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Analysis and Fringe Field Scaling of a Legacy Set of Electrostatic Deflector Aberration Formulas

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Abstract

We performed an analysis of the derivation of first and second order analytic aberration formulas by Wollnik (1965) for the case of electrostatic deflectors in the horizontal plane. We found that these aberration formulas are valid for the main field of the deflector; however, they do not account for any fringe field effects. To address this issue, we modified the aberration formulas from Wollnik (1965) for a hard edge fringe field by scaling the particle inclinations at the entrance and exit edges of the deflector. These modified aberration formulas fully agree with electrostatic aberration formulas derived by Valetov and Berz (in this volume), as well as with differential-algebraic (DA) calculations of electrostatic deflector aberrations using the code *COSY INFINITY*.

Keywords: electrostatic deflectors, aberrations, fringe fields, energy conservation
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Contents

1 Introduction

Valetov and Berz (in this volume) derived first and second order aberration formulas for electrostatic deflectors and found a very high agreement between them and aberrations calculated by the code *COSY INFINITY* (Makino & Berz, 2006) using differential-algebraic (DA) transfer map methods. On the other hand, Valetov and Berz (in this volume) found a significant discrepancy with the analytic aberration formulas from Wollnik (1965) ("Wollnik's paper"), as well as with the program *GIOS* that uses the aberration formulas from Wollnik's paper. This discrepancy was in second order horizontal aberrations $(x|xa)$, $(a|xx)/2$, $(a|xa)$, and $(a|aa)/2$ (see Secs. 2 and 5 for the notation).

The purpose of this work is to find and address the reason for this discrepancy. We will first verify the charged particle Lagrangian used in Wollnik's paper. Next, we will check that the Taylor expansions of the Lagrangian to third order and the resulting expansions of the ODEs of motion to second order in Wollnik's paper are correct. We will then ascertain that the variation of parameters to obtain the aberration formulas was done correctly, and we will find that the analytic aberration formulas in Wollnik's paper are correct for the main field of the electrostatic deflector.

Aberrations of a particle optical element generally include both main and fringe field effects, with the exception of cases where the entire relevant motion occurs in the main field. The simplest model of a fringe field is the hard edge fringe field model, where the fringe field is approximated by a step function. In *COSY INFINITY*'s beamline coordinate system particle coordinates infinitesimally before and after a hard edge fringe field are the same because of the definition of the coordinate system. However, the beamline coordinates in Wollnik's paper do not have this property, which necessitates scaling of the momentum-like coordinates at the entrance and exit edges of the deflector to account for refractive effects necessarily arising from the change of electrostatic potential experienced by a particle. We scaled the momentum-like inclination coordinate α for a hard edge fringe field in aberration formulas from Wollnik's paper. The resulting modified aberration formulas are in a full agreement with aberration formulas derived by Valetov and Berz (in this volume) and with the code *COSY INFINITY*.

Wollnik's paper derives first and second order aberration formulas for electrostatic deflectors and magnetic dipoles with arbitrary inhomogeneity coefficients and non-relativistic equations of motion. Per the impetus of our study, the scope of the analyses in this work will be the derivation of electrostatic deflectors aberrations for motion in the horizontal plane.

2 Notation and the Coordinate System

Wollnik's paper considers nonrelativistic particles of mass $m = m_0(1+\gamma)$, charge e in elementary charge units e_0, and kinetic energy $U = U_0(1+\delta)$. For the purpose of this study, we will perform the analyses for particles without mass or energy deviations, and we will set $\gamma = 0$ and $\delta = 0$ when using or citing formulas from Wollnik's paper. Thus, all particles are launched with the reference kinetic energy U_0. We will use U for the position-dependent kinetic energy of non-reference particles.

Wollnik's paper begins with a cylindrical coordinate system (r, z, θ), where r is the distance to the center of curvature of the deflector or dipole, z is the vertical transverse coordinate, and θ is the arc's central angle. The reference orbit has the coordinates $(r, z) = (r_0, 0)$. The aberration formulas in Wollnik's paper are derived in the dimensionless coordinate system

$$(u, v, w) = \left(\frac{r}{r_0} - 1, \frac{z}{r_0}, \theta\right), \tag{1}$$

which is related to *COSY INFINITY*'s coordinates (x, y, s) in the main field of an electrostatic deflector or magnetic dipole with curvature radius r_0 as

$$(u, v, w) = \frac{1}{r_0}(x, y, s + \text{const}). \tag{2}$$

When using the notation from Wollnik's paper, we will minimize the number of notation definitions: for example, Wollnik's paper denotes $k_1 = \sqrt{2-c}$ and $s_1 = \sin(k_1 w)$, but we will use the full expression $\sin\left(\sqrt{2-c}w\right)$ to avoid introducing k_1 and s_1.

For reference, *COSY INFINITY*'s beamline coordinate system uses coordinates (Berz & Makino, 2017)

$$\begin{aligned} r_1 &= x, & r_2 &= a = p_x/p_0, \\ r_3 &= y, & r_4 &= b = p_y/p_0, \\ r_5 &= l = -(t-t_0)\,v_0\tfrac{\gamma}{1+\gamma}, & r_6 &= \delta_K = \tfrac{K-K_0}{K}. \end{aligned}$$

Coordinates x and y are the transverse Frenet-Serret position coordinates with the x axis pointing outwards relative to the center of curvature, p is the momentum, K is the kinetic energy, v is the velocity, t is the time of flight, and γ is the Lorentz factor. Index 0 refers to the reference particle. The arc length coordinate in *COSY INFINITY* is denoted by s.

For any $f, g \in C^n\left(\mathbb{R}^k\right)$, where n is the order and k is the number of variables, will use the DA equivalence relation $f =_n g$ to denote that $f(0) = g(0)$ and all partial derivatives of f and g agree at 0 up to order n. See Berz (1999) for detailed information on DA algebra.

