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Thired Order Transfer Matrix Elements of Octopoles
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ABSTRACT:
The matrix elements of the third order transport matrices for electrostatic and magnetic octopoles are derived. They are needed in ion optical calculations, if octopoles are used as correctors of image aberrations.

Transfer-Matrix-Elemente 3. Ordnung von Oktopolen

## ZUSAMMENFASSUNG:

Die Matrixelemente der Transportmatrizen 3. Ordnung werden für elektrostatische und magnetische Oktopole abgeleitet. Sie werden in ionenoptischen Berechnungen benötigt, wenn Oktopole zur Korrektur von Bildfehlern verwendet werden.

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## 1.) INTRODUCTION

To correct the third order image aberrations of ion optical systems without affecting the imaging in lower orders, octapole elements must be used ${ }^{1)}$. The most converientway to calculate image aberrations uses the transfer matrix formalism ${ }^{2}, 3$ ). For its use the third order transfer matrix elements of octopole correctors must be known.

## 2.) DIFFERENTIAL EQUATIONS OF MOTION

We start from the third order equation of motion of charged particles in an octopole field:

$$
\begin{align*}
x^{\prime \prime} & =3 k^{2} x y^{2}-k^{2} x^{3} \\
y^{\prime \prime} & =3 k^{2} x^{2} y-k^{2} y^{3} \tag{1}
\end{align*}
$$

This is a special case of eqs. ( $13 \mathrm{a}, \mathrm{b}$ ) of ref. 4. In analogy to the quadrupole ${ }^{+}$and hexapole strength (eqs. (23) and (25) of ref. 5) we introduce the octopole strength parameter

$$
\begin{align*}
\mathrm{k}^{2} & =\frac{\mathrm{e}}{\mathrm{p}_{0}} \cdot \frac{\mathrm{~B}_{0}}{\mathrm{r}^{3}} & \text { in the magnetic case } \\
\text { or } & \mathrm{k}^{2}=\frac{e}{\mathrm{p}_{0} \cdot v_{0}} \cdot \frac{U_{0}}{4 r^{4}} & \text { in the electrostatic case, } \tag{2}
\end{align*}
$$

Here the particle momentum $p_{0}$, the particle velocity $v_{0}$, the magnetic field strenght of the pole $B_{o}$, the electrical tension of the pole $U_{o}$ and the aperture radius $r$ are used. The orientation of the octopole system within the coordinate system is shown in fig. 1. The primes in eq. (1) denote differentiation with respect to the direction of the $z$-axes.

## 3.) TAYLOR EXPANSION

We consider a ray which starts at the coordinates $x_{0}, y_{0}$ with the angles $x_{0}^{\prime}=\alpha_{0}$ and $y_{o}^{\prime}=\beta_{0}$ and with a momentum spread $\delta_{0}$. Along the particle ray path

[^0]the coordinates $x, x^{\prime}, y, y^{\prime}$ and $\delta$ are functions of $Z$. If the ray is a paraxial ray, that means in the neighbourhood of the central symmetric axis $\mathrm{x}=0, \mathrm{y}=0$, with small angles $\mathrm{x}_{0}^{\prime}$ and $\mathrm{y}_{0}^{\prime}$ we may develope these functions $x, x^{\prime}, y, y^{\prime}, \delta$ in Taylor series of the original coordinates $x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}$ and $\delta_{0}$, breaking after the third order. The expansion has the form
\[

$$
\begin{equation*}
i=\sum(i / j) j+\sum(i / j k) j k+\sum(i / j k l) j k l+\ldots \tag{3}
\end{equation*}
$$

\]

with $i=x, x^{\prime}, y, y^{\prime}, \delta$
and $j, k, I=x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}, \delta_{0}$
in analogy to eq. (32) of ref. 5. The parentheses (i/j), (i/jk) and (i/jkl) are symbols for the Taylor coefficients, i identifies the coordinate represented by the expansion, while $j, k, l$ indicate the term in question. These Taylor coefficients are just the first, second and third order matrix elements in the transport matrix theory and are functions of $Z$, which must be determined.

## 4.) EVALUATION OF THE COEFFICIENTS OF FIRST AND SECOND ORDER

To evaluate the coefficients, we differentiate eq.(3) twice and substitute these expansions in the left and right hand side of eqs. (1), breaking after the third order terms.

