Quadrupoles, to Third Order

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1 Introduction

I derive the third order optics of quadrupoles. I transform away the derivatives of the strength function, and thus demonstrate that third order aberrations are insensitive to fringe field shaping. The results can be used for efficient tracking to third order or for simple and quick evaluation of nonlinear effects.

This is an extension to my work of 1997[1], which covered both electrostatic and magnetic quads, but only for the non-relativistic case.

2 Theory

A particle of charge $q$ and mass $m$ has canonical pairs of coordinates $((x, P_x), (y, P_y), (z, P_z), (t, E))$. The equation coupling these is

\[ (E - q\Phi)^2 - |\vec{P} - q\vec{A}|^2 c^2 = m^2 c^4. \]  

Here, $\Phi$ and $\vec{A}$ are respectively the scalar and vector potentials; both are functions of $(x, y, z)$, and both are zero on the reference particle’s orbit.

Let us use units for time, energy and potential that sets resp. $c = 1$, $m = 1$, $q = 1$. This is permissible as long as we consider no processes that change mass or charge.

\[ (E - \Phi)^2 - |\vec{P} - \vec{A}|^2 = 1. \]  

To find the Hamiltonian $H = E$, solve for $E$:

\[ H(x, P_x, y, P_y, z, P_z; t) = \Phi + \sqrt{1 + |\vec{P} - \vec{A}|^2} \]
2.1 In Frenet-Serret Frame

The reference orbit is assumed to be in one plane and is generally curved with curvature \( h = 1/\rho \). The transformation is conventionally made to the Frenet-Serret coordinate system where the longitudinal coordinate \( s \) is in the reference orbit direction, so \( h = h(s) \), \( x \) is radially outward, and \( y \) is perpendicular to the bend plane. Ruth\(^2\) shows that then the Hamiltonian is

\[
H(x, P_x, y, P_y, s, P_s; t) = \Phi + \sqrt{1 + (P_x - A_x)^2 + (P_y - A_y)^2 + \frac{(P_s - A_s)^2}{1 + hx}} \tag{4}
\]

As conventional in beam and accelerator physics, we use the longitudinal coordinate \( s \) as independent variable. Then the Hamiltonian is \(-P_s\):

\[
H(x, P_x, y, P_y, t; E; s) = -A_s - (1 + hx)\sqrt{(E - \Phi)^2 - 1 - (P_x - A_x)^2 - (P_y - A_y)^2} \tag{5}
\]

2.2 In Differential Coordinates

The “reference particle” has \( x = y = 0 \) and \( P_x = P_y = 0 \). In the following, we use the traditional symbols \( \beta, \gamma \) and hence also \( \beta \gamma \) for the reference particle’s speed, energy, and momentum, respectively.

The Hamiltonian is awkward because it mixes small dynamic quantities \( x, y, P_x, P_y \) with a large one \( E \). We only care about particles with a small \( \Delta E \) deviation from the reference energy \( \gamma \), and a small \( \Delta t \) deviation from the reference time \( t_0 = s/\beta \). We do this with a canonical transformation from \((t, -E)\) to \((\Delta t, -\Delta E)\). The generating function is

\[
F(t, -\Delta E) = \left(t - \frac{s}{\beta}\right)(-\Delta E - \gamma) \tag{6}
\]

The new Hamiltonian is

\[
\tilde{H}_s = H_s + \frac{\partial F}{\partial s} = H_s + \frac{\gamma + \Delta E}{\beta} \tag{7}
\]

Furthermore, we introduce new coordinates \((\tau, P_\tau)\) in place of \((\Delta t, \Delta E)\), with \( \tau = \beta \Delta t, P_\tau = \Delta E/\beta \). This results in a new “time” coordinate \( \tau \) being the distance ahead of the reference particle, and the “energy” coordinate being the momentum deviation w.r.t. the reference particle.
The Hamiltonian is then
\[ \tilde{H}_s(x, P_x, y, P_y, \tau, P_\tau; s) = \]
\[ P_\tau - A_s - (1 + hx) \sqrt{(\gamma + \beta P_\tau - \Phi)^2 - 1 - (P_x - A_x)^2 - (P_y - A_y)^2} \]  \hspace{1cm} (8)