3 Equivalence of Charged Particle Lagrangians

3.1 Lagrangian From Wollnik's Paper

Wollnik's paper uses the Lagrangian

$$F = \left[\frac{ee_0}{U_0}\varphi\left\{(1+u)^2 + u'^2 + v'^2\right\}\right]^{\frac{1}{2}} - \frac{ee_0}{\sqrt{2mU_0}}(1+u)\,A_w, \tag{3}$$

where A_w is the w component of magnetic potential $(0, 0, A_w)$ and φ is the electrostatic potential

$$\varphi(u,v) = r_0 E_0 \sum_{i,k=0}^{+\infty} e_{ik} u^i v^k. \tag{4}$$

Wollnik's paper restricts the electromagnetic field to separate cases of an electrostatic deflector and a magnetic dipole, of which we consider the electrostatic deflector case.

For the expansion of the electrostatic potential in eq. 4, Wollnik specifies several first coefficients e_{ik} as

$$\begin{aligned} e_{00} &= \frac{1}{2}, \\ e_{10} &= -1, \\ e_{20} &= \frac{1}{2}(1+c), \quad & e_{02} &= -\frac{1}{2}c, \\ e_{30} &= \frac{1}{6}\bar{c}, & e_{12} &= -\frac{1}{2}(\bar{c}+2+c), \end{aligned} \tag{5}$$

where c and $\bar{c}$ are inhomogeneity coefficients. These coefficients are

$$\begin{aligned} c &= -\left[\frac{\partial E_u}{\partial u}\frac{1}{E_0}\right]_{u=v=0} - 1, \\ \bar{c} &= -\left[\frac{\partial^2 E_u}{\partial u^2}\frac{1}{E_0}\right]_{u=v=0}, \end{aligned} \tag{6}$$

where E_u is the u component of electrostatic field.

Comparing Wollnik's electrostatic potential expansion in eq. 4 with the radial electrostatic field expansion

$$E\left(x\right)=E_0\left[1-\sum_{j=1}^{N}n_j\left(\frac{x}{r_0}\right)^j\right]+O\left(x^{N+1}\right) \tag{7}$$

in *COSY INFINITY*'s notation (Berz & Makino, 2017), we obtain the following relations between the inhomogeneity coefficients:

$$\begin{aligned} c &= n_1-1, \\ \bar{c} &= 2n_2. \end{aligned} \tag{8}$$

The Lagrangian in eq. 3 has a quite different appearance from the well-known form (Valetov & Berz, in this volume)

$$L\left(\vec{r},\vec{\mathrm{v}},t\right)=\frac{m\mathrm{v}^2}{2}+ee_0\vec{A}\cdot\vec{\mathrm{v}}-ee_0\tilde{\varphi} \tag{9}$$

of the non-relativistic Lagrangian of a charged particle, where $\vec{r}$ is the particle's position, $\vec{A}$ is the vector potential, $\vec{\mathrm{v}}$ is the particle's velocity, and $\tilde{\varphi}$ is the scalar potential.

We also note that the electrostatic field expansion in eq. 4 is not zero at the reference orbit, as required by the beam physics convention. Additionally, Newton's second law for the u coordinate of the reference particle gives

$$\begin{aligned} m\frac{d^2u}{dt^2}r_0 &= \frac{2}{r_0}U_0-\left[\frac{ee_0}{r_0}\frac{\partial\varphi}{\partial u}\right]_{u=v=0}= \\ &= \frac{2}{r_0}U_0+ee_0E_0=0, \end{aligned} \tag{10}$$

from where

$$U_0=-\frac{1}{2}E_0ee_0r_0. \tag{11}$$

However, this expression has the opposite sign of the equation (6e) in Wollnik's paper for the reference particle, which is

$$U_0=\frac{1}{2}E_0ee_0r_0. \tag{12}$$

This issue is resolved by noting that the electrostatic potential in eq. 4 satisfies Maxwell's equations and Newton's second law and is zero at the reference orbit if we redefine the electrostatic potential as

$$\begin{aligned} \tilde{\varphi}\left(u,v\right) &= U_0-\varphi\left(u,v\right)= \\ &= U_0-r_0E_0\sum_{i,k=0}^{+\infty}e_{ik}u^iv^k. \end{aligned} \tag{13}$$

With this redefinition of the electrostatic potential, the Lagrangian from eq. 3 assumes the form

$$F=\left[\frac{U_0-ee_0\tilde{\varphi}}{U_0}\left\{\left(1+u\right)^2+u'^2+v'^2\right\}\right]^{\frac{1}{2}}-\frac{ee_0}{\sqrt{2mU_0}}\left(1+u\right)A_w. \tag{14}$$

3.2 Lagrangian Derived by Changing the Independent Variable

In contrast to the Lagrangian from Wollnik's paper, the nonrelativistic Lagrangian of a charged particle in *COSY INFINITY*'s beamline coordinate system is (Valetov & Berz, in this volume)

$$L^{\mathrm{C,s}}\left(\vec{r},\vec{\mathrm{v}}^{\mathrm{s}},s\right)=\frac{1}{\dot{s}}\left(\frac{m\left(\mathrm{v}^{\mathrm{s}}\right)^2}{2}\dot{s}^2+ee_0\vec{A}^{\mathrm{C}}\cdot\vec{\mathrm{v}}^{\mathrm{C,s}}\dot{s}-ee_0\tilde{\varphi}^{\mathrm{C}}\right), \tag{15}$$

where the superscript C refers to *COSY INFINITY*'s beamline coordinate system, the superscript s denotes that arc length s is the independent variable, and the overdot denotes derivative by time t.

This Lagrangian was obtained from the Lagrangian in the Cartesian laboratory coordinate system (LCS) by coordinate transformations including a change of the independent variable from time t to arc length s, making t a position variable and dt/ds the respective momentum-like coordinate. Thus, when applying the Euler–Lagrange equation to the Lagrangian in eq. 15, partial derivatives by variables other than $\dot{s}$ are not applied to $\dot{s}$. The resulting equations of motion contain $\dot{s}$, where $\dot{s}$ can be expressed in terms of the position coordinates (e.g., u and v) using the conservation of energy.

