# INTRINSIC THIRD ORDER ABERRATIONS IN ELECTROSTATIC AND MAGNETIC QUADRUPOLES 

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## Abstract

## 2 THEORY

### 2.1 Electrostatic

When using the longitudinal position as independent variable, the Hamiltonian $H$ is just the longitudinal momentum:

$$
\begin{equation*}
H=-\sqrt{p_{0}^{2}-2 m q \Phi-p_{x}^{2}-p_{y}^{2}} \tag{1}
\end{equation*}
$$

The electrostatic potential is $\Phi(x, y, z)$ and $p_{0}$ is the reference momentum. We will benefit from cleaner and more transparent notation if momenta are measured in units of $p_{0}$. This has the additional benefit that to first order, $p_{x}=x^{\prime}$. Additionally, we let the potential $\Phi$ in units of the reference kinetic energy $p_{0}^{2} /(2 m)$. Then

$$
\begin{equation*}
H=-\sqrt{1-\Phi-p_{x}^{2}-p_{y}^{2}} \tag{2}
\end{equation*}
$$

We expand the square root to 4 th order in coordinates and ignore the constant:

$$
\begin{equation*}
H \approx \frac{1}{2}\left(\Phi+p_{x}^{2}+p_{y}^{2}\right)+\frac{1}{8}\left(\Phi+p_{x}^{2}+p_{y}^{2}\right)^{2} \tag{3}
\end{equation*}
$$

To the same order, Laplace's equation gives for the expansion of the quadrupole potential:

$$
\begin{equation*}
\Phi=V(z)\left(x^{2}-y^{2}\right)-\frac{V^{\prime \prime}(z)}{12}\left(x^{4}-y^{4}\right) \tag{4}
\end{equation*}
$$

The final Hamiltonian, correct to $4^{\text {th }}$ order is

$$
\begin{align*}
H= & \frac{1}{2}\left[V\left(x^{2}-y^{2}\right)-\frac{V^{\prime \prime}}{12}\left(x^{4}-y^{4}\right)+p_{x}^{2}+p_{y}^{2}\right] \\
& +\frac{1}{8}\left[V\left(x^{2}-y^{2}\right)+p_{x}^{2}+p_{y}^{2}\right]^{2} \tag{5}
\end{align*}
$$

The trouble with applying this to simple cases like thin lenses and hard-edge limits is the presence of $V^{\prime \prime}(z)$, which becomes singular in those limits. In most cases, one sacrifices physical insight and simply traces particles with this Hamiltonian, using a more-or-less realistic function $V(z)$. For example, the approach taken in GIOS[1] is to leave it up to the user to specify 'fringe field integrals' such as $\int V^{2} d z$ through the fringe fields. However, this leaves much room for error; different integrals may not be realistic or consistent with each other. Moreover, if one needs to solve Laplace's equation to find fringe field integrals, one might as well use the solution directly in a ray-tracing code. If one does go through this exercise, one discovers that the higher order aberrations are relatively insensitive to the 'hardness' of the quadrupole edges. This leads one
to suspect that the aberrations are dominated by an intrinsic effect which has nothing to do with the detailed shape of the fringing field. Such is indeed the case.

It turns out to be possible to find a canonical transformation which eliminates the derivatives of $V(z)$. In our case, we wish to retain terms to $4^{\text {th }}$ order in the Hamiltonian ( $3^{\text {rd }}$ order on force), and the transformation $\left(x, p_{x}, y, p_{y}\right) \rightarrow$ $\left(X, P_{X}, Y, P_{Y}\right)$ has generating function

$$
\begin{align*}
& G\left(x, P_{X}, y, P_{Y}\right)=x P_{X}+y P_{Y}+\frac{V^{\prime}}{24}\left(x^{4}-y^{4}\right)+ \\
& -\frac{V}{6}\left(x^{3} P_{X}-y^{3} P_{Y}\right) \tag{6}
\end{align*}
$$

To the same order, this yields the transformation

$$
\begin{align*}
x & =X+\frac{V}{6} X^{3} \\
p_{x} & =P_{X}-\frac{V}{2} X^{2} P_{X}+\frac{V^{\prime}}{6} X^{3} \tag{7}
\end{align*}
$$

The $y$-transformation is obtained by replacing $x, p_{x}, X, P_{X}$ with $y, p_{y}, Y, P_{Y}$ and $V$ with $-V$. Note that outside the quadrupole, the transformed coordinates are the same as the original ones.

