beam. This mode of increasing the contrast in an electron microscope is referred to as zero loss imaging [1]. The first instruments that filtered inelastically scattered electrons out of the beam were high pass energy filters. One simply applied a retarding potential barrier which could only be overcome by electrons that had not suffered an appreciable energy loss in the object [2,3]. These early techniques have been replaced by energy

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filters which select parts of the energy loss spectrum by a narrow selection slit. For this purpose bending magnets or electrostatic deflectors have to be used to produce dispersion. An energy selection slit is then placed in a plane where the beam of electrons with nominal energy is as narrow as possible. Since the object size is magnified by the intermediate magnification at the position of the filter, whereas the defraction image is demagnified by that number, the electron beam has a waist at an image of the defractive plane. There is another more subtle reason why the energy selection plane has to be an image of the defraction plane. The energy which is selected has to be the same for all electrons, no matter at which spot of the object they originated. This property is referred to as isochromaticity [1]. Therefore, the field ray has to intersect the optic axis at the energy selection plane, which is then equivalent to a defraction plane. After the energy selection has been performed at that plane, a projector system has to transfer an achromatic image of the object to the detector plane. The image has to be achromatic in order not to be blurred by the energy band which can pass the selection slit.

An energy filter cannot only be used for increasing the contrast of an electron microscopic picture but also for element specific imaging. One simply accelerates the electrons to an energy which is too high by an amount ΔE so that only those electrons which lose the energy ΔE by inelastic scattering pass the energy selection slit and form the image. If one takes a picture with ΔE just above a characteristic energy level of an atomic element, predominantly electrons scattered inelastically at such atoms form the image. If one performs background subtraction by taking into account an image with ΔE just below that characteristic excitation energy, one obtains an image of atoms which are all of one elemental type.

Finally a third important application of energy filters should be mentioned. If the projection system after the filter can image the energy selection plane on the detector, then the energy loss spectrum of the object or of a small object detail can be recorded and used to analyze elemental composition. The requirements on an imaging energy filter are therefore the following:

(1) The dispersion at the image of the object behind the filter has to vanish.

(2) This achromatic image should be stigmatic and round, so that a round projector system can image it to the detector plane.

(3) The filter should not introduce dominant aberrations at the object image.

(4) In the section of dispersion, the energy selection plane has to be an image of the defraction plane, or an image of the object if the microscope is operated in defraction mode.

(5) The dispersion at the energy selection plane should be large.

(6) The filter should not introduce dominant aberrations at the energy selection plane.

The achromatic image of the object can be a virtual image located inside the filter [4], the image of the defraction plane, however, has to be located in a field free region, in order to position the energy selection slit. It is advantageous if the object image in front of the filter is located in a field free region since introducing grids at that position can be very useful for aligning the energy filter [5,1].

It was emphasized already in [6] that symmetric filter arrangements can lead to a cancellation of some disturbing aberrations. Therefore, we want to analyze systematically which implications various symmetries will have for the electrons motion. Some of the results have already been obtained by the Eikonal method [1] or the map method [7]. Here we want to show how to combine both methods to uncover implications of symmetry in a very straightforward fashion.

2. The paraxial optics, fundamental rays, and aberrations

The motion of charged particles through particle optical systems can be described by a transport function which takes initial phase space coordinates $\vec{z}_i$ of particle in front of the system into final coordinates $\vec{z}_f = \vec{M}_t(\vec{z}_i)$ behind it. The Taylor polynomial of $\vec{M}(\vec{z})$ to an order n is often referred to as the nth order Taylor transport function. The coefficients of this polynomial are related to the aberrations of various orders. The phase space coordinates which we will consider in this article are the transverse positions x and y, the corresponding

normalized canonical momenta $a = p_x/p_0$ and $b = p_y/p_0$, where p_0 is the kinetic momentum of a reference particle, and the relative deviation κ from the reference energy. Evaluating the transfer map to first order defines the so-called paraxial optics.