The Lagrangian of a charged particle from eq. 15 can be rewritten [for example, $dx/dt = r_0 du/dt = du/dw \cdot r_0 \cdot dw/dt$] using the beamline coordinate system from Wollnik's paper as

$$L^{\mathrm{W,w}}\left(\vec{r}, \vec{\mathrm{v}}^{\mathrm{w}}, w\right) = \frac{1}{\dot{w}}\left(\frac{m\left(\mathrm{v}^{\mathrm{w}}\right)^2 r_0^2}{2}\dot{w}^2 + ee_0\vec{A}^{\mathrm{W}} \cdot \vec{\mathrm{v}}^{\mathrm{W,w}} r_0 \dot{w} - ee_0\tilde{\varphi}^{\mathrm{W}}\right), \tag{16}$$

where the superscript W denotes Wollnik's coordinate system and the superscript w indicates that w is the independent variable.

3.3 Lagrangian Derived Using Maupertuis's Principle

The Lagrangian in eq. 3 from Wollnik's paper, unlike the Lagrangian in eq. 16, does not use time t as a position variable and does not contain $\dot{w}$. However, because time t is a position variable in eq. 16, simply replacing $\dot{w}$ by its expression in terms of u and v in this Lagrangian would result in incorrect equations of motion. A natural idea to address this issue would be to modify our Lagrangian from eq. 16 in a way that after replacing $\dot{w}$ by its expression in terms of u and v applying the Euler–Lagrange equation would give the correct equations of motion.

Such a modification of the Lagrangian can be obtained using Maupertuis's principle. In particular, Pars (1965) proposed a modified Lagrangian

$$\Lambda = \frac{dt}{d\tau}\left(L' + h\right), \tag{17}$$

where L' is the Lagrangian expressed in a new coordinate system with an independent variable τ (which is $\tau = w$ in Wollnik's paper and $\tau = s$ in *COSY INFINITY*'s beamline coordinate system), t is the independent variable in the original coordinate system, and h is a parameter with the constraint $h = U_0$ that should be applied to the equations of motion produced using the Euler–Lagrange equation.

We bring our Lagrangian from eq. 16 to the form of eq. 17, obtaining

$$\Lambda = \frac{m\left(\mathrm{v}^{\mathrm{w}}\right)^2 r_0^2}{2}\dot{w} + ee_0\vec{A}^{\mathrm{W}} \cdot \vec{\mathrm{v}}^{\mathrm{W,w}} r_0 - \frac{1}{\dot{w}}ee_0\tilde{\varphi}^{\mathrm{W}} + \frac{1}{\dot{w}}h. \tag{18}$$

Considering that the reference energy

$$U_0 = \frac{m\left(\mathrm{v}^{\mathrm{w}}\right)^2 r_0^2}{2}\dot{w}^2 + ee_0\tilde{\varphi}^{\mathrm{W}} \tag{19}$$

is constant, we can equivalently apply the constraint $h = U_0$ before the Euler–Lagrange equation, obtaining a simpler Lagrangian

$$\Lambda = m\left(\mathrm{v}^{\mathrm{w}}\right)^2 r_0^2 \dot{w} + ee_0\vec{A}^{\mathrm{W}} \cdot \vec{\mathrm{v}}^{\mathrm{W,w}} r_0, \tag{20}$$

which has resemblance to the modified Wollnik's Lagrangian from eq. 14.

The prime notation will be used to denote derivatives by w. Using the Frenet–Serret theorem (Valetov & Berz, in this volume), we express velocity $\vec{\mathrm{v}}^{\mathrm{w}}$in terms of u, v, their derivatives, and the independent variable w as

$$
\begin{aligned}
r_0 \vec{\mathrm{v}}^{\mathrm{w}}(w) &= \frac{d}{dw}\vec{r}(w) = \\
&= \frac{d}{dw}\left(\vec{r}_0(w) + u(w)\, r_0 \vec{e}_u(w) + v(w)\, r_0 \vec{e}_v(w)\right) = \\
&= (1 + u(w))\, r_0 \vec{e}_w(w) + u'(w)\, r_0 \vec{e}_u(w) + v'(w)\, r_0 \vec{e}_v(w)\,,
\end{aligned}
\tag{21}
$$

where $\vec{r}(w)$ is the radius vector of the considered particle, $\vec{r}_0(w)$ is the reference particle's radius vector, and $\vec{e}_u$ and $\vec{e}_v$ are basis vectors of the u and v axes.

We express $\dot{w}$ in terms of position coordinates u and v, reference kinetic energy U_0, and potential energy V as

$$
\begin{aligned}
\dot{w} &= \frac{\vec{\mathrm{v}}^{\mathrm{ct}}}{r_0 \vec{\mathrm{v}}^{\mathrm{w}}} = \\
&= \frac{\sqrt{\frac{2}{m}(U_0 - V)}}{r_0 \sqrt{(1+u)^2 + u'^2 + v'^2}},
\end{aligned}
\tag{22}
$$

where the superscript ct refers to the Cartesian LCS and the expression for v^{w} from eq. 21 was used.

Applying the expression of $\dot{w}$ from eq. 22 to the Lagrangian in eq. 20, assuming $\vec{A}^{\mathrm{W}} = -(0, 0, A_w)$ similarly to the redefinition of the electostatic potential in eq. 13, we see that Wollnik's Lagrangian F (both the original form in eq. 3 and with the redefined electrostatic field in eq. 14) is the Lagrangian Λ from eq. 20 scaled by a constant coefficient $\sqrt{2mU_0}r_0$:

$$
\begin{aligned}
\Lambda &= m\left(\mathrm{v}^{\mathrm{w}}\right)^2 r_0^2 \dot{w} + e e_0 \vec{A}^{\mathrm{W}} \cdot \vec{\mathrm{v}}^{\mathrm{W,w}} r_0 = \\
&= \sqrt{2m} r_0 \sqrt{U_0 - V} \sqrt{(1+u)^2 + u'^2 + v'^2} - e e_0 (1+u)\, r_0 A_w = \\
&= \sqrt{2mU_0} r_0 F.
\end{aligned}
\tag{23}
$$

3.4 Conclusion on the Lagrangians

The Lagrangian of a charged particle used in Wollnik's paper with the beamline coordinate system (u, v, w) is equivalent to the Lagrangians based on Valetov and Berz (in this volume), where derivation is performed by changing the independent variable. Wollnik's Lagrangian in eq. 3 can be obtained from our Lagrangian in eq. 16 by eliminating the dependent variables t and dt/dw using Maupertuis's principle and considering Wollnik's definition of the electrostatic potential.

