

Matrix Representation for Calculation of the Second-Order Aberration in Ion Optics

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Dedicated to Prof. J. MATTAUCH on his 70th birthday

The matrix representation for calculating the ion trajectory is extended to include the second-order aberration terms.

Properties of the matrix and relations between its elements are discussed.

As an example of the application of the matrix method, the second-order coefficients of a homogeneous magnetic field of arbitrary shape are derived and the relations between the matrix elements and HINTENBERGER's notations are shown.

The particle trajectory near the optical axis can be expressed by a linear function of initial angle, position and velocity. In this case the matrix representation^{1, 2} is very useful to determine the focusing condition or to calculate the dispersion factor and other optical properties. It is the most important advantage of this method that the trajectory through the complex field combination in tandem can be expressed easily by manipulation of the transfer matrices of various parts of the system.

For a more precise calculation of the trajectory, the second-order approximation is required, and these second-order terms give the mathematical aberration if the first-order focusing conditions are fulfilled.

When mass spectrographs with high resolving power or high optical brightness are designed, the second-order terms can not be neglected, though its calculation is a very tedious work.

The second-order coefficients of the double focusing mass spectrograph which consists of a cylindrical electrostatic field followed by a homogeneous magnetic field have been investigated by HINTENBERGER and KÖNIG³. They proposed several analyser systems which eliminate the second-order aberrations.

It is possible to calculate the aberration of more complex analyser systems by HINTENBERGER's method, e. g. the aberration for a mass spectrograph which consists of two electrostatic fields and a magnetic field. It is, however, rather difficult to generalize their expressions for the second-order coefficients.

If the matrix method is applicable to the second-order calculation as well as to the first-order approximation, it may be very useful. In this report the transfer matrices, extended to include conveniently the second-order terms, are proposed and some of their applications are presented.

1. Transfer Matrix and the Second-Order Terms

Now we take a trajectory of a particle whose velocity is given by v_0 , the central velocity, and define this trajectory to be the optical axis of the field and call the beam on this axis the central beam. For simplicity, we only consider the motion of particles in the plane on which the optical axis lies. The particle may be characterized by the displacement x from the optical axis, the angle α between this axis and the direction of motion and its velocity v . We consider a particle characterized by x_0 , α_0 , v , at the entrance of the field. The displacement x and the angle α of this particle at the exit of the field may be given as functions of the initial conditions x_0 , α_0 , v ,

$$x = X(x_0, \alpha_0, v), \quad (1)$$

$$\alpha = A(x_0, \alpha_0, v). \quad (2)$$

If the displacement x is small compared with the bending radius in the field, and the angle α and the velocity deviation are small, too, these functions may be expanded in power series of x_0 , α_0 , and β , where β is defined by

$$v = v_0(1 + \beta), \quad \beta \ll 1. \quad (3)$$

¹ S. PENNER, Rev. Sci. Instr. **32**, 150 [1961].

² D. LUCKEY, Techniques of High Energy Physics, Interscience Publishers, New York 1961 (Edited by DAVID M. RITSON).

³ H. HINTENBERGER and L. A. KÖNIG, Z. Naturforschg. **12 a**, 773 [1957].



To obtain the second-order solution, we drop all terms higher than second order in x_0 , α_0 and β . Then,

$$x = A_{11} x_0 + A_{12} \alpha_0 + A_{13} \beta + A_{14} x_0^2 + A_{15} x_0 \alpha_0 + A_{16} \alpha_0^2 + A_{17} x_0 \beta + A_{18} \alpha_0 \beta + A_{19} \beta^2, \quad (4)$$

$$\alpha = A_{21} x_0 + A_{22} \alpha_0 + A_{23} \beta + A_{24} x_0^2 + A_{25} x_0 \alpha_0 + A_{26} \alpha_0^2 + A_{27} x_0 \beta + A_{28} \alpha_0 \beta + A_{29} \beta^2. \quad (5)$$

In first-order theory a vector space is chosen whose components are x , α , and β , and the field is represented by a matrix transformation of this vector. In order to extend the matrix method to the second-order theory, the vector space has to be extended to a nine-dimensional one. The components of this nine-dimensional vector are x , α , β , x^2 , $x\alpha$, α^2 , $x\beta$, $\alpha\beta$, β^2 . Then a field is represented by a matrix transformation of this vector. The elements of the first row of this matrix are the A_{1j} 's of Eq. (4) and the elements of the second row are the A_{2j} 's of Eq. (5). Provided the velocity of the particles is not changed at the entrance and the exit of field, the matrix elements of the third row are zero except $A_{33} = 1$.