In the Eikonal method, the paraxial optics is used to define four fundamental rays. They are an arbitrary set of four linearly independent paraxial trajectories and therefore all solve the linearized equation of motion. In an electron microscope it is useful to choose two fundamental rays in the x and two in the y section with the following properties: The so-called axial fundamental rays in these two sections are called w_α and w_β and intersect the optical axis in the object plane with slope 1. The other two fundamental rays w_γ and w_δ are called field rays since they intersect the optic axis at the source and have transverse positions 1 at the object plane. An arbitrary particle trajectory can then be described in terms of initial transverse positions and momenta in the object plane and its relative energy deviation κ. Also other conventions are possible, however, whichever convention is taken, we take care that the Wronski determinants $w_\gamma w'_\alpha - w'_\gamma w_\alpha$ and $w_\delta w'_\beta - w'_\delta w_\beta$, which are invariant along the optic axis, are equal to one and that all other Wronski determinants are equal to zero.

Every trajectory is defined by its starting conditions, and the phase space coordinates are therefore functions of $\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa$, and the longitudinal coordinate s along the optic axis. At every point s along the optical axis one can then find four constants $\gamma, \alpha, \delta, \beta$ which define the transverse positions and normalized momenta of a particle's trajectory as a linear combination of the fundamental rays and their derivatives

$$\begin{pmatrix} x(s) \\ y(s) \end{pmatrix} = \gamma(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w_\gamma(s)$$
$$+ \alpha(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w_\alpha(s)$$
$$+ \delta(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w_\delta(s)$$
$$+ \beta(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w_\beta(s) \quad (1)$$

$$\begin{pmatrix} a(s) \\ b(s) \end{pmatrix} = \gamma(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w'_\gamma(s)$$
$$+ \alpha(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w'_\alpha(s)$$

$$+ \delta(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w'_\delta(s)$$
$$+ \beta(\gamma_i, \alpha_i, \delta_i, \beta_i, \kappa, s)w'_\beta(s). \quad (2)$$

To include the energy deviation in our considerations, we construct the five-dimensional vector $\vec{\zeta}^{\,T} = (\gamma, \alpha, \delta, \beta, \kappa)$. These five coordinates are functions of the initial conditions. Therefore, we have constructed a map which transports the coefficients of Eqs. (1) and (2) from the initial plane into a final plane by $\vec{\zeta}_f = \vec{M}(\vec{\zeta}_i)$. Dealing with this transfer map is much simpler than dealing with the previously mentioned transfer function $\vec{M}_t$ for the phase space coordinates $\vec{z}$ since the linear part of the newly defined transfer map has the simple matrix representation

$$\mathbf{L}(d, \tilde{d}) = \begin{pmatrix} 1 & 0 & 0 & 0 & d \\ 0 & 1 & 0 & 0 & \tilde{d} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (3)$$

where $dw_\gamma + \tilde{d}w_\alpha$ describes the linear dispersion. Furthermore, the transfer map $\vec{M}$ has the advantage that it does not change in a field free region. The transfer map is related to the phase space transport function $\vec{M}_t$ via the fundamental rays in the initial and final plane, characterized by the coordinate s_i and s_f, via

$$\mathbf{W}(s) = \begin{pmatrix} w_{\gamma x}(s) & w_{\alpha x}(s) & 0 & 0 & 0 \\ w'_{\gamma x}(s) & w'_{\alpha x}(s) & 0 & 0 & 0 \\ 0 & 0 & w_{\delta y}(s) & w_{\beta y}(s) & 0 \\ 0 & 0 & w'_{\delta y}(s) & w'_{\beta y}(s) & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (4)$$

$$\vec{M}_t(\vec{z}) = \mathbf{W}(s_f)\vec{M}(\mathbf{W}(s_i)^{-1}\vec{z}). \quad (5)$$

The nonlinear Taylor coefficients of the function $\vec{M}(\vec{\zeta})$ in the final plane are referred to as aberrations of the system. We introduce a five-dimensional vector of integers $\vec{k}^T = (k_\gamma, k_\alpha, k_\delta, k_\beta, k_\kappa)$ and write monomials of the five initial coefficients as $\vec{\zeta}_i^{\,\vec{k}}$. The Taylor coefficient are indicated by a letter for the coordinate and by the monomial, which we set

in parentheses. The first component of the Taylor transfer map is for example $\sum_{\vec{k}} \vec{\zeta}^{\vec{k}} (\gamma, \vec{\zeta}^{\vec{k}})$.