4 Third Order Expansions of the Equivalent Lagrangians

Following Wollnik's paper, we obtained third order Taylor expansions for Wollnik's Lagrangian F (as stated in eq. 3) and our Lagrangian Λ (both versions: eq. 18 and eq. 20).

For Wollnik's Lagrangian F, we used Wollnik's definition of the electrostatic potential φ from eq. 4. For our Lagrangian Λ, we used the form $\tilde{\varphi} = U_0 - \varphi$ of the electrostatic potential from eq. 13, as well as the expression for $\dot{w}$ from eq. 22. The expression for the reference kinetic energy U_0 from eq. 12 was used for the Lagrangians F and Λ.

The third order DA vectors representing the Lagrangians F and Λ in terms of variables u, v, u', and v' are the right-hand side of

$$
\begin{aligned}
F =_3 \Lambda =_3\ & 1 + \frac{1}{2}(c-2)\, u^2 - \frac{c}{2} v^2 + \frac{1}{2} u'^2 + \frac{1}{2} v'^2 + \\
&+ \left(c + \frac{\bar{c}}{6}\right) u^3 - \frac{1}{2}(2 + 3c + \bar{c})\, u v^2 - u\left(u'^2 + v'^2\right),
\end{aligned}
\tag{24}
$$

in agreement with the third order expansion of the Lagrangian F in eq. (5) of Wollnik's paper, with the difference that Wollnik also considered particles with energy offsets $\delta \neq 0$. Wollnik used the parameter

$$\eta = r_0 E_0 \frac{e e_0}{2U_0 (1+\delta)} \tag{25}$$

to describe the energy offsets, which is $\eta = 1$ for $\delta = 0$.

5 First Order Expansion of the ODEs of Motion and Their Solution

Continuing to follow Wollnik's paper, by applying the Euler–Lagrange equation to the second order truncation of the Lagrangian's expansion from eq. 24, we obtained first order Taylor expansions of the ODEs of motion in terms of u, v, and their derivatives:

$$\begin{aligned} u'' &= (c-2)\, u, \\ v'' &= -cv, \end{aligned} \tag{26}$$

which agree with eq. (7) in Wollnik's paper (scope of comparison $\delta = 0$). Considering the relations between Wollnik's electrostatic potential inhomogeneity coefficients c, $\bar{c}$ and *COSY INFINITY*'s inhomogeneity coefficients n_1, n_2 stated in eq. 8, this also agrees with the first order terms of the expansion of the ODE of motion in the horizontal plane from Valetov and Berz (in this volume).

In addition to position coordinates u and v, Wollnik's paper uses momentum-like inclination coordinates α and β:

$$\begin{aligned} \alpha &= \frac{du}{dw}\frac{r_0}{r} = u'\left(1 - u + O\left(u^2\right)\right), \\ \beta &= \frac{dv}{dw}\frac{r_0}{r} = v'\left(1 - v + O\left(v^2\right)\right). \end{aligned} \tag{27}$$

We obtained the solution of the first order expansion of the ODE of motion for u as follows:

$$\begin{aligned} {}^1u(w) &= u_2 \cos\left(\sqrt{2-c}w\right) + \alpha_2 \frac{1}{\sqrt{2-c}} \sin\left(\sqrt{2-c}w\right), \\ {}^1\alpha(w) &= -u_2\sqrt{2-c}\sin\left(\sqrt{2-c}w\right) + \alpha_2 \cos\left(\sqrt{2-c}w\right), \end{aligned} \tag{28}$$

where (u_2, α_2) are the initial values of u and α, which agrees with eqns. (10u) and (19u) of Wollnik's paper (scope of comparison $\delta = 0$).

Following Wollnik and Berz (1985), we will use the notation

$$(r_i | r_{j_1} \cdots r_{j_n}) = \left(\frac{\partial^n \left(\mathcal{M}(\vec{r})\right)_i}{\partial r_{j_1} \cdots \partial r_{j_n}}\right)_{\vec{r}=0} \tag{29}$$

for partial derivatives of the transfer map $\vec{r} \mapsto \mathcal{M}(\vec{r})$, where $\vec{r}$ is a coordinate vector $\vec{r} = (r_1, \ldots, r_{2m})$ and $2m$ is the number of phase space coordinates. Aberration coefficients are described by the respective coefficients $(r_i | r_{j_1} \cdots r_{j_n})$ as

$$\frac{1}{j_1! \cdots j_n!} (r_i | r_{j_1} \cdots r_{j_n}). \tag{30}$$

From eq. 28, the first order aberrations are

$$(u|u) = \cos\left(\sqrt{2-c}w\right), \tag{31a}$$

$$(u|\alpha) = \frac{1}{\sqrt{2-c}} \sin\left(\sqrt{2-c}w\right), \tag{31b}$$

$$(\alpha|u) = -\sqrt{2-c}\sin\left(\sqrt{2-c}w\right), \tag{31c}$$

$$(\alpha|\alpha) = \cos\left(\sqrt{2-c}w\right), \tag{31d}$$

in agreement with the first order aberration formulas obtained by Valetov and Berz (in this volume) (scope of comparison $\delta = 0$).

6 Second Order Expansion of the ODEs of Motion

We applied the Euler–Lagrange equation to the third order expansion of the Lagrangian from eq. 24, obtaining

$$u'' - (c-2)\,u = 2uu'' + u'^2 - v'^2 + \frac{1}{2}\,(6c+\bar{c})\,u^2 - \frac{1}{2}\,(2+3c+\bar{c})\,v^2 = \bar{F}\,(w)\,, \tag{32}$$

and

$$v'' + cv = 2u'v' + 2uv''0 - (2+3c+\bar{c})\,uv = \tilde{F}\,(w)\,, \tag{33}$$

which agree with the equations at the bottom of p. 216 of Wollnik's paper (scope of comparison $\delta = 0$). In the following, we only consider motion in the horizontal transverse plane (i.e. the u–α plane).