The square of x is calculated from Eq. (4). Dropping the higher-order terms we obtain

$$x^2 = A_{11}^2 x_0^2 + 2 A_{11} A_{12} x_0 \alpha_0 + A_{12}^2 \alpha_0^2 + 2 A_{11} A_{13} x_0 \beta + 2 A_{12} A_{13} \alpha_0 \beta + A_{13}^2 \beta^2.$$

Then the matrix elements of the fourth row are as follows:

$$\begin{aligned} A_{41} &= A_{42} = A_{43} = 0, \\ A_{44} &= A_{11}^2, & A_{45} &= 2 A_{11} A_{12}, & A_{46} &= A_{12}^2, \\ A_{47} &= 2 A_{11} A_{13}, & A_{48} &= 2 A_{12} A_{13}, & A_{49} &= A_{13}^2. \end{aligned}$$

The other matrix elements are obtained similarly. Then the transfer matrix in general is given by

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} & A_{17} & A_{18} & A_{19} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} & A_{26} & A_{27} & A_{28} & A_{29} \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{11}^2 & 2 A_{11} A_{12} & A_{12}^2 & 2 A_{11} A_{13} & 2 A_{12} A_{13} & A_{13}^2 \\ 0 & 0 & 0 & A_{11} A_{21} & A_{11} A_{22} + A_{12} A_{21} & A_{12} A_{22} & A_{11} A_{23} + A_{21} A_{13} & A_{12} A_{23} + A_{22} A_{13} & A_{13} A_{23} \\ 0 & 0 & 0 & A_{21}^2 & 2 A_{21} A_{22} & A_{22}^2 & 2 A_{21} A_{23} & 2 A_{22} A_{23} & A_{23}^2 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{11} & A_{12} & A_{13} \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{21} & A_{22} & A_{23} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (6)$$

The simplest one is the transfer matrix through a region of no field, which is given by

$$\begin{pmatrix} 1 & L & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2L & L^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & L & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & L & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (7)$$

where L is the length of the field-free region.

We have calculated all the matrix elements from those of the first and the second row, which may be obtained by solving the equation of motion in the second-order approximation. It is however interesting to see that the matrix elements of the second

row can in the case of sector fields also be calculated from the matrix elements of the first row. Since α is written approximately in the form

$$\alpha = \frac{dx}{ds} + O_3 \left(\frac{dx}{ds} \right)$$

where ds and dx are the components of a line element parallel and perpendicular to the optical axis respectively, it is given by the calculation of dx/ds in the second-order approximation as well as in linear approximation. If the optical axis is the arc of radius r_0 , α is given by

$$\alpha = \frac{dx}{ds} = \frac{dx}{r_0 d\varphi} \left(1 - \frac{x}{r_0} \right) \quad (8)$$

where φ is the deflection angle. — Hence

$$\begin{aligned} \alpha &= A_{11}' x_0 + A_{12}' \alpha_0 + A_{13}' \beta + \left(A_{14}' - \frac{A_{11} A_{11}'}{r_0} \right) x_0^2 + \left(A_{15}' - \frac{(A_{11} A_{12})'}{r_0} \right) x_0 \alpha_0 \\ &\quad + \left(A_{16}' - \frac{A_{12} A_{12}'}{r_0} \right) \alpha_0^2 + \left(A_{17}' - \frac{(A_{11} A_{13})'}{r_0} \right) x_0 \beta + \left(A_{18}' - \frac{(A_{12} A_{13})'}{r_0} \right) \alpha_0 \beta + \left(A_{19}' - \frac{A_{13} A_{13}'}{r_0} \right) \beta^2 \end{aligned} \quad (9)$$

where the prime denotes $\frac{1}{r_0} \frac{d}{d\varphi}$.

Equating coefficients of Eq. (5) and Eq. (9) we obtain

$$\begin{aligned} A_{21} &= A_{11}', & A_{22} &= A_{12}', & A_{23} &= A_{13}', \\ A_{24} &= A_{14}' - \frac{A_{11} A_{11}'}{r_0}, & & & A_{25} &= A_{15}' - \frac{(A_{11} A_{12})'}{r_0}, \\ A_{26} &= A_{16}' - \frac{A_{12} A_{12}'}{r_0}, & & & A_{27} &= A_{17}' - \frac{(A_{11} A_{13})'}{r_0}, \\ A_{28} &= A_{18}' - \frac{(A_{12} A_{13})'}{r_0}, & & & A_{29} &= A_{19}' - \frac{A_{13} A_{13}'}{r_0}. \end{aligned} \quad (10)$$

We have confined the problem to a two-dimensional motion. In the case of a three-dimensional motion it becomes more complicated. As we treat the motion of charged particles near the optical axis, the field may be expanded in power series around this axis. Provided the field is mirror symmetric about the plane on which the optical axis lies, the vector component of the field parallel or perpendicular to the plane of symmetry is expressed in first-order approximation by only one coordinate in the respective direction. Therefore, the motion parallel or perpendicular to the plane on which the optical axis lies can be determined independently. But in the second-order approximation the second-order terms in the power series expansion of the field component contain the square and cross terms of the coordinates perpendicular to each other. Hence three components have to be added to the vector space in general, and the transfer matrix becomes twelve-dimensional. If the field is homogeneous in the direction perpendicular to the plane on which the optical axis lies, for example a homogeneous magnetic field or a cylindrical electrostatic field, the second-order terms of the field do not contain the terms relating to the coordinate of this direction. Then the field is represented by the nine-dimensional transfer matrix.