3. Symmetric systems

3.1. Mid-section symmetry

To avoid confusion, we use the convention that sections are surfaces that contain the optical axis whereas planes are perpendicular to it. Usually all optical elements which are used in filters have a section of symmetry. The x direction is taken to lie in this symmetry section, whereas the y coordinate is transverse to it, and one chooses the first pair of fundamental rays in the x and the second pair in the y section. Mid-section symmetry then implies that a sign change of the initial δ_i and β_i has to result merely in a sign change of the final δ_f and β_f, whereas γ_f and α_f do not change. This results in the well-known condition

$$\vec{M}(\mathbf{R}\vec{\zeta}) = \mathbf{R}\vec{M}(\vec{\zeta}), \quad \mathbf{R} = \text{diag}(1, 1, -1, -1, 1). \quad (6)$$

This simple condition is only stated for completeness and implies the following conditions for the aberrations:

$$(\gamma, \vec{\zeta}^{\vec{k}}) = 0, \quad (\alpha, \vec{\zeta}^{\vec{k}}) = 0 \quad \text{if } k_y + k_b = \text{odd} \quad (7)$$

$$(\delta, \vec{\zeta}^{\vec{k}}) = 0, \quad (\beta, \vec{\zeta}^{\vec{k}}) = 0 \quad \text{if } k_y + k_b = \text{even}. \quad (8)$$

3.2. Mirror symmetry and point symmetry

Similar implications result from other symmetries. Here we consider systems with one mirror plane or one point of symmetry. Fig. 1 shows schematically the two possibilities of arranging two dispersive systems symmetrically.

In order to take advantage of the symmetry, the image planes of the object in front of the filter and behind the filter have to be arranged symmetrically also. The same has to be true for the images of the defraction plane. The object image is characterized by the condition that the axial rays w_α and w_β are zero. Similarly the defraction plane is characterized by the fact that the field rays w_γ and w_δ are zero. The symmetry then implies that in the x as well as in the y section, one of the fundamental rays is symmetric with respect to the image plane and the
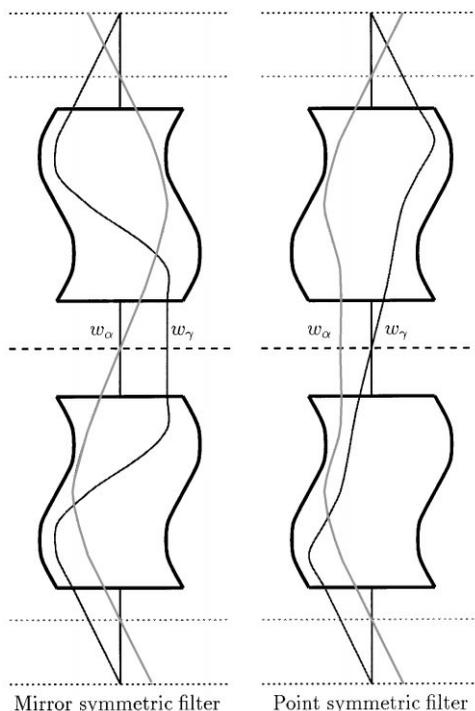
Fig. 1. Schematic illustration of mirror- and point-symmetric filters. The image planes of the object and of the source are indicated as well as the fundamental rays in the section of dispersion.

other is antisymmetric with respect to that plane. For this argument it is essential that the linear approximation implies that the negative of a fundamental ray is also a paraxial trajectory.