This yields the transformed Hamiltonian $H^{*}$ :

$$
\begin{align*}
H^{*} & =\frac{V}{2}\left(X^{2}-Y^{2}\right)+\frac{1}{2}\left(P_{X}^{2}+P_{Y}^{2}\right)+ \\
& +\frac{1}{8}\left(P_{X}^{2}+P_{Y}^{2}\right)^{2}-\frac{V}{4}\left(X^{2}+Y^{2}\right)\left(P_{X}^{2}-P_{Y}^{2}\right) \\
& +\frac{7 V^{2}}{24}\left(X^{4}+Y^{4}\right)-\frac{V^{2}}{4} X^{2} Y^{2} \tag{8}
\end{align*}
$$

We can identify the terms: the first two are the usual linear ones; the third term is not related to the electric field (it is small and due to the fact that $x^{\prime} \neq p_{x}$ or, equivalently, $\tan \theta \neq \sin \theta$ ); the $4^{\text {th }}$ term is also small and arises because a particle going through the quadrupole at an angle is inside the quad for slightly longer than one which remains on axis. See ref. [3] for more complete physical derivation of the individual terms.

The dominating higher order terms are the last two terms in eqn. 8. Since there are no derivatives of $V$, we can directly write down the aberrations in the thin-lens limit:

$$
\begin{equation*}
\Delta p_{x}=\frac{-1}{f^{2} L}\left(\frac{7}{6} x^{3}-\frac{1}{2} x y^{2}\right) \tag{9}
\end{equation*}
$$

with a similar expression for $\Delta p_{y} . L$ and $f$ are the quadrupole's effective length and focal length. The fractional focal error is found by dividing by the linear part $\Delta_{0} p_{x}=$ $-x / f$ :

$$
\begin{equation*}
\frac{\Delta f_{x}}{f}=\frac{1}{f L}\left(\frac{7}{6} x^{2}-\frac{1}{2} y^{2}\right) \tag{10}
\end{equation*}
$$

for $x$, and similarly for $y$.

### 2.2 Magnetic

In magnetic fields, the canonical momentum $\vec{p}$ contains the vector potential $\vec{A}$ so that the time-based Hamiltonian is

$$
\begin{equation*}
H_{\tau}=\frac{1}{2 m}|\vec{p}-q \vec{A}|^{2} \tag{11}
\end{equation*}
$$

As before, we use the invariant $p_{0} \equiv \sqrt{2 m H_{\tau}}$ to normalize the momenta, convert to $z$ as independent variable, and expand the square root, keeping terms up to $4^{\text {th }}$ order:

$$
\begin{align*}
H & \approx-A_{z}+\frac{1}{2}\left[\left(p_{x}-A_{x}\right)^{2}+\left(p_{y}-A_{y}\right)^{2}\right]+ \\
& +\frac{1}{8}\left[\left(p_{x}-A_{x}\right)^{2}+\left(p_{y}-A_{y}\right)^{2}\right]^{2} \tag{12}
\end{align*}
$$

To this order, the vector potential for quadrupole strength $k(z)$ is

$$
\begin{align*}
& A_{x}=-\frac{k^{\prime}}{4} x y^{2}, \quad A_{y}=\frac{k^{\prime}}{4} x^{2} y  \tag{13}\\
& A_{z}=-\frac{k}{2}\left(x^{2}-y^{2}\right)+\frac{k^{\prime \prime}}{48}\left(x^{4}-y^{4}\right)
\end{align*}
$$

and the Hamiltonian can be written:

$$
\begin{align*}
H & =\frac{1}{2}\left[k\left(x^{2}-y^{2}\right)-\frac{k^{\prime \prime}}{24}\left(x^{4}-y^{4}\right)+p_{x}^{2}+p_{y}^{2}\right]+ \\
& +\frac{k^{\prime} x y}{4}\left(y p_{x}-x p_{y}\right)+\frac{1}{8}\left(p_{x}^{2}+p_{y}^{2}\right)^{2} \tag{14}
\end{align*}
$$

The generating function which will eliminate derivatives of $k$ is

$$
\begin{align*}
& G\left(x, P_{X}, y, P_{Y}\right)=x P_{X}+y P_{Y}+\frac{k^{\prime}}{48}\left(x^{4}-y^{4}\right)+ \\
& -\frac{k}{12}\left[\left(x^{3}+3 x y^{2}\right) P_{X}-\left(3 x^{2} y+y^{3}\right) P_{Y}\right] \tag{15}
\end{align*}
$$

which, to the same order yields transformation

$$
\begin{align*}
x & =X+\frac{k}{12}\left(X^{3}+3 X Y^{2}\right)  \tag{16}\\
p_{x} & =P_{X}-\frac{k}{4}\left[\left(X^{2}+Y^{2}\right) P_{X}-2 X Y P_{Y}\right]+\frac{k^{\prime}}{12} X^{3}
\end{align*}
$$

and similarly for $\left(y, p_{y}\right)$. The transformed Hamiltonian is

$$
\begin{align*}
H^{*} & =\frac{k}{2}\left(X^{2}-Y^{2}\right)+\frac{1}{2}\left(P_{X}^{2}+P_{Y}^{2}\right)+ \\
& +\frac{1}{8}\left(P_{X}^{2}+P_{Y}^{2}\right)^{2}-\frac{k}{4}\left(X^{2}+Y^{2}\right)\left(P_{X}^{2}-P_{Y}^{2}\right) \\
& +\frac{k^{2}}{12}\left(X^{4}+Y^{4}\right)+\frac{k^{2}}{2} X^{2} Y^{2} \tag{17}
\end{align*}
$$