Collecting the terms with the same power in the particle ray origin coordinates $x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}, \delta_{0}$, a second order differential equations is obtained for each Taylor coefficient. For the first order coefficients this is of the type

$$
\begin{equation*}
(i / j) "=0 \tag{4}
\end{equation*}
$$

with $i=x, x^{\prime}, y, y^{\prime}, \delta$
$j=x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}, \delta_{0}$
The solutions are obtained by integrating twice, which leads to the general form

$$
(i / j)=c_{1} \cdot z+c_{2}
$$

for $i=x, x^{\prime}, y, y^{\prime}, \delta$
and $j=x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}, \delta_{0}$
with two integration constants $c_{1}$ and $c_{2}$ for each coefficient. The constants are determined by the boundary conditions, demanding that for $\mathrm{k}^{2} \rightarrow 0$ the octopole must behave like a drift path of the same length $Z$. This yields

$$
\begin{array}{ll}
\left(x / x_{0}\right)=1 & \left(y / y_{0}\right)=1  \tag{5a}\\
\left(x / x_{0}^{\prime}\right)=z & \left(y / y_{0}^{\prime}\right)=z
\end{array}
$$

and their nonvanishing derivatives

$$
\begin{equation*}
\left(x^{\prime} / x_{0}^{\prime}\right)=1 \quad\left(y^{\prime} / y_{0}^{\prime}\right)=1 \tag{5b}
\end{equation*}
$$

As the energy spread is not affected by a drift path, also

$$
\begin{equation*}
\left(\delta / \delta_{0}\right)=1 \tag{5c}
\end{equation*}
$$

All non listed matrix elements of first order are identically zero.

Collecting the terms of second order in the starting coordinates, we get

$$
\begin{equation*}
(i / j, k) "=0 \tag{6}
\end{equation*}
$$

```
for i = x, x', y, y', \delta
    j,k = x x, x', yo, y',
```

With the same boundary conditions as for the first order coefficients we find, that all integration constants of the second order coefficients are zero, thus

$$
\begin{equation*}
(i / j, k)=0 \tag{7}
\end{equation*}
$$

$$
\text { for } \begin{aligned}
i & =x, x^{\prime}, y, y^{\prime}, \delta \\
j, k & =x_{0}, x_{0}^{\prime}, y_{0}, y_{0}^{\prime}, \delta_{0}
\end{aligned}
$$

## 5.) THIRD ORDER COEFFICIENTS

Collecting the terms of third order in the starting coordinates and making use of eqs. ( $5 a, b, c$ ) we derive the following differential equations for the third order coefficients

$$
\begin{aligned}
\left(x / x_{0} x_{0} x_{0}\right)^{\prime \prime} & =-k^{2}\left(x / x_{0}\right)^{3}+3 k^{2}\left(x / x_{0}\right)\left(y / x_{0}\right)^{2}=-k^{2} \\
\left(x / x_{0} x_{0} x_{0}^{\prime}\right)^{\prime \prime} & =-3 k^{2}\left(x / x_{0}\right)^{2}\left(x / x_{0}^{\prime}\right)+3 k^{2}\left(x / x_{0}^{\prime}\right)\left(y / x_{0}\right)^{2}+6 k^{2}\left(x / x_{0}\right)\left(y / x_{0}\right)\left(y / x_{0}^{\prime}\right) \\
& =-3 k^{2} z
\end{aligned}
$$