There are now two possibilities in each section; either one chooses the antisymmetric or the symmetric fundamental ray to define the object image. To describe these choices of symmetry, we introduce the factors s_α and s_β. They are 1 if the corresponding fundamental ray, w_α or w_β, is symmetric and -1 if that ray is antisymmetric. Fig. 1 shows schematically the fundamental rays and the image planes. We let $\vec{M}(\vec{\zeta})$ be the transfer map from in front of the filter to behind the filter. As mentioned previously one does not have to specify the exact plane to which the transfer map refers since in our formalism the transfer map does not change in a field free region. Furthermore, we let $\vec{M}_1$ be the transfer map of the first half of the symmetric

arrangement and $\vec{M}_2$ that of the second half. Due to the symmetry of the fields and the fundamental rays, $\vec{M}_2$ can be used to determine $\vec{M}_1$. In case of the mirror symmetric system

$$\vec{M}_1(\vec{\zeta}) = \mathbf{S}\vec{M}_2^{-1}(\mathbf{S}\vec{\zeta}), \quad \mathbf{S} = \text{diag}(-s_\alpha, s_\alpha, -s_\beta, s_\beta, 1). \tag{9}$$

Similarly $\vec{M}_1(\vec{\zeta})$ of the point symmetric system is given by

$$\vec{M}_1(\vec{\zeta}) = \mathbf{P}\vec{M}_2^{-1}(\mathbf{P}\vec{\zeta}), \quad \mathbf{P} = \text{diag}(s_\alpha, -s_\alpha, -s_\beta, s_\beta, 1). \tag{10}$$

4. Implications of symmetry

To obtain the matrix representation of the linear transfer map of the mirror symmetric system, we use Eq. (3) and get

$$M = \mathbf{L}(d, \tilde{d})\mathbf{S}\mathbf{L}(-d, -\tilde{d})\mathbf{S}$$
$$= \mathbf{L}(d, \tilde{d})\mathbf{L}(s_\alpha d, -s_\alpha \tilde{d})$$
$$= \mathbf{L}((1 + s_\alpha)d, (1 - s_\alpha)\tilde{d}) \tag{11}$$

where $s_\alpha d$ and $-s_\alpha \tilde{d}$ describe the dispersion in the center of the filter. The dispersion (γ, κ) at the image of the object behind the filter is only zero, which is the first requirement mentioned in the introduction, if $s_\alpha = -1$ and therefore the fundamental ray w_α has to be antisymmetric in the case of mirror symmetry. This result is well known and can easily be obtained by considering that the integral over the bending field times the sine like ray w_α is proportional to the dispersion. This formula is derived from the equation of motion, however, as we see here, the special form of the equation of motion is not important for this conclusion. In any system with mirror symmetry the dispersion would always be zero for antisymmetric w_α, independent of the equation of motion, as long as this equation is invariant under a change of the time direction.

The total point-symmetric system has a linear transfer map represented by the matrix

$$M = \mathbf{L}(d, \tilde{d})\mathbf{P}\mathbf{L}(-d, -\tilde{d})\mathbf{P}$$
$$= \mathbf{L}((1 - s_\alpha)d, (1 + s_\alpha)\tilde{d}). \tag{12}$$

The ray w_α has to be symmetric in this case in order to make the objects image achromatic by symmetry. It follows that $\mathbf{P} = \mathbf{S}$ is identical for all imaging filters. We do not have to consider mirror- and point-symmetric systems separately any longer. This simple analysis already reveals that all implications of symmetry are identical for these two types of symmetry, including cancellation of aberrations. For simplicity, we will continue to use the matrix $\mathbf{S}$ and imply that $s_\alpha = -1$.

In order to analyze aberrations, we have to find the Taylor polynomial of the inverse map $\vec{M}_2^{-1}$. For this purpose one separates the transfer map of the second system into a linear and a nonlinear part $\vec{M}_2(\vec{\zeta}) = \mathbf{L}(d, \tilde{d})\vec{\zeta} + N(\vec{\zeta})$. As first pointed out in Ref. [8], the inverse to order n of the Taylor map is then given by

$$\mathbf{L}(-d, -\tilde{d})\left[\vec{\zeta} + \sum_{j=1}^{n} (-N(\mathbf{L}(-d, -\tilde{d})\vec{\zeta}))^j\right]. \tag{13}$$

Here the exponent j of a map indicates the jth composition of the map with itself. The transfer map of a symmetric filter is therefore given by

$$\{\mathbf{L}(d, \tilde{d})\vec{\zeta} + \vec{N}(\vec{\zeta})\} \circ \left\{\mathbf{S}\mathbf{L}(-d, -\tilde{d})\right.$$
$$\left.\left[\mathbf{S}\vec{\zeta} + \sum_{j=1}^{n} (-N(\mathbf{L}(-d, -\tilde{d})\mathbf{S}\vec{\zeta}))^j\right]\right\} \tag{14}$$

where the circle $\circ$ indicates the composition of functions.