2.3 Re-Normalize Momenta

We now change the units of momentum to $\beta \gamma$. This will have the advantage that outside of the regions of electric and magnetic fields, we have $P_x = x'$, $P_y = y'$, $P_\tau = \Delta P/P$ where primes are derivatives w.r.t. $s$. Further, we rescale scalar potential by a factor $\beta^2 \gamma$, and vector potential by a factor $\beta \gamma$. The result is

\[ H = P_\tau - A_s - (1 + hx) \sqrt{\frac{1}{\beta} + \beta(P_\tau - \Phi)} - \frac{1}{\beta^2 \gamma^2} - (P_x - A_x)^2 - (P_y - A_y)^2 \]  \hspace{1cm} (9)

or

\[ H = P_\tau - A_s - (1 + hx) \sqrt{1 + 2(P_\tau - \Phi) + \beta^2(P_\tau - \Phi)^2 - (P_x - A_x)^2 - (P_y - A_y)^2} \]  \hspace{1cm} (10)

This is the general Hamiltonian. It is exact.

2.4 Potentials’ Scales

For handy reference, here are the definitions of the scaled potentials in terms of the unscaled (subscript u):

\[ \Phi = \frac{q}{\beta^2 \gamma mc^2} \Phi_u(x, y, s), \]
\[ \vec{A} = \frac{q}{\beta \gamma mc} \vec{A}_u(x, y, s) \]  \hspace{1cm} (11)

2.5 Relativistic Limits

This $H$ also has the nice feature that the non-relativistic and ultra-relativistic limits are simple:

\[ \beta \ll 1 : H = P_\tau - A_s - (1 + hx) \sqrt{1 + 2(P_\tau - \Phi) - (P_x - A_x)^2 - (P_y - A_y)^2} \]
\[ \gamma \gg 1 : H = P_\tau - A_s - (1 + hx) \sqrt{(1 + P_\tau - \Phi)^2 - (P_x - A_x)^2 - (P_y - A_y)^2} \]  \hspace{1cm} (12)
2.6 Example: Field-free, curvature-free

\[ \tilde{H}_s = P_\tau - \sqrt{1 + 2P_\tau + \beta^2P^2_\tau - P^2_x - P^2_y} \]  

(13)

Then \( P'_x = P'_y = P'_\tau = 0 \), and to first order:

\[ x' = \frac{\partial H}{\partial P_x} = \frac{P_x}{\sqrt{1 + 2P_\tau + \beta^2P^2_\tau - P^2_x - P^2_y}} \approx P_x \]  

(14)

and similar for \( y' \),

\[ \tau' = 1 - \frac{1 + \beta^2P_\tau}{\sqrt{1 + 2P_\tau + \beta^2P^2_\tau - P^2_x - P^2_y}} \approx \frac{P_\tau}{\gamma^2} \]  

(15)

2.7 Straight elements, ignore longitudinal

Let us now confine ourselves to straight elements \( (h = 0) \) and concentrate only on transverse. Then for magnetic elements, we have

\[ H = -A_s - \sqrt{1 - (P_x - A_x)^2 - (P_y - A_y)^2} \]  

(16)

and for electrostatic elements, we have

\[ H = -\sqrt{1 - 2\Phi + \beta^2\Phi^2 - P^2_x - P^2_y} \]  

(17)

3 Electrostatic Quads

Compared with equation 2 of the 1997 paper\(^1\), we notice an extra term \( \beta^2\Phi^2 \) in the square root of eqn.\(^1\).