7 Wollnik's Solution of the Second Order ODEs of Motion

To solve the second order expansion of the ODEs of motion from the equations at the bottom of p. 216 in Wollnik's paper, which take the form of eqns. 32 and 33 for $\delta = 0$, Wollnik applied the method of variation of parameters from Hildebrand (1949). We reconstruct Wollnik's solution for $u\,(w)$ by following both Wollnik (1965) and Hildebrand (1949) as follows.

First, we consider the linear aspect

$$u'' - (c-2)\,u = \bar{F}\,(w) \tag{34}$$

of eq. 32. We have its general homogeneous solution in eq. 28, and we seek a solution of eq. 32 as

$${}^2u\,(w) = u_2\,(w)\cos\left(\sqrt{2-c}w\right) + \frac{1}{\sqrt{2-c}}\alpha_2\,(w)\sin\left(\sqrt{2-c}w\right). \tag{35}$$

Eq. 34 represents one condition for $u_2\,(w)$ and $\alpha_2\,(w)$, and we use

$$u_2'\,(w)\cos\left(\sqrt{2-c}w\right) + \frac{1}{\sqrt{2-c}}\alpha_2'\,(w)\sin\left(\sqrt{2-c}w\right) = 0 \tag{36}$$

as a second condition.

We arrive to the system of equations

$$\begin{aligned} u_2'\,(w)\cos\left(\sqrt{2-c}w\right) + \frac{1}{\sqrt{2-c}}\alpha_2'\,(w)\sin\left(\sqrt{2-c}w\right) &= 0, \\ u_2'\,(w)\cos'\left(\sqrt{2-c}w\right) + \frac{1}{\sqrt{2-c}}\alpha_2'\,(w)\sin'\left(\sqrt{2-c}w\right) &= \bar{F}\,(w)\,. \end{aligned} \tag{37}$$

The solution of this system of equations for $u_2\,(w)$ and $\alpha_2\,(w)$ is

$$\begin{aligned} u_2\,(w) &= \int_0^w \left(-\frac{1}{\sqrt{2-c}}\sin\left(\sqrt{2-c}w\right)\right)\bar{F}\,(w)\,dw + c_1, \\ \alpha_2\,(w) &= \int_0^w \cos\left(\sqrt{2-c}w\right)\bar{F}\,(w)\,dw + c_2, \end{aligned} \tag{38}$$

where c_1 and c_2 are integration constants.

Denoting the initial values as $u_2 = {}^2u\,(0)$ and $\alpha_2 = {}^2\alpha\,(0)$, inserting eq. 38 into eq. 35, and setting $w = 0$ in the resulting expressions for ${}^2u\,(w)$ and its derivative ${}^2u'\,(w)$, we found

$$\begin{aligned} c_1 &= u_2, \\ c_2 &= \alpha_2\,(1+u_2)\,, \end{aligned} \tag{39}$$

and obtained the general solution of eq. 34 as

$$\begin{aligned}
{}^{2}u\left(w\right) = {}^{1}u\left(w\right) + \frac{1}{\sqrt{2-c}}\alpha_2 u_2 \sin\left(\sqrt{2-c}w\right) + \\
+ \frac{1}{\sqrt{2-c}}\Big(\sin\left(\sqrt{2-c}w\right)\int_0^w \cos\left(\sqrt{2-c}w\right)\bar{F}\left(w\right)dw - \\
- \cos\left(\sqrt{2-c}w\right)\int_0^w \sin\left(\sqrt{2-c}w\right)\bar{F}\left(w\right)dw\Big),
\end{aligned} \tag{40}$$

where ${}^{1}u\left(w\right)$ is the first order solution from eq. 28. The term $\alpha_2 u_2 \sin\left(\sqrt{2-c}w\right)/\sqrt{2-c}$ does not appear in eq. (11u) of Wollnik's paper; however, the aberration formulas of eq. (12u) in Wollnik's paper fully agree with eq. 40.

In Wollnik's paper, the solution of the first order expansion of the ODE of motion for $u\left(w\right)$ is then inserted into the nonlinear expression for $\bar{F}\left(w\right)$ at the bottom of p. 216 of Wollnik's paper, which corresponds here to inserting eq. 28 into the nonlinear aspect

$$2uu'' + u'^2 - v'^2 + \frac{1}{2}\left(6c+\bar{c}\right)u^2 - \frac{1}{2}\left(2+3c+\bar{c}\right)v^2 = \bar{F}\left(w\right) \tag{41}$$

of eq. 32. From the result of the integration, we extracted expressions for the second order aberrations of u:

$$\begin{aligned}
\frac{1}{2}\left(u|uu\right) = \left[u^2\right]\left({}^{2}u\left(w\right)\right) = \\
= \frac{1}{3}\frac{1}{2-c}\left(2\left(9c+\bar{c}-6\right) + \left(12c+\bar{c}-12\right)\cos\left(\sqrt{2-c}w\right)\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right),
\end{aligned} \tag{42a}$$

$$\begin{aligned}
\left(u|u\alpha\right) = \left[u\alpha\right]\left({}^{2}u\left(w\right)\right) = \\
= \frac{1}{3}\frac{1}{\left(2-c\right)^{3/2}}\left(\bar{c}+9c-6+\left(12-12c-\bar{c}\right)\cos\left(\sqrt{2-c}w\right)\right)\sin\left(\sqrt{2-c}w\right),
\end{aligned} \tag{42b}$$

$$\begin{aligned}
\frac{1}{2}\left(u|\alpha\alpha\right) = \left[\alpha^2\right]\left({}^{2}u\left(w\right)\right) = \\
= \frac{1}{3}\frac{1}{\left(2-c\right)^2}\left(6c+\bar{c}-\left(12c+\bar{c}-12\right)\cos\left(\sqrt{2-c}w\right)\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right),
\end{aligned} \tag{42c}$$

where $\left[z\right]f$ denotes the Taylor series coefficient of z in f.