5. Symmetry-induced cancellation of aberrations

When a system is found which satisfies the mentioned conditions for the paraxial rays, higher-order effects limit the resolution and the energy width of the system. Since dipoles have to be used to create dispersion, second-order aberrations are limiting. It has therefore been suggested to cancel as many of the leading aberrations by employing symmetric magnetic arrangements. Other aberrations can be canceled by symmetrically arranged multipoles. When all second-order aberrations are canceled, the third-order aberrations are dominant.

Some of these aberrations, however, again cancel by symmetry. Here we derive a formula for the leading-order m of the transfer map of a symmetric system. It therefore is assumed that all aberrations up to order m are canceled by symmetry and multipoles. Writing the leading-order contribution of $\vec{N}(\vec{\zeta})$ as $\vec{N}_m(\vec{\zeta})$, we only have to consider $\vec{M}_2 = \mathbf{L}(d, \tilde{d})\vec{\zeta} + \vec{N}_m(\vec{\zeta})$ and its inverse up to order m given by $\mathbf{L}(-d, -\tilde{d})[\vec{\zeta} - \vec{N}_m(\mathbf{L}(-d, -\tilde{d})\vec{\zeta})]$. The transfer map of the symmetric system is therefore to leading order m equal to

$$
\begin{aligned}
\vec{M} = {}_m&\{\mathbf{L}(d, \tilde{d})\vec{\zeta} + \vec{N}_m(\vec{\zeta})\} \\
&\circ \{\mathbf{SL}(-d, -\tilde{d})(\mathbf{S}\vec{\zeta} - \vec{N}_m(\mathbf{L}(-d, -\tilde{d})\mathbf{S}\vec{\zeta})\} \\
= {}_m&\mathbf{L}(0, 2\tilde{d})\vec{\zeta} + \{\vec{N}_m(\vec{\zeta}) - \mathbf{L}(0, 2\tilde{d})\mathbf{S}\vec{N}_m(\mathbf{S}\vec{\zeta})\} \\
&\circ \{\mathbf{L}(-d, \tilde{d})\vec{\zeta}\}. \quad (15)
\end{aligned}
$$

Since the relative energy deviation κ does not change in an electron microscopic filter, the fifth component of N_m vanishes, and the mth-order part of the filter's transfer map is given by

$$
\vec{K}(\mathbf{L}(-d, \tilde{d})\vec{\zeta}) \quad \text{with} \quad \vec{K}(\vec{\zeta}) = \vec{N}_m(\vec{\zeta}) - \mathbf{S}\vec{N}_m(\mathbf{S}\vec{\zeta}). \quad (16)
$$

Therefore the symmetry implies that the following geometric aberrations vanish:

$$
\begin{aligned}
(\gamma, \vec{\zeta^k}) &= 0 \quad \text{if } (-1)^{k_z}(-s_\beta)^{k_\delta}(s_\beta)^{k_\beta} = 1 \\
(\alpha, \vec{\zeta^k}) &= 0 \quad \text{if } (-1)^{k_z}(-s_\beta)^{k_\delta}(s_\beta)^{k_\beta} = -1 \\
(\delta, \vec{\zeta^k}) &= 0 \quad \text{if } -s_\beta(-1)^{k_z}(-s_\beta)^{k_\delta}(s_\beta)^{k_\beta} = 1 \\
(\beta, \vec{\zeta^k}) &= 0 \quad \text{if } -s_\beta(-1)^{k_z}(-s_\beta)^{k_\delta}(s_\beta)^{k_\beta} = -1. \quad (17)
\end{aligned}
$$

Cancellations of aberrations which include chromatic effects are somewhat harder to obtain since a cancellation of these aberrations in $\vec{K}(\vec{\zeta})$ does not imply their cancellation in the transfer map of the complete filter. This is due to the fact that composing $\vec{K}$ with $\mathbf{L}(-d, \tilde{d})\vec{\zeta}$ can reintroduce these aberrations.