Notice the similarity to eqn. 8: in fact all terms are identical except the last two, which only differ in their coefficients. Applying the same procedure as in the electrostatic case, we write down the fractional change in focusing strength:

$$
\begin{equation*}
\frac{\Delta f_{x}}{f}=\frac{1}{f L}\left(\frac{1}{3} x^{2}+y^{2}\right) \tag{18}
\end{equation*}
$$

## 3 DISCUSSION

Formulas 10 and 18 are handy for quickly evaluating the importance of $3^{\text {rd }}$ order aberration. They also show that for fixed focal length, the only way of reducing the aberration is by lengthening the quadrupole; the fraction of aperture used is not important; for a given effective length, the absolute size of the aperture is not important; the shape of the ends of the electrode is not important.

Comparing the two formulas, we see that for roundish beams ( $x \approx y$ ), electrostatic and magnetic quads yield similar aberrations: they are in the ratio of $\frac{7}{6}: \frac{4}{3}$. For cases where one transverse dimension is large compared with the other, and it is important to maintain the quality in the larger dimension, magnetic quads are better by a factor of $\frac{7}{2}$. However, for the more common case where it is more important to maintain the quality of the higher quality dimension, electrostatic quads win by a factor of 2 .
Results from using the above Hamiltonians are in agreement with those from using the commonly used codes GIOS and COSY, provided fringe field cards are used. In both of those codes it is possible to perform a $3^{\text {rd }}$ order calculation with quads which have no fringe fields. This gives incorrect and actually completely unphysical results. In essence, omitting the fringe field cards in those codes describes a situation where the particle traverses nonMaxwellian fields. For example, GIOS, since it does not use the scalar value of the potential field, does not obey conservation of energy when fringe field cards are omitted.

The hard-edge case is correctly described in GIOS by including fringe field cards and setting the quadrupole aperture to zero, or, equivalently, setting all the fringe field integrals to zero. This is a useful approximation since the results are usefully close to reality and yet one needs not worry about specifying realistic fringe field integrals. This does not work in COSY, since a zero aperture forces an infinitesimal integration step-size. A better solution would be to build in the hard-edge kicks and use these as default when no fringe field is specified.

The required hard-edge kicks at the entrance to the quadrupole are derived directly from equations 7 and 16. The reason is that we know that the transformed coordinates ( $X, P_{X}, Y, P_{Y}$ ) do not experience any singular forces in the hard-edge limit. Therefore, the kicks for those coordinates are all zero. So the kicks for the untransformed $\left(x, p_{x}, y, p_{y}\right)$ for the electrostatic case are,

$$
\begin{align*}
\Delta x & =\frac{V}{6} x^{3} \\
\Delta p_{x} & =\frac{-V}{2} x^{2} p_{x} \\
\Delta y & =\frac{-V}{6} y^{3}  \tag{19}\\
\Delta p_{y} & =\frac{V}{2} y^{2} p_{y}
\end{align*}
$$

and for the magnetic case are,

$$
\begin{align*}
\Delta x & =\frac{k}{12}\left(x^{3}+3 x y^{2}\right) \\
\Delta p_{x} & =\frac{-k}{4}\left[\left(x^{2}+y^{2}\right) p_{x}-2 x y p_{y}\right] \\
\Delta y & =\frac{-k}{12}\left(3 x^{2} y+y^{3}\right)  \tag{20}\\
\Delta p_{y} & =\frac{k}{4}\left[\left(x^{2}+y^{2}\right) p_{y}-2 x y p_{x}\right]
\end{align*}
$$

The kicks at the exit are, of course, opposite in sign. These agree with the GIOS case of zero fringe field integrals. See ref. [1].

## 4 REFERENCES

[1] H. Matsuda and H. Wollnik Third Order Transfer Matrices for the Fringing Field of Magnetic and Electrostatic Quadrupole Lenses NIM 103, p. 117 (1972).
[2] M. Berz Computational Aspects of Design and Simulation: COSY INFINITY NIM A298, p. 473 (1990).
[3] R. Baartman Aberrations in Electrostatic Quadrupoles TRI-DN-95-21 (TRIUMF internal note, 1995).