Applying the formula for α from eq. 27 to the evaluated integral in eq. 40, we obtained the second order aberrations of α:

$$\begin{aligned}
\frac{1}{2}\left(\alpha|uu\right) = \left[u^2\right]\left({}^{2}\alpha\left(w\right)\right) = \left[u^2\right]\left(\frac{{}^{2}u'\left(w\right)}{1+{}^{2}u\left(w\right)}\right) = \\
= \frac{1}{6}\frac{1}{\sqrt{2-c}}\left(6c+\bar{c}+2\left(9c+\bar{c}-6\right)\cos\left(\sqrt{2-c}w\right)\right)\sin\left(\sqrt{2-c}w\right),
\end{aligned} \tag{42d}$$

$$\begin{aligned}
\left(\alpha|u\alpha\right) = \left[u\alpha\right]\left({}^{2}\alpha\left(w\right)\right) = \left[u\alpha\right]\left(\frac{{}^{2}u'\left(w\right)}{1+{}^{2}u\left(w\right)}\right) = \\
= \frac{2}{3}\frac{1}{2-c}\left(9c+\bar{c}-6\right)\left(1+2\cos\left(\sqrt{2-c}w\right)\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right),
\end{aligned} \tag{42e}$$

$$\begin{aligned}
\frac{1}{2}\left(\alpha|\alpha\alpha\right) = \left[\alpha^2\right]\left({}^{2}\alpha\left(w\right)\right) = \left[\alpha^2\right]\left(\frac{{}^{2}u'\left(w\right)}{1+{}^{2}u\left(w\right)}\right) = \\
= \frac{2}{3}\frac{1}{\left(2-c\right)^{3/2}}\left(9c+\bar{c}-6\right)\sin\left(\sqrt{2-c}w\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right).
\end{aligned} \tag{42f}$$

The aberrations in eq. 42 agree with the results on p. 217 of Wollnik (1965). Considering the ODEs of motion in *COSY INFINITY*'s beamline coordinate system (Valetov & Berz, in this volume), the transformation of the aberration formulas from Wollnik's coordinates (u, α) to *COSY INFINITY*'s beamline coordinates (x, a) is performed using the relations $x = ur_0$ and

$$\begin{aligned} \alpha &= \frac{du}{dw}\frac{r_0}{r} = \\ &= \frac{1}{1+hx}\frac{dx}{ds} = \\ &= a\zeta, \end{aligned} \tag{43}$$

where h is the curvature of the reference orbit and ζ is the scaled longitudinal component of momentum

$$\zeta = \frac{p_s}{p_0} = \sqrt{\frac{\eta}{\eta_0} - a^2 - b^2}. \tag{44}$$

Outside the field of the electrostatic deflector we have $\zeta =_2 1$, and as the expansion of ζ from Valetov and Berz (in this volume) shows, $\zeta =_2 1 - hx$ inside the main field of the electrostatic deflector. The derivation of aberration formulas in Wollnik's paper considers only the main field and does not consider fringe field effects, i.e. the aberrations are for initial and final coordinates infinitesimally inwards of the hard edge fringe fields at the entrance and exit edges of the electrostatic deflector, respectively. Thus, the expression $\alpha =_2 (1 - hx)\, a$ can be used to transform the first and second order aberration formulas of eqns. 31 and 42 from Wollnik's coordinates (u, α) to *COSY INFINITY*'s coordinates (x, a).

Having performed the transformation, we found that eqns. 31 and 42 fully agree with the analytic aberration formulas derived by Valetov and Berz (in this volume). Because of the definition of variables in *COSY INFINITY*'s beamline coordinate system, the transfer map for the hard edge fringe field is identity in *COSY INFINITY*'s coordinates, i.e. coordinates (x, a) infinitesimally outwards and inwards of the hard edge fringe field are the same. This can be shown by performing the derivations for momentum scaling similar to those in Sec. 8 for *COSY INFINITY*'s coordinate system. Hence, the aberration formulas in Wollnik's paper are valid in *COSY INFINITY*'s beamline coordinates for electrostatic deflectors with hard edge fringe fields with the caveat that the coordinate transformation from (u, α) to (x, a) must be performed infinitesimally inwards of the fringe field (with $\alpha =_2 (1 - hx)\, a$).

However, aberration formulas should normally account for all relevant effects, including hard edge fringe fields at a minimum, in order to account for energy conservation by considering the diffractive effects of the change in potential. Transforming the aberration formulas of eqns. 31 and 42 from Wollnik's coordinates (u, α) to *COSY INFINITY*'s coordinates (x, a) infinite with initial and final coordinates infinitesimally outwards of the hard edge fringe field at the entrance and exit edges of the electrostatic deflector, i.e. with $\alpha =_2 a$, we observed a discrepancy in second order aberrations $(x|xa)$, $(a|xx)/2$, $(a|xa)$, and $(a|aa)/2$ compared to aberrations computed numerically using *COSY INFINITY* and the analytic aberration formulas derived by Valetov and Berz (in this volume). We also found that the resulting aberration formulas do not satisfy the first and second order symplecticity conditions (Berz, 1999; Wollnik & Berz, 1985)

$$\begin{aligned} g_1 &= (x|x)\,(a|a) - (a|x)\,(x|a) - 1 = 0, \\ g_2 &= (x|x)\,(a|xa) - (a|x)\,(x|xa) + (x|xx)\,(a|a) - (a|xx)\,(x|a) = 0, \\ g_3 &= (x|x)\,(a|aa) - (a|x)\,(x|aa) + (x|xa)\,(a|a) - (a|xa)\,(x|a) = 0. \end{aligned} \tag{45}$$

8 Scaling of Wollnik's Aberration Formulas to Account for a Fringe Field Effect

In the coordinate system of Wollnik's paper, coordinates (u, α) need to be transformed at the entrance and exit edges of the electrostatic deflector to produce aberrations for a deflector with a hard edge fringe field, accounting for the diffractive effects of the change in potential using energy conservation. The inclination angle scaling that occurs in this context is analogous to refraction in light optics: when a ray hits the surface at an angle, its inclination angle changes. The reason behind this is ultimately that the speed of light changes when transitioning from one medium to the other, which affects the longitudinal momentum.