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

\[ H \approx \frac{1}{2}(2\Phi - \beta^2\Phi^2 + P^2_x + P^2_y) + \frac{1}{8}(2\Phi + P^2_x + P^2_y)^2. \]  

(18)

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

\[ \Phi = \frac{k(s)}{2}(x^2 - y^2) - \frac{k''(s)}{24}(x^4 - y^4). \]  

(19)

\(^1\)There is also a factor of 2 because the scaling of eqn.\(^1\) differs from the 1997 scaling by this factor
The expanded Hamiltonian, correct to 4\textsuperscript{th} order is

\[ H = \frac{k(x^2 - y^2)}{2} + \frac{P^2_x}{2} + \frac{P^2_y}{2} + \frac{(P^2_x + P^2_y)^2}{8} \frac{k(x^2 - y^2)(P^2_x + P^2_y)}{4} + \frac{k^2(x^2 - y^2)^2}{8\gamma^2} - \frac{k''(x^4 - y^4)}{24}. \]  

(20)

3.1 \( k'' \) is a “Fringe Field Effect”? 

The trouble with applying this to simple cases like thin lenses and hard-edge limits is the presence of \( k''(s) \), 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 \( k(s) \). For example, the approach taken in GIOS\textsuperscript{3} is to leave it up to the user to specify ‘fringe field integrals’ such as \( \int k^2 ds \) through the fringe fields. However, this leaves one quite vulnerable to 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.

3.2 \( k'' \) can be transformed out! 

It turns out to be possible to find a canonical transformation which eliminates the derivatives of \( k(s) \). In our case, we wish to retain terms to 4\textsuperscript{th} order in the Hamiltonian (3\textsuperscript{rd} order on force), and the transformation \((x, P_x, y, P_y) \rightarrow (X, P_X, Y, P_Y)\) has generating function

\[ G(x, P_x, y, P_y) = xP_x + yP_y + \frac{k'}{24}(x^4 - y^4) - \frac{k}{6}(x^3P_x - y^3P_y). \]  

(21)
To the same order, this yields the transformation

\[ x = X + \frac{k}{6}X^3 \]
\[ P_x = P_X - \frac{k}{2}X^2P_X + \frac{k'}{6}X^3. \]  

(22)

The \( y \)-transformation is obtained by replacing \( x, P_x, X, P_X \) with \( y, P_y, Y, P_Y \) and \( k \) with \(-k\). Note that outside the quadrupole, the transformed coordinates are the same as the original ones.

This yields the transformed Hamiltonian \( H^* \):

\[ H^* = \frac{k}{2}(X^2 - Y^2) + \frac{1}{2}(P_X^2 + P_Y^2) + \frac{1}{8}(P_X^2 + P_Y^2)^2 - \frac{k}{4}(X^2 + Y^2)(P_X^2 - P_Y^2) + \frac{(7 - 3\beta^2)k^2}{24}(X^4 + Y^4) - \frac{(1 - \beta^2)k^2}{4}X^2Y^2. \]  

(23)

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 \( x' \neq P_x \) or, equivalently, \( \tan \theta \neq \sin \theta \)); the 4th 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. [4] for more complete physical derivation of the individual terms.

### 3.3 Thin lens, Hard Edge Formulae

The dominating higher order terms are the last two terms in eqn. 23. Since there are no derivatives of \( k \), we can directly write down the aberrations in the thin-lens limit:

\[ \Delta P_x = \frac{-1}{f^2L} \left( \frac{7 - 3\beta^2}{6}x^3 - \frac{1 - \beta^2}{2}xy^2 \right), \]  

(24)

with a similar expression for \( \Delta P_y \). \( L \) and \( f \) are the quadrupole’s length and focal length. (Actually, it is more accurate to replace \( \frac{1}{f^2L} \) with \( \int k^2ds \).)

The fractional focal error is found by dividing by the linear part \( \Delta_0P_x = -x/f \):

\[ \frac{\Delta f_x}{f} = \frac{1}{fL} \left( \frac{7 - 3\beta^2}{6}x^2 - \frac{1 - \beta^2}{2}y^2 \right) \]  

(25)

for \( x \), and similarly for \( y \).
3.4 Physical Interpretation: Speed Effect

It is interesting and instructive to deconstruct the final result \[24\] to derive physical origins for these terms. We do this in the thin lens limit.