2. Some Properties of Transfer Matrices

In the case of the first order approximation it is well known that the transfer matrix has a determinant $+1$. It is derived directly from LIOUVILLE's theorem. This result is easily extended to the nine-dimensional transfer matrices of the second-order approximation theory, because the following relation holds for the minor determinant

$$\begin{vmatrix} A_{44} & A_{45} & A_{46} \\ A_{54} & A_{55} & A_{56} \\ A_{64} & A_{65} & A_{66} \end{vmatrix} = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix}^3 = 1. \quad (11)$$

In the course of designing an analyser system, it is often desired to have the transfer matrix of the field whose bending direction is different from the

preceding field. In this case we can change the signs of x and α at the entrance and change them again as before after passing through the field. It is convenient to write this process in the following matrix form:

$$[A_i] = [E_{--}] \cdot [A] \cdot [E_{--}] \quad (12)$$

where $[A_i]$ is the matrix for the inverted bending field and $[E_{-}]$ is defined as follows:

$$[E_{--}] = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Now take a field represented by a transfer matrix $[A]$ and retrace the trajectory from exit to entrance. This process can be considered as the inverse transformation. Therefore the transfer matrix $[A_r]$ for this process is given by the inverse matrix:

$$[A_r] = [A]^{-1}$$

that is:

$$[A_r] \cdot [A] = [E],$$

where $[E]$ is the unit matrix. The transfer matrix $[A_m]$ of the field which is a mirror image of the given field $[A]$ where the reflection is made about a plane perpendicular to the optical axis, is equal to $[A_r]$ except the sign of α . Hence we have to change the sign of α at the entrance and again change it at the exit as before. In matrix form this statement becomes

$$[A_m] = [E_{+-}] \cdot [A]^{-1} \cdot [E_{+-}] \quad (15)$$

where

[illegible]

At the exit side we can derive a similar transfer matrix from geometrical considerations. But as leaving the field is the mirror image of entering the field, the transfer matrix for the rotation of the exit edge is easily derived from Eq. (15) and from the inverse matrix of $[\vartheta']$, provided ϑ' is replaced by the exit angle ϑ'' .

The result is

$$[\vartheta''] = \begin{pmatrix} 1 & 0 & 0 & \frac{\tan \vartheta''}{2r} & 0 & 0 & 0 & 0 & 0 \\ \frac{\tan \vartheta''}{r} & 1 & 0 & -\frac{\tan^2 \vartheta''}{2r^2} & -\frac{\tan^2 \vartheta''}{r} & 0 & -\frac{\tan \vartheta''}{r} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\tan \vartheta''}{r} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \left(\frac{\tan \vartheta''}{r}\right)^2 & 2\frac{\tan \vartheta''}{r} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\tan \vartheta''}{r} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (20)$$

The entry angle ϑ' and the exit angle ϑ'' are taken as positive if the optical axis is on the side of the normal toward the center of curvature of the optical axis in the field. It should be noted that the transfer matrices for the entrance edge and that for the exit edge are expressed by the same matrix in first-order theory with exception of the rotation angle, but in the second-order approximation these matrices are quite different. The transfer matrix $[S]$ for the homogeneous magnetic field with entry angle ϑ' and exit angle ϑ'' is obtained by multiplying $[A]$ on the right with $[\vartheta']$ and on the left with $[\vartheta'']$.

$$[S] = [\vartheta''] \cdot [A] \cdot [\vartheta']. \quad (21)$$

If the field boundary is not rectilinear but curvilinear, the radius of curvature of the field boundary has to be considered in the second-order approximation.

Now we consider the magnetic field with linear boundary which is tangent to the real field boundary at the entrance of optical axis to the field region, and compare the trajectory of a particle in this imaginary field with that in the real field with curvilinear boundary.

Let us characterize the particle by x_1, α_1, v on B_1 in the former case and by x_2, α_2, v in the latter case.