Let the subscripts i and f denote initial and final coordinates, i.e. coordinates at the entrance and exit edges of the deflector, and let the subscripts I and O denote positions infinitesimally inwards and outwards of the hard edge fringe field, respectively. Taking into account that (u, w) are essentially *COSY INFINITY*'s coordinates (x, s) scaled by r_0 inside the deflector, we consistently extend them to have $(u, w) = (x, s)/r_0$ both inside and outside the deflector. (See Sec. 2 for a definition of *COSY INFINITY*'s beamline coordinate system.) Thus $u = 0$ at the reference orbit both inside and outside of the electrostatic deflector, $w_{\mathrm{iI}} = w_{\mathrm{iO}}$, and $w_{\mathrm{fI}} = w_{\mathrm{fO}}$. The inclination α outside of the hard edge fringe field is expressed as $\alpha = du/dw$ because there the reference orbit curvature is zero.

For position coordinate u, we have $u_{\mathrm{iI}} = u_{\mathrm{iO}}$ and $u_{\mathrm{fI}} = u_{\mathrm{fO}}$ because positions are continuous functions of time. Now, consider a longitudinal z axis with the origin $z = 0$ at the intersection of the hard edge fringe field and the reference orbit at the entrance edge of the deflector. For convenience, we also let $w = 0$ at the entrance edge of the deflector. Outside the field of the deflector (at $w, z < 0$), the electrostatic field is zero, and from eq. 13 for the main field ($w, z > 0$), the horizontal transverse component of the electrostatic field in the horizontal plane is

$$\begin{aligned} E_u(u, w) &= -\frac{\partial \tilde{\varphi}(u)}{r_0 \partial u} H(w) = \\ &= -H(w) E_0 \left(1 - (c+1)u - \frac{\bar{c}u^2}{2} + O\left(u^3\right)\right), \end{aligned} \tag{46}$$

where $H(w)$ is the Heaviside function

$$H(w) = \int_{-\infty}^{w} \delta(\bar{w})\, d\bar{w} = \begin{cases} 1 & \text{for } w > 0, \\ 0 & \text{for } w < 0, \end{cases} \tag{47}$$

and $\delta(w)$ is Dirac's delta function.

The fringe field has a longitudinal component $E_z(u, z)$, and in the hard edge fringe field model the fringe field is localized at $z = 0$. By the Maxwell–Faraday equation, we have

$$\left[\frac{\partial E_{(r_0 u)}}{\partial z} - \frac{\partial E_z}{\partial (r_0 u)}\right]_{z=0} = 0, \tag{48}$$

from where we obtain for the hard edge fringe field

$$E_z(u, z) = -\delta(z) \int_0^u r_0 d\bar{u} E_0 \left(1 - (c+1)\bar{u} - \frac{\bar{c}\bar{u}^2}{2} + O\left(\bar{u}^3\right)\right). \tag{49}$$

There are no such delta function–like forces acting transversely, and thus $\dot{u}_{\mathrm{i}} = \dot{u}_{\mathrm{iI}} = \dot{u}_{\mathrm{iO}}$ and $\dot{u}_{\mathrm{f}} = \dot{u}_{\mathrm{fI}} = \dot{u}_{\mathrm{fO}}$; however, due to the delta function–like longitudinal component of the electrostatic field the longitudinal component of velocity changes: $r\dot{w}_{\mathrm{iI}} \neq r_0 \dot{w}_{\mathrm{iO}}$ and $r\dot{w}_{\mathrm{fI}} \neq r_0 \dot{w}_{\mathrm{fO}}$. Integrating Newton's second law of motion yields

$$\dot{w}_{\mathrm{iI}}(1 + u_{\mathrm{i}}) = \dot{w}_{\mathrm{iO}} - \frac{e e_0 E_0}{m r_0 \dot{w}_{\mathrm{iO}}} u_{\mathrm{i}} + O\left(u_{\mathrm{i}}^2\right). \tag{50}$$

Considering that the reference orbit curvature is zero outside of the fringe field and Newton's second law

$$\frac{m r_0^2 \dot{w}_0^2}{r_0} = e e_0 E_0 \tag{51}$$

for the reference particle, the kinetic energy outside the fringe field of the deflector is

$$U_0 = \frac{m r_0^2 \left(1 + u_{\mathrm{i}}'^2\right) \dot{w}_{\mathrm{iO}}^2}{2} = \frac{1}{2} E_0 e e_0 r_0. \tag{52}$$

Applying this expression to eq. 50, we obtain the second order DA representation

$$\dot{w}_{\mathrm{iI}}\left(1+u_{\mathrm{i}}\right)=_2 \dot{w}_{\mathrm{iO}}\left(1-u_{\mathrm{i}}\right). \tag{53}$$

Similarly, $\dot{w}_{\mathrm{fI}}\left(1+u_{\mathrm{f}}\right)=_2 \dot{w}_{\mathrm{fO}}\left(1-u_{\mathrm{f}}\right)$.

Finally, applying these transformation expressions for $\dot{w}$ and $\dot{u}$ to obtain transformations for α, we have

$$\begin{aligned}\alpha_{\mathrm{iO}} &=_2 \frac{du_{\mathrm{iO}}}{dw_{\mathrm{iO}}} =_2 \\ &=_2 \frac{1-u_{\mathrm{i}}}{1+u_{\mathrm{i}}}\frac{du_{\mathrm{iI}}}{dw_{\mathrm{iI}}} =_2 \\ &=_2 \left(1-u_{\mathrm{i}}\right)\alpha_{\mathrm{iI}}\end{aligned} \tag{54}$$

and, similarly,

$$\alpha_{\mathrm{fO}} =_2 \left(1-u_{\mathrm{f}}\right)\alpha_{\mathrm{fI}}. \tag{55}$$

We note that for *COSY INFINITY*'s beamline coordinate system, derivations similar to the above produce $(x,a)_{\mathrm{iO}} = (x,a)_{\mathrm{iI}}$ and $(x,a)_{\mathrm{fO}} = (x,a)_{\mathrm{fI}}$, showing that no momentum scaling is necessary for a hard edge fringe field in *COSY INFINITY*'s coordinate system due to its definition of coordinates.