Referring to the untransformed Hamiltonian \[20\], we can identify the term with $\gamma^{-2}$ as due to a “velocity-gain” effect: particles entering the electric field have their speed changed because of longitudinal field, for example, those entering near the like-charged electrode are slowed so spend a longer than normal time in the focusing field. This effect disappears in ultra-relativistic limit. The contribution to $P_x$ from this effect in thin lens limit is

$$\Delta P_x |_{dv} = -\frac{x(x^2 - y^2)}{2\gamma^2} \int k^2 ds,$$ \[26\]

leaving only $\frac{2}{3}x^3$ inside the parentheses of eqn.\[24\] to account for.

3.5 Physical Interpretation: $k''$ Effect

The direct effect of the $k''$ term in the potential and the Hamiltonian \[20\] can be found from integrating by parts:

$$\Delta P_x |_{k''} = -\int \frac{\partial H}{\partial x} \big|_{k''} ds = \frac{1}{6} \int k'' x^3 ds = -\frac{1}{2} \int k' x^2 x' ds$$

$$\approx -\frac{1}{2} \int k x^2 x'' ds \approx \frac{1}{2} \int k x^3 ds \approx -\frac{x^3}{2} \int k^2 ds$$ \[27\]

3.6 Physical Interpretation: $\Delta x$ Effect

The remainder is now $-\frac{x^3}{6} \int k^2 ds$. This originates from a small, subtle and largely overlooked effect; I overlooked it in my earlier work\[4\]. It originates from a shift in $x$ experienced in the quad.

From \[27\] above, we also find

$$x'' = \frac{k'' x^3}{6}$$ \[28\]

which in thin lens approx can be integrated directly to obtain

$$\Delta x = \frac{k x^3}{6}.$$ \[29\]
Another way to see this is from eqn. 22. Since the transformed variable $X$ does not see any shifts due to derivatives of $k$, it is unaffected on passing through the fringe field. But if $X$ is not shifted, then $x$ must be shifted by $kx^3/6$.

As $x$ is shifted, there results a different overall focus effect $\Delta P_x = k\Delta x$:

$$\Delta P_x|_{dx} \approx -\frac{x^3}{6} \int k^2 ds.$$  \hfill (30)

Equations 26, 27, 30, when summed, give 24. Q.E.D.

## 4 Magnetic Quads, Scalar Potential

We can use the same scalar potential for magnetic as for electrostatic (19), but rotated by $\pi/4$:

$$\Psi(x, y, s) = k(s)xy - \frac{k''(s)}{12}xy(x^2 + y^2)$$  \hfill (31)

To find the vector potential, we follow Venturini-Abell-Dragt (VAD) and express it first in polar coordinates:

$$\Psi(r, \theta, s) = \left(\frac{k}{2}r^2 - \frac{k''}{24}r^4\right) \sin 2\theta$$  \hfill (32)

### 4.1 Vector Potential, Gauge Choice

But instead of VAD’s gauge condition $A_\theta = 0$, we set $A_r = 0$. Then

$$B_\theta = -\frac{\partial A_s}{\partial r} = \frac{1}{r} \frac{\partial \Psi}{\partial \theta}$$

$$B_s = \frac{1}{r} \frac{\partial (rA_\theta)}{\partial r} = \frac{\partial \Psi}{\partial s}$$  \hfill (33)

and we can find $\vec{A}$ simply by integrating. This results in

$$A_\theta = \frac{k'}{8}r^3 \sin 2\theta$$

$$A_s = \left(-\frac{k'}{2}r^2 + \frac{k''}{48}r^4\right) \cos 2\theta$$  \hfill (34)
or in Cartesian:

\[
\vec{A} = \left( -\frac{k'}{4} x y^2, \frac{k'}{4} x^2 y, -\frac{k}{2} (x^2 - y^2) + \frac{k''}{48} (x^4 - y^4) \right)
\]  

(35)