and similarly

$$
\begin{aligned}
& \left(x / x_{0} x_{0}^{\prime} x_{0}^{\prime}\right)^{\prime \prime}=-3 k^{2} z^{2} \\
& \left(x / x_{0} y_{0} y_{0}\right)^{\prime \prime}=3 k^{2} \\
& \left(x / x_{o} y_{o} y_{o}^{\prime}\right)^{\prime \prime}=6 \mathrm{k}^{2} Z \\
& \left(x / x_{0} y_{0}^{\prime} y_{0}^{\prime}\right)^{\prime \prime}=3 k^{2} z^{2} \\
& \left(x / x_{0}^{\prime} x_{0}^{\prime} x_{0}^{\prime}\right)^{\prime \prime}=-k^{2} z^{3} \\
& \left(x / x_{0}^{\prime} y_{o} y_{0}\right)^{\prime \prime}=3 k^{2} Z \\
& \left(x / x_{0}^{1} y_{0}^{0} y_{0}^{\prime}\right)^{\prime \prime}=6 k^{2} z^{2} \\
& \left(x / x_{0}^{\prime} y_{o}^{\prime} y_{0}^{\prime}\right)^{\prime \prime}=3 k^{2} z^{3} \\
& \left(y / x_{0} x_{0} y_{0}\right)^{\prime \prime}=3 k^{2} \\
& \left(y / x_{0} x_{0} y_{0}^{\prime}\right)^{\prime \prime}=3 k^{2} z \\
& \left(y / x_{0} x_{0}^{\prime} y_{0}\right)^{\prime \prime}=6 k^{2} z \\
& \left(y / x_{0} x_{0}^{\prime} y_{0}^{\prime}\right)^{\prime \prime}=6 k^{2} z^{2} \\
& \left(y / x_{0}^{\prime} x_{0}^{\prime} y_{0}\right)^{\prime \prime}=3 k^{2} z^{2} \\
& \left(y / x_{0}^{1} x_{0}^{\prime} y_{0}^{\prime}\right)^{\prime \prime}=3 k^{2} z^{3} \\
& \left(y / y_{0} y_{0} y_{0}\right)^{\prime \prime}=-k^{2} \\
& \left(y / y_{0} y_{o} y_{0}^{\prime}\right)^{\prime \prime}=-3 k^{2} z \\
& \left(y / y_{0} y_{o}^{1} y_{o}^{\prime}\right)^{\prime \prime}=-3 k^{2} z^{2} \\
& \left(y / y_{o}^{1} y_{o}^{1} y_{o}^{\prime}\right)^{\prime \prime}=-k^{2} z^{3}
\end{aligned}
$$

The second derivatives of all other third order coefficients vanish.

Integration of the first of eqs. (8) gives

$$
\left(x / x_{0} x_{o} x_{0}\right)=-\frac{1}{2} k^{2} z^{2}+c_{1} z+c_{2}
$$

with $c_{1}, a_{2}$ integration constants, which may be determined from the boundary conditions. For the limits $\mathrm{k}^{2} \rightarrow 0$ and $\mathrm{Z} \rightarrow 0$ the third order coefficients must vanish, hence $c_{1}=0$ and $c_{2}=0$. This holds in the same manner for all other third order coefficients and leads to

$$
\begin{align*}
& \left(x / x_{0} x_{0} x_{0}\right)=-\frac{1}{2} k^{2} z^{2} \quad\left(y / x_{0} x_{0} y_{0}\right)=\frac{3}{2} k^{2} z^{2} \\
& \left(x / x_{0} x_{o} x_{o}^{\prime}\right)=-\frac{1}{2} k^{2} z^{3} \quad\left(y / x_{o} x_{o} y_{o}^{\prime}\right)=\frac{1}{2} k^{2} z^{3} \\
& \left(x / x_{0} x_{0}^{\prime} x_{0}^{\prime}\right)=-\frac{1}{4} k^{2} z^{4} \quad\left(y / x_{0} x_{0}^{\prime} y_{0}\right)=k^{2} z^{3} \\
& \left(x / x_{0} y_{o} y_{o}\right)=\frac{3}{2} k^{2} z^{2} \quad\left(y / x_{0} x_{o}^{\prime} y_{0}^{\prime}\right)=\frac{1}{2} k^{2} z^{4} \\
& \left(x / x_{0} y_{o} y_{o}^{\prime}\right)=k^{2} z^{3} \quad\left(y / x_{0}^{\prime} x_{o}^{\prime} y_{o}\right)=\frac{1}{4} k^{2} z^{4}  \tag{9}\\
& \left(x / x_{o} y_{o}^{\prime} y_{o}^{\prime}\right)=\frac{1}{4} k^{2} z^{4} \quad\left(y / x_{0}^{\prime} x_{o}^{\prime} y_{o}^{\prime}\right)=\frac{3}{20} k^{2} z^{5} \\
& \left(x / x_{0}^{\prime} x_{0}^{\prime} x_{0}^{\prime}\right)=-\frac{1}{20} k^{2} z^{5} \quad\left(y / y_{o} y_{o} y_{o}\right)=-\frac{1}{2} k^{2} z^{2} \\
& \left(x / x_{0}^{\prime} y_{o} y_{0}\right)=\frac{1}{2} k^{2} z^{3} \quad\left(y / y_{0} y_{0} y_{0}^{\prime}\right)=-\frac{1}{2} k^{2} z^{3} \\
& \left(x / x_{o}^{\prime} y_{o} y_{o}^{\prime}\right)=\frac{1}{2} k^{2} z^{4} \quad\left(y / y_{o} y_{o}^{\prime} y_{o}^{\prime}\right)=-\frac{1}{4} k^{2} z^{4} \\
& \left(x / x_{0}^{\prime} y_{o}^{\prime} y_{o}^{\prime}\right)=\frac{3}{20} k^{2} z^{5} \quad\left(y / y_{o}^{\prime} y_{o}^{\prime} y_{o}^{\prime}\right)=-\frac{1}{20} k^{2} z^{5}
\end{align*}
$$