In the field of electron microscopy the Eikonal method has been used to show which aberrations vanish identically due to symmetry conditions. Also within this formalism this is especially simple for geometric aberrations. In Refs. [9,10] it was found numerically that the chromatic aberrations of magnification $(\gamma, \gamma\kappa)$ and $(\delta, \delta\kappa)$ are very small

when all geometric aberrations of second order vanish due to symmetry or due to sextupole correction field. Only later [1] it was deduced from the Eikonal method that these chromatic aberrations are related to the geometric aberrations in the case of symmetric systems and therefore have to vanish when all geometric second-order aberrations are corrected.

Similarly, Eq. (16) reveals that a correction of all non-vanishing aberrations in $\vec{K}$ by means of multipoles automatically compensates all chromatic aberrations which can be reintroduced by composition of $\vec{K}$ with $\mathbf{L}(d, \tilde{d})$. These are the aberrations $(\gamma, \gamma\kappa)$, $(\alpha, \alpha\kappa)$, $(\delta, \delta\kappa)$, $(\beta, \beta\kappa)$, and $(\gamma, \kappa\kappa)$. In second order, the leading order in uncorrected filters, solely symmetry considerations revile the following five correlated aberrations:

$$
(\gamma, \gamma\kappa) = (\gamma, \gamma\alpha)\tilde{d} \quad (18)
$$

$$
(\alpha, \alpha\kappa) = 2(\alpha, \alpha\alpha)\tilde{d} \quad (19)
$$

$$
(\delta, \delta\kappa) = (\delta, \delta\alpha)\tilde{d} \quad (20)
$$

$$
(\beta, \beta\kappa) = (\beta, \beta\alpha)\tilde{d} \quad (21)
$$

$$
(\gamma, \kappa\kappa) = 2\{(\gamma, \alpha\kappa)_2 - (\gamma, \gamma\alpha)_2 d\}\tilde{d} = (\gamma, \alpha\kappa)\tilde{d} \quad (22)
$$

where the index 2 indicates an aberration coefficient of $\vec{M}_2$. Except for the last relation, this was already shown in a more complicated way by analyzing the third-order Eikonal [1].

6. The symplectic symmetry

The transfer function $\vec{M}_t$ for phase space coordinates $\vec{z}$ is symplectic since particle motion in electron microscopes can be described by a Hamiltonian [11]. This means that the Jacobian of $\vec{M}_t$ is a symplectic matrix. If we consider κ as a parameter, we obtain the four-dimensional transfer map $\vec{M}$ as in Eq. (5) by

$$
\mathbf{W}(s) = \begin{pmatrix}
w_{\gamma x}(s) & w_{\alpha x}(s) & 0 & 0 \\
w'_{\gamma x}(s) & w'_{\alpha x}(s) & 0 & 0 \\
0 & 0 & w_{\delta x}(s) & w_{\beta x}(s) \\
0 & 0 & w'_{\delta x}(s) & w'_{\beta x}(s)
\end{pmatrix} \quad (23)
$$

$$
\vec{M}_t(\vec{z}, \kappa) = \mathbf{W}(s_f)\vec{M}(\mathbf{W}(s_i)^{-1}\vec{z}, \kappa). \quad (24)
$$

Since we chose the fundamental ray to have a Wronski determinant of 1 in the x and the y section, and since the Wronski determinant does not change from the initial position s_i to the final position s_f, the matrices $\mathbf{W}(s_f)$ and $\mathbf{W}(s_i)^{-1}$ are both symplectic. Therefore also the transfer map $\vec{M}$ is symplectic

$$\partial_{\vec{\zeta}}\vec{M}^T\mathbf{J}(\partial_{\vec{\zeta}}\vec{M}^T)^T = \mathbf{J},$$

$$\mathbf{J} = \mathrm{diag}\left(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\right). \qquad (25)$$

Since the Jacobian of the first-order transfer map is the identity matrix, the symplectic symmetry entails for the leading order

$$\partial_{\vec{\zeta}}\vec{N}_m^T\mathbf{J} = (\partial_{\vec{\zeta}}\vec{N}_m^T\mathbf{J})^T. \qquad (26)$$