It is interesting to compare this with the VAD\textsuperscript{5} vector potential

\[
\vec{A} = \left( \frac{k'}{4} \left( x^3 - xy^2 \right), \frac{k'}{4} \left( x^2 y - y^3 \right), -\frac{k}{2} (x^2 - y^2) + \frac{k''}{12} (x^4 - y^4) \right)
\]  

(36)

The two vector potentials differ by the gradient of the following function:

\[
\chi(x, y, s) = \frac{1}{16} \left( x^4 - y^4 \right) k'
\]  

(37)

4.2 Lorenz Gauge

Neither of these two vector potentials satisfy \( \nabla \cdot \vec{A} = 0 \), the Lorenz gauge. We can add any multiple of \( \chi \) and it turns out that adding \( \nabla \chi/3 \) to eqn.\textsuperscript{35} does satisfy Lorenz gauge to required order:

\[
\vec{A} = \left( \frac{k'}{4} \left( x^3 - xy^2 \right), \frac{k'}{4} \left( x^2 y - y^3 \right), -\frac{k}{2} (x^2 - y^2) + \frac{k''}{24} (x^4 - y^4) \right)
\]  

(38)

4.3 Magnetic Hamiltonian

I choose to use eqn.\textsuperscript{35} because it’s the simplest. Then the Hamiltonian can be written:

\[
H = \frac{k(x^2 - y^2)}{2} + \frac{P_x^2}{2} + \frac{P_y^2}{2} + \\
\left( \frac{P_x^2 + P_y^2}{8} \right)^2 + \frac{k' xy (y P_x - x P_y)}{4} - \frac{k'' (x^4 - y^4)}{48}
\]  

(39)

The generating function which will eliminate derivatives of \( k \) is

\[
G(x, P_x, y, P_y) = x P_x + y P_y + \frac{k'}{48} (x^4 - y^4) + \\
- \frac{k}{12} \left[ (x^3 + 3xy^2) P_x - (3x^2 y + y^3) P_y \right]
\]  

(40)
which, to the same order yields transformation

\[ x = X + \frac{k}{12}(X^3 + 3XY^2) \]
\[ P_x = P_X - \frac{k}{4} \left[ (X^2 + Y^2)P_X - 2XYP_Y \right] + \frac{k'}{12}X^3, \tag{41} \]

and similarly for \((y, P_y)\). The transformed Hamiltonian is

\[ H^* = \frac{k}{2}(X^2 - Y^2) + \frac{1}{2}(P_X^2 + P_Y^2) + \]
\[ + \frac{1}{8}(P_X^2 + P_Y^2)^2 - \frac{k}{4}(X^2 + Y^2)(P_X^2 - P_Y^2) \]
\[ + \frac{k^2}{12}(X^4 + Y^4) + \frac{k^2}{2}X^2Y^2. \tag{42} \]

Notice the similarity to eqn. 23: 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 find

\[ \Delta P_x = -\int k^2 ds \left( \frac{x^3}{3} + xy^2 \right) \tag{43} \]

Or the fractional change in focusing strength:

\[ \frac{\Delta f_x}{f} = \frac{1}{fL} \left( \frac{x^2}{3} + y^2 \right) \tag{44} \]

where \(L\) is the effective length.
References

[1] R. Baartman. Intrinsic Third Order Aberrations in Electrostatic and Magnetic Quadrupoles. In Proc. Particle Accelerator Conference, 12-16 May 1997, Vancouver, British Columbia, Canada, pages 1415–1417. IEEE, 1997.

[2] Ronald D Ruth. Single particle dynamics and nonlinear resonances in circular accelerators. In Lecture Notes in Physics, pages 37–63. Springer, 1986.

[3] H Matsuda and H Wollnik. Third order transfer matrices for the fringing field of magnetic and electrostatic quadrupole lenses. Nuclear Instruments and Methods, 103(1):117–124, 1972.

[4] R. Baartman. Aberrations in Electrostatic Quadrupoles. Technical Report TRI-DN-95-21, TRIUMF, 1995.

[5] M Venturini, D Abell, and A Dragt. Map computation from magnetic field data and application to the lhc high-gradient quadrupoles.