The expansion coefficients of the angles $x$ ' and $y^{\prime}$ are gained by differentiation:

$$
\begin{align*}
& \left(x^{\prime} / x_{0} x_{0} x_{0}\right)=-k^{2} z \\
& \left(y_{0}^{\prime} / x_{0} x_{0} y_{0}\right)=3 k^{2} z \\
& \left(x^{\prime}\left(x_{0} x_{0} x_{o}^{\prime}\right)=-\frac{3}{2} k^{2} z^{2}\right. \\
& \left(y_{0}^{1} / x_{0} x_{0} y_{o}^{\prime}\right)=\frac{3}{2} k^{2} z^{2} \\
& \left(x^{\prime} / x_{o} x_{o}^{\prime} x_{0}^{\prime}\right)=-k^{2} z^{3} \\
& \left(y_{0}^{\prime} / x_{0} x_{0}^{\prime} y_{o}\right)=3 k^{2} z^{2} \\
& \left(x^{\prime} / x_{0} y_{o} y_{o}\right)=3 k^{2} z \\
& \left(y_{o}^{\prime} / x_{o} x_{o}^{\prime} y_{o}^{\prime}\right)=2 k^{2} z^{3} \\
& \left(x^{\prime} / x_{0} y_{o} y_{0}^{\prime}\right)=3 k^{2} z^{2}  \tag{10}\\
& \left(y_{o}^{\prime} / x_{o}^{\prime} x_{o}^{\prime} y_{o}\right)=k^{2} z^{3} \\
& \left(x^{\prime} / x_{o} y_{o}^{\prime} y_{o}^{\prime}\right)=k^{2} z^{3} \\
& \left(y_{0}^{\prime} / x_{0}^{\prime} x_{0}^{\prime} y_{0}^{\prime}\right)=\frac{3}{4} k^{2} z^{4} \\
& \left(x^{\prime} / x_{0}^{\prime} x_{0}^{\prime} x_{0}^{\prime}\right)=-\frac{1}{4} k^{2} z^{4} \\
& \left(y_{0}^{\prime} / y_{o} y_{o} y_{o}\right)=-k^{2} z \\
& \left(x^{\prime} / x_{o}^{\prime} y_{o} y\right)=\frac{3}{2} k^{2} z^{2} \\
& \left(y_{0}^{\prime} / y_{o} y_{\circ} y_{o}^{\prime}\right)=-\frac{3}{2} k^{2} z^{2} \\
& \left(x^{\prime} / x_{o}^{\prime} y_{o} y_{o}^{\prime}\right)=2 k^{2} z^{3} \\
& \left(y_{0}^{\prime} / y_{o} y_{o}^{\prime} y_{o}^{\prime}\right)=-k^{2} z^{3} \\
& \left(x^{\prime} / x_{o}^{\prime} y_{o} y_{o}^{\prime}\right)=\frac{3}{4} k^{2} z^{4} \\
& \left(y_{o}^{\prime} / y_{o}^{\prime} y_{o}^{\prime} y_{o}^{\prime}\right)=-\frac{1}{4} k^{2} z^{4}
\end{align*}
$$

All non-listed matrix elements are identically zero.

## 6.) RANGE OF VALIDITY

These coefficients deduced in eqs. (9) and (10) are correct also in the relativistic case, if the relativistic momentum $p_{0}$ is used in eq. (2). Computations with these coefficients should give approximately correct results only if the octopoles used are sufficiently long (compared to the aperture diameter), as fringing field effects are not included. But this seems no serious disadvantage, as in most cases octopoles serve only as correctors with relative small field strength.
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Fig.1. Orientation of octopoles relative to the coordinate system. a) magnetic and b) electrostatic octopole.


[^0]:    ${ }^{+}$Note the different definition of the quadrupole strength in eq. (1-10) of ref. 6.