Therefore the potential problem $\vec{N}_m = -\mathbf{J}\partial_{\vec{\zeta}}E(\vec{\zeta})$ has a unique solution $E(\vec{\zeta})$ which is a homogeneous polynomial of order $m + 1$. This function $E(\vec{\zeta})$ is the leading order of the Eikonal used in the Eikonal method. For the coordinates γ, α, δ, β the symplectic symmetry has the surprisingly simple form to leading order

$$-k_\gamma(\gamma, \vec{\zeta}^{(k_\gamma, k_\alpha-1, k_\delta, k_\beta, k_\kappa)^T}) = k_\alpha(\alpha, \vec{\zeta}^{(k_\gamma-1, k_\alpha, k_\delta, k_\beta, k_\kappa)^T})$$

$$(27)$$

$$-k_\delta(\delta, \vec{\zeta}^{(k_\gamma, k_\alpha, k_\delta, k_\beta-1, k_\kappa)^T}) = k_\beta(\beta, \vec{\zeta}^{(k_\gamma, k_\alpha, k_\delta-1, k_\beta, k_\kappa)^T}).$$

$$(28)$$

These relations are much simpler than the corresponding relations derived by the conventional map method [12]. Due to this simplicity it is often convenient to use solely the coefficients of the Eikonal indicated by $E_{\zeta^{\vec{k}}}$ rather than the aberration coefficients. Then the symplectic condition is implied in all conclusions automatically. For example, the five correlated second-order aberrations reduce to only three correlations,

$$E_{\gamma\alpha\kappa} = 2E_{\gamma\alpha\alpha}\tilde{d}, \quad E_{\delta\beta\kappa} = E_{\alpha\delta\beta}\tilde{d}, \quad E_{\alpha\kappa\kappa} = 2E_{\alpha\alpha\kappa}\tilde{d}. \quad (29)$$

7. Conclusion

We have introduced the convention of fundamental rays to define coordinates of motion and have constructed a transfer map which transports these coordinates. This mixture of the Eikonal and the map method allowed us to draw conclusions about the implications of symmetries in imaging filters in a very straight forward way. Some of these conclusions had not been derived before since they were not accessible in such a simple fashion. Furthermore, we showed how the symplectic symmetry leads to the simple relations between leading-order aberrations of the Eikonal method.

References

[1] H. Rose, D. Krahl, Electron Optics of Imaging Energy Filters, Springer Series in Optical Sciences, vol. 71, Springer, Berlin, Heidelberg, 1995, pp. 43–149 (chapter 2).

[2] H. Börsch, Optik 5 (1949) 436.

[3] G. Möllenstedt, O. Rang, Z. Angewandte Physik 3 (1951) 187.

[4] R. Castaing, L. Henry, Filtrage magnétique de vitesses en microscopie électronique, J. Microscopie 3 (1964) 133.

[5] S. Kujawa, D. Krahl, H. Niedrig, E. Zeitler, Optik 86 (1990) 39.

[6] H. Rose, W. Pejas, Optik 54 (1979) 235.

[7] W.S. Wan, M. Berz, Analytical theory of arbitrary-order achromats, Phys. Rev. E 54 (1996) 2870.

[8] G.H. Hoffstätter, Rigorous bounds on survival times in circular accelerators and efficient computation of fringe-field transfer maps, Ph.D. Thesis, Michigan State University, East Lansing, MI 48824, USA, 1994.

[9] S. Lanio, Optimierung abbildender Energiefilter für die analytische Elektronenmikroskopie, Ph.D. Thesis, TH Darmstadt, Germany, 1986.

[10] R. Degenhardt, Korrektur von Aberrationen in der Teilchenoptik mit Hilfe von Symmetrien, Ph.D. Thesis, Technische Hochschule Darmstadt, 1992.

[11] H. Goldstein, Classical Mechanics, second ed., Addison-Wesley, Reading/MA, USA, 1980.

[12] H. Wollnik, M. Berz, Nucl. Instr. and Meth. 238 (1985) 127.