To account for energy conservation by considering the diffractive effects of the change in potential in the entrance and exit fringe fields using the hard edge model, the second order aberration formulas from eq. 42, to which we refer here by the subscript W, have to be modified using eqns. 54 and 55 as follows:

$$\begin{aligned}\frac{1}{2}(u|uu) &= \frac{1}{2}(u|uu)_{\mathrm{W}} = \\ &= \frac{\left(2\left(9c+\bar{c}-6\right)+\left(12c+\bar{c}-12\right)\cos\left(\sqrt{2-c}w\right)\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right)}{3\left(2-c\right)},\end{aligned} \tag{56a}$$

$$\begin{aligned}(u|u\alpha) &= (u|u\alpha)_{\mathrm{W}} + (u|\alpha)_{\mathrm{W}} = \\ &= \frac{\left(6c+\bar{c}-\left(12c+\bar{c}-12\right)\cos\left(\sqrt{2-c}w\right)\right)\sin\left(\sqrt{2-c}w\right)}{3\left(2-c\right)^{3/2}},\end{aligned} \tag{56b}$$

$$\begin{aligned}\frac{1}{2}(u|\alpha\alpha) &= \frac{1}{2}(u|\alpha\alpha)_{\mathrm{W}} = \\ &= \frac{\left(6c+\bar{c}-\left(12c+\bar{c}-12\right)\cos\left(\sqrt{2-c}w\right)\right)\sin^2\left(\frac{1}{2}\sqrt{2-c}w\right)}{3\left(2-c\right)^{2}},\end{aligned} \tag{56c}$$

$$\begin{aligned}\frac{1}{2}(\alpha|uu) &= \frac{1}{2}(\alpha|uu)_{\mathrm{W}} - (u|u)_{\mathrm{W}}(\alpha|u)_{\mathrm{W}} = \\ &= \frac{\left(6c+\bar{c}\right)\left(\sin\left(\sqrt{2-c}w\right)+\sin\left(2\sqrt{2-c}w\right)\right)}{6\sqrt{2-c}},\end{aligned} \tag{56d}$$

$$\begin{aligned}(\alpha|u\alpha) &= (\alpha|u\alpha)_{\mathrm{W}} + (\alpha|\alpha)_{\mathrm{W}} - (u|u)_{\mathrm{W}}(\alpha|\alpha)_{\mathrm{W}} - (u|\alpha)_{\mathrm{W}}(\alpha|u)_{\mathrm{W}} = \\ &= \frac{\left(6c+\bar{c}\right)\left(\cos\left(\sqrt{2-c}w\right)-\cos\left(2\sqrt{2-c}w\right)\right)}{3\left(2-c\right)},\end{aligned} \tag{56e}$$

$$\begin{aligned}\frac{1}{2}(\alpha|\alpha\alpha) &= \frac{1}{2}(u|\alpha\alpha)_{\mathrm{W}} - (u|\alpha)_{\mathrm{W}}(\alpha|\alpha)_{\mathrm{W}} = \\ &= \frac{\left(9c+\bar{c}-6-\left(6c+\bar{c}\right)\cos\left(\sqrt{2-c}w\right)\right)\sin\left(\sqrt{2-c}w\right)}{3\left(2-c\right)^{3/2}}.\end{aligned} \tag{56f}$$

The first order aberrations from eq. 31 are valid for the hard edge fringe field model of the electrostatic deflector without modifications. We checked that a transformation of eq. 31 and 56 from Wollnik's coordinates (u,α) to *COSY INFINITY*'s beamline coordinates (x,a) using the relations $x=r_0u$ and $a =_2 \alpha$, which are valid outside of the fringe field, results in a full agreement with the analytic aberration formulas derived by

Valetov and Berz (see eqns. 44 and 45 of Valetov and Berz, in this volume). Eqns. 31 and 56 also satisfy analytically and numerically the first and second order symplecticity conditions of eq. 45, in contrast to the unscaled aberration formulas from eqns. 31 and 42.

9 Conclusion

We have analyzed the derivations of first and second order aberration formulas from Wollnik's paper (Wollnik, 1965) for motion in the horizontal transverse plane of charged particles of reference energy traversing an electrostatic deflector with arbitrary inhomogeneity coefficients c and $\bar{c}$.

We found that the Lagrangian, the third order expansion of the Lagrangian, and the first and second order expansions of the ODEs of motion in Wollnik's paper are valid. The first and second order aberrations the horizontal transverse plane u–α for electrostatic deflectors are correct in Wollnik's paper; however, they only consider the main field, whereas it is generally necessary to consider fringe field effects for aberration formulas to be valid. To assure a proper consideration of energy conservation, we modified these aberrations to account for the diffractive effects of the change in potential, using the hard edge fringe field model, and obtaining eqns. 28 and 56.

See Valetov and Berz (in this volume) for a comparison of electrostatic spherical and cylindrical deflector test cases comprising (1) the analytic aberration formulas for electrostatic deflectors derived by Valetov and Berz (in this volume), (2) numerical differential-algebraic calculation of aberrations using the code *COSY INFINITY*, (3) the analytic aberrations from Wollnik's paper (eqns. 31 and 42), (4) the code *GIOS*, and (5) the analytic formulas from Wollnik's paper scaled to account for a hard edge fringe field (eqns. 31 and 56). Valetov and Berz (in this volume) also provide tracking pictures obtained using the aberrations of each test case. As these test cases demonstrate, the scaled aberration formulas from eqns. 31 and 56 fully agree with the analytic aberration formulas derived by Valetov and Berz (eqns. 44 and 45 of Valetov and Berz, in this volume) and with the code *COSY INFINITY*. The scaled aberration formulas from eqns. 31 and 56 satisfy the first and second order symplecticity conditions.

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