If these trajectories coincide in the magnetic field, the following relations are derived from geometrical

considerations:

$$x_1 = x_2, \quad \alpha_1 = \alpha_2 + \frac{1}{2R'r \cos^3 \vartheta'} x_2^2$$

where R' is the radius of curvature of the field boundary. This transformation is expressed by the following matrix:

$$[R'] = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2R'r \cos^3 \vartheta'} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (22)$$

At the exit side a similar transfer matrix is easily derived from the inverse matrix of (22) by use of Eq. (15) provided ϑ' and R' are replaced by the parameters of the exit side ϑ'' and R'' . R' and R'' are taken as positive if the field is convex. Therefore the transfer matrix $[T]$ of a homogeneous magnetic field of arbitrary shape is given as follows:

$$[T] = [R''] \cdot [S] \cdot [R'] \\ = [R''] \cdot [\vartheta''] \cdot [A] \cdot [\vartheta'] \cdot [R']. \quad (23)$$

The matrix elements T_{1j} and T_{2j} agree with the second-order coefficients which have been derived by HINTENBERGER and KÖNIG⁴. Here we only show the relation between the matrix elements and HINTENBERGER's notations.

$$\begin{aligned} T_{11} &= \mu_{1b}, & T_{12} &= r \mu_{1a}, & T_{13} &= r \mu_{2a}, \\ T_{14} &= \frac{1}{r} \mu_{11c}, & T_{15} &= \mu_{11b}, & T_{16} &= r \mu_{11a}, \\ T_{17} &= \mu_{12b}, & T_{18} &= r \mu_{12a}, & T_{19} &= r \mu_{22a}, \\ T_{21} &= \frac{1}{r} \nu_{1b}, & T_{22} &= \nu_{1a}, & T_{23} &= \nu_{2a}, \\ T_{24} &= \frac{1}{r^2} \nu_{11c}, & T_{25} &= \frac{1}{r} \nu_{11b}, & T_{26} &= \nu_{11a}, \\ T_{27} &= \frac{1}{r} \nu_{12b}, & T_{28} &= \nu_{12a}, & T_{29} &= \nu_{22a}. \end{aligned} \quad (24)$$

The calculation of the second-order aberration of a MATTAUCH-HERZOG type mass spectrograph which consists of two electrostatic fields followed by a homogeneous magnetic field by the matrix method is a good example and will be reported in another paper by the author.

⁴ L. A. KÖNIG and H. HINTENBERGER, Z. Naturforschg. **12 a**, 377 [1957].

4. Conclusion

It is very complicated to calculate the second-order aberrations of complex analyser systems and mistakes are liable to be made.

Even if the matrix method is used the tediousness of the calculation is not altered.

The usefulness of the matrix representation comes from the fact that the over-all transfer matrix of the total system is easily written as a product of the transfer matrices of various parts of the system.

Hence the calculation of the second-order aberration is reduced to the mere mechanical calculation of matrix products.

For the case of the numerical calculation by digital computer, the matrix method may be advantageous to programming.

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Mattauch-Herzog Type Mass Spectrograph with a Two Stage Electrostatic Field

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Dedicated to Prof. J. MATTAUCH on his 70th birthday

The most important advantage of the MATTAUCH-HERZOG type mass spectrograph is double focusing for all masses. One disadvantage, however, is the fact that the energy slit cannot control the velocity spread (β) independently of beam divergence (α). This disadvantage is removed by substituting a two-stage electrostatic field for the usual single one.

General formulae for determining the distances between the elements of the optical system are derived.

Combinations of two cylindrical electrostatic fields with equal radii are chosen as a practical example. The condition to be fulfilled for a physically significant solution and the resolving power of this system are discussed.

The study of the second-order aberrations shows that α^2 focusing for all masses can be achieved under suitable conditions. In addition, $\alpha\beta$ and β^2 aberrations can be made to vanish simultaneously at a point on the focal plane.

The design parameters are numerically computed and tabulated for several favorable examples. The total image defect is calculated for a typical example, and found to be very small for a wide range of masses.

Recently increasing interest has been shown in the potentiality of spark source mass spectrometry for the chemical analysis of solids.

An ion beam produced by a spark source, however, has a wide energy spread. Therefore, a double focusing mass spectrometer is required. In addition the intensity of an ion beam emerging from a spark source fluctuates rapidly and the spark produces considerable RF noise, so that electrical detection is prevented and photographic recording is inevitable.

A MATTAUCH-HERZOG type mass spectrograph¹ is especially well suited for this purpose, because it shows double focusing for all masses along a straight line.

One disadvantage of this type of instrument, however, is the fact that the energy slit cannot control the energy spread independently of beam divergence. Therefore, even if the energy slit is narrowed to infinitesimal width, the ion beam which enters the magnetic field still has a wide energy spread.

The author noticed that by substituting a combination of two electrostatic deflection fields for a single one in the usual MATTAUCH-HERZOG type mass spectrograph, the disadvantage mentioned above could be removed by setting an energy slit between the two electrostatic fields^{1a}.

¹ J. MATTAUCH and R. HERZOG, Z. Phys. **89**, 786 [1934].

^{1a} I. TAKESHITA, Z. Naturforschg. **20 a**, 624 [